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Kinetic Study of the Effect of Potassium-Containing Compounds (Potassium Superoxide, KO_2; Potassium Bicarbonate, $KHCO_3$; and Potassium Carbonate, KCO_3) on the Combustion Properties of Hydrogen and Methane Flames.

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Abstract

Potassium-containing compounds are effective, non-toxic, environmentally-friendly fire suppression agents, offering a promising alternative to halon agents. These compounds are still under investigation and are not yet widely commercially available.

This study investigates the kinetic interactions of potassium-containing compounds, specifically potassium superoxide (KO_2), potassium bicarbonate ($KHCO_3$), and potassium carbonate (KCO_3) within hydrogen, (H_2) and methane (CH_4) flames through numerical simulations using the Ansys Chemkin-Pro2019R2 software.

The thesis introduces a testing program evaluating the performance of potassium oxide (K_2O) on wood and pool fires. The results demonstrate that the activation of K_2O instantly extinguished the flames and inhibited re-ignition for approximately 25-30 minutes.

Using two different reaction mechanisms, numerical methods were used to estimate the properties of the H_2 flame. The first mechanism utilised was GRI-Mech version 3.0, specifically designed to model the combustion of both hydrocarbons and H_2 and the second employed a reduced mechanism proposed by Hadi for H_2 combustion. The results obtained are in agreement with the findings of the literature.

Reactions involving potassium species were incorporated into both the GRI-Mech and Hadi's reduced mechanism. The study found acceptable numerical results for H_2 flame properties, confirming the merged mechanisms' validity.

The study investigates the inhibition effects of KO_2, $KHCO_3$, and KCO_3 mole fractions on the characteristics of H_2 and CH_4 flames. This is done based on the GRI-Mech/K-species reaction mechanism through numerical simulations. The study predicts the laminar burning velocity (S_L) and the flame concentration of the hydroxyl radical (OH) in different equivalence ratios (0.9, 1, 1.1).

For H_2 flames, KO_2 proved to be the most effective agent, with higher inhibition effectiveness observed in lean mixtures. The analysis of reaction pathways at various concentrations of KO_2 revealed a substantial influence on H_2 flame pathways, even at low concentrations. Furthermore, the adiabatic flame temperature of the H_2 flame was affected by the KO_2 mole fraction.

In the context of CH_4 flames, both KCO_3 and $KHCO_3$, based on S_L, exhibit the capability to reduce the S_L of CH_4. However, when considering the reduction of OH, the performances of $KHCO_3$ and KCO_3 prove comparable.

Limited mole fractions of KCO_3 prove useful for studying their effect on CH_4 flames in a broad range of equivalence ratios. Both KCO_3 and $KHCO_3$ demonstrate a uniform impact on the adiabatic flame temperature of CH_4 flames.

KCO_3 and $KHCO_3$ exhibit different effects on CH_4 flames, with $KHCO_3$ demonstrating greater efficacy. Numerical simulations indicate $KHCO_3$ significantly affects CH_4 flames, correlating with literature findings on flame speed reduction and inhibition reactions.

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Nomenclature

Symbol	Description	Units
S_L	Laminar Burning Velocity	cm/s
δ	Thickness of reaction zone	units of length
^{r}	The average magnitude of fuel consumption rate over the entire flame	mol/cm^3.s
Tig	Ignition temperature	K
Tr	Temperature of the reactant mixture	K
Tp	Temperature of the combustion products	K
C	Concentration	mol/m^3
R	Rate of Reaction	mol/s
LFL	Lower Flammability Limit	%
UFL	Upper Flammability Limit	%
A	The pre-exponential factor of Arrhenius equation	(kmol/m³)(1-m)/s (depends on reaction)
E	Activation energy	cal/mol
T	Temperature	K
t	Time	s
R	Gas constant	J/mol.K
K	Rate constant	Depending on reaction order
μm	Micrometer	measures small lengths, like diameters
V	Volum	m³
ρ	Density	kg/m³
m	Mass	kg
Per Miller	unit of enthalpy	kcal/mol
Q	The amount of heat produced or released	J
ΔT	Temperature rise of the fuel	°C
H	Specific enthalpy	kcal/mol
Cp	The specific molar heat capacity	J/mol.K
AFT	Adiabatic Flame Temperature	K
ε/k-B	The Lennard-Jones potential well depth	K
k_B	Boltzmann Constant	ergs/K
σ	The Lennard-Jones collision diameter	Angstrom
α	The polarizability	cubic Angstroms
μ	The Dipole moment	Debye
Zrot	The rotational relaxation collision number	

r_k	Production rate	mol/(cm$^3 s$)
v_{ki}	Stoichiometric coefficient	
q_i	Rate of progress variable for the reaction	
$a_1, a_2, \ldots, a_6$	Numerical coefficients	
k_{f_i}	Forward rate constant for reaction ith	depends on reaction
X	Concentration of the species involved in the reaction	depends on reaction
k_{r_i}	Reverse rate constant of the i th reaction	depends on reaction
k_{c_i}	Equilibrium constant	depends on reaction
k_{p_i}	Equilibrium constant in pressure units for the i th reaction	depends on reaction
A_C	Cross-sectional area of the flame front	cm^2
ρ	Density of the unburned gas adjacent to the flame front	kg/m³
$\frac{dm}{dt}$	mass flow rate of the unburned gas in the flame front	kg/s

Abbreviation

Symbol	Description
NFPA	The National Fire Protection Association
IMO	International Maritime Organization-Atlantic
ISO	The International Standards Organization
PGA	Pyrotechnically Generated Aerosols
Gri-mech	Gas Research Institute
LLNL	Lawrence Livermore National Laboratory
AFFF	Aqueous Film-Forming Foam
CAFS	Compressed Air-Foam Systems
BC powder	Potassium Bicarbonate
ABC	Mono-Ammonium Phosphate
ABS	American Bureau of Shipping
DTA	Differential Thermal Analysis
TG	Thermogravimetry
MCPVT	the modified closed pressure vessel test
SNLL	Sandia National Laboratories
CFD	Computational Fluid Dynamics
LSU	Louisiana State University
NASA	National Aeronautics and Space Administration

Chemical Formula

H_2: Hydrogen
O_2: Oxygen
OH: Hydroxyl radical
H: Hydrogen atom
HO_2: Hydroperoxyl radical
H_2O_2: Hydrogen peroxide
N_2: Nitrogen gas
H_2O: Water
HCO: Formyl radical
CO: Carbon monoxide
CO_2: Carbon dioxide
CH_4: Methane
CH_3: Methyl radical
C_2H: Ethynyl radical
C_2H_6: Ethane
C_2H_5: Ethyl Radical
C_2H_4: Ethylene
C_2H_3: Vinyl radical
C_2H_2: Acetylene
C_3H_7: propyl
C_3H_8: Propane
CH_2O: Formaldehyde
CH_3O: Methoxy radical
CH_3OH: Methanol
CH_3CO: Acetyl
CH_3CO_3: Methyl percarbonate
CH_3CO_3H: Methyl percarbonic acid
CH_3O_2: Methyl peroxy
CH_3O_2H: Methyl peroxy acid
$C_2H_5O_2H$: Ethyl peroxy acid
$C_2H_5O_2$: Ethyl peroxide
C_2H_5O: Ethyl alcohol (Ethanol)
C_2H_5OH: Ethyl alcohol (Ethanol)
SC_2H_5O: Ethyl thio peroxide
PC_2H_5O: Ethyl peroxythioformate
CH_2HCO: Formaldehyde oxime
CN - Cyanide
HCN - Hydrogen cyanide
NO - Nitric oxide
H_2CN Radical: Cyanamide Radical
NH: Ammonia
NO: Nitric Oxide
HCNO: Fulminic Acid

C: Carbon
HOCN: Fulminic Acid
HNCO: Isocyanic Acid
NCO: Cyanate
N_2O: Nitrous Oxide
NH_2: Amide
HNO: Nitroxyl
NO_2: Nitrogen Dioxide
C_2N_2: Cyanogen
NNH: Diazene (or Diimide)
NH_3: Ammonia
N_2H_2: Dihydrodiazene
C_2H_3O: Acetyl Radical
C_3H_6OH: Propanol
$C_3H_5O_2$: Methyl Acetate
C_3H_5O: Acetoxypenta-1,3-diene
$NC_3H_7O_2$: Nitropropylene
$NC_3H_7O_2H$: Nitropropane
NC_3H_7O: N-Propoxy
IC_4H_5: I-Buten-3-ynyl Radical
NC_4H_5: N-Buten-3-ynyl Radical
C_6H_5: Phenyl Radical
C_4H_4: 1-Buten-3-ynyl Radical
C_3H_3: Propargyl Radical
C_3H_6: Propylene
C_3H_8: Propane
IC_3H_7: I-Propyl Radical
NC_3H_7: N-Heptyl Radical
SC_3H_5: 1-Buten-3-yl Radical
PC_3H_4: Propyne
TC_3H_5: 2-Buten-3-yl Radical
C_3H_6O: Propylene Oxide
C_3H_2: Propadiene
C_4H_2: Diacetylene
C_4H_8: 1-Butene
$C_2C_4H_8$: Cis-1,2-Dimethylcyclopropane
C_4H_5: 1,3-Butadiene
C_4H: Butadienyl Radical
C_6H_6: Benzene
C_3H_5: Propargyl Radical
C_3H_4: Allene. C_4H_6: 1,3-Butadiene
IC_4H_3: Isocyanoallene
NC_4H_3: Isocyanopropadiene
C_6H_5O: Phenoxy Radical
CH_3NO_3: Methyl Nitrate
CH_2NO_3: Formaldehyde Nitrate
HONO: Nitrous Acid
AR: Argon
NO_3: Nitrate

HNO_3: Nitric Acid
N_2H_3: Diamide
N_2H_4: Hydrazine
CNN: Cyanogen
HCNN: Hydrogen Cyanide
HCCOH: Methylene Formate
N_2O_4: Dinitrogen Tetroxide
N_2O_3: Dinitrogen Trioxide
N_2O_5: Dinitrogen Pentoxide
NH_2OH: Hydroxylamine
HNOH: Hydroxylamine
H_2NO: Hydroxylamine
HNNO: Hydroxylamine
C_2H_5CHO: Acetaldehyde
C_2H_5CO: Acetaldehyde
H_2CNO: Methanamide
CH_3NO: Methanamide
HCNH cis: Cyclopropanimine
HNCN: Hydrogen Isocyanide
NCN: Isocyanogen
HE: Helium
K: Potassium
PN: Potassium Nitrate
HKO: Potassium hydroxide
HK: Potassium hydride
KO: Potassium monoxide
K_2O: Potassium oxide
KO_3: Potassium ozonide
KO_2: Potassium super-oxide
K_2O_2: Potassium Peroxide
$KHCO_3$: Potassium bicarbonate
KCO_3: Potassium carbonate
K_2CO_3: Dipotassium carbonate
$K_2H_2O_2$: Dipotassium peroxide

Chapter 1

Introduction

Accidental fires are among the most common and destructive disasters in industrial and domestic environments. The search for safer, environmentally friendly, and more effective fire suppression agents has been a driving force behind innovations in combustion science and industrial safety. A notable turning point in this journey was the international discontinuation of halon, an effective but environmentally harmful fire suppressant Pitts et al. (1991). This decision highlighted the need for alternative agents that could safeguard lives and property without detrimental effects on the ozone layer. Potassium-containing compounds have emerged as potential candidates for influencing combustion dynamics.

Aerosol fire suppressants currently under investigation include micron-sized alkali metal salts, such as potassium carbonate. Alkali metal salts, notably sodium and potassium bicarbonate, have been employed as fire suppressants since at least the early 1940s, with the first NFPA standard for these agents issued in 1955. Their effectiveness in fire suppression has been well-recognized for decades. Since the 1980s, research into aerosol fire suppression has increasingly focused on micron-sized alkali metal salts delivered in a gaseous medium. This shift is due to a better understanding of the inverse relationship between particle size and suppression efficacy. Additionally, alkali metal salt aerosol extinguishers have gained renewed attention because they are relatively cost-effective and have been endorsed by organizations like the U.S. Environmental Protection Agency as safe and effective alternatives to Halon 1301 Sheehan (2013).

Condensed aerosols based on potassium-containing compounds were selected as fire suppression agents because of several key factors. Unlike halon compounds, these aerosols do not deplete the ozone layer, making them environmentally friendly alternatives that align with global efforts to reduce ozone-depleting substances. They also have a significantly lower global warming potential, contributing to a lesser impact on climate change.

The efficiency and performance of potassium compounds in fire suppression are notable. These compounds are highly effective at extinguishing fires by interfering with the chemical reactions within the flame. Their versatility allows them to be used for various types of fires, including Class A (solids), Class B (flammable liquids and gases),

and Class C (electrical fires) fires, making them suitable for different fire scenarios. Furthermore, potassium-containing compounds exhibit low toxicity, making them safer for use in occupied spaces than some Halon alternatives, which can harm human health. The residue left by these aerosols is generally less harmful and easier to clean, reducing potential damage to sensitive equipment and environments and making post-fire cleanup more manageable Sheehan (2013).

Potassium species-based fire suppression systems are often more cost-effective in the long term compared to halon systems. Factors such as the cost of the agent, system maintenance, and potential environmental fines associated with halon use contribute to their economic advantage Kibert & Dierdorf (1993).

This study adds to the body of knowledge by constructing a detailed kinetic model of potassium-containing compounds. The primary goal is to obtain deeper insight into how potassium-containing compounds such as superoxide (KO_2), potassium bicarbonate ($KHCO_3$), and potassium carbonate (KCO_3) influence combustion properties by analysing the flame temperature, the speed of the flame, the limit of flammability and the reaction pathways.

1.1 Background

Fires, as defined by the National Fire Protection Association NFPA (2016), are rapid oxidation processes driven by a chemical reaction that releases light and heat in varying intensities. This definition underscores the dynamic and transformative nature of fires, which can range from small controlled flames to large destructive conflagrations.

The essence of fire hinges on a delicate balance among four fundamental elements, often represented as the "fire tetrahedron" O'Connor (2022) in Figure 1.1. These elements are fuel, oxidiser, heat, and a chemical chain reaction. In combustion, fuel donates electrons to the oxidiser (typically oxygen) during the combustion reaction. Fuels can exist in three states: solid, liquid, or gas. Combustion occurs when the matter in a solid or liquid state is converted to a gaseous state, where both the fuel and the oxidiser are present in the gaseous form, facilitating recombination.

Regarding the oxidiser, air naturally contains around 21% oxygen, along with 78% nitrogen and 1% other elements. Although oxygen is the most common oxidiser, substances such as ammonium nitrate and chlorine can also serve as oxidising agents ABS (2015).

Heat is the energy source that ignites and sustains the combustion process. It's necessary to raise the fuel to its ignition temperature and maintain the chemical reaction. Heat sources can vary and include flames, sparks, electrical arcs, or radiant heat. The amount of heat produced depends on factors such as fuel type, fuel concentration, and oxygen supply. Once the fuel reaches its ignition point, it can undergo self-sustaining combustion, continuing to burn as long as there is an adequate supply of heat, fuel, and

oxygen Hurley et al. (2015). It begins when the fuel and oxidiser combine and react, producing heat and other products. As the reaction progresses, intermediate species and radicals, continue to react with more fuel and oxidiser, perpetuating the combustion process. This self-sustaining chain reaction is a key characteristic of combustion ABS (2015).

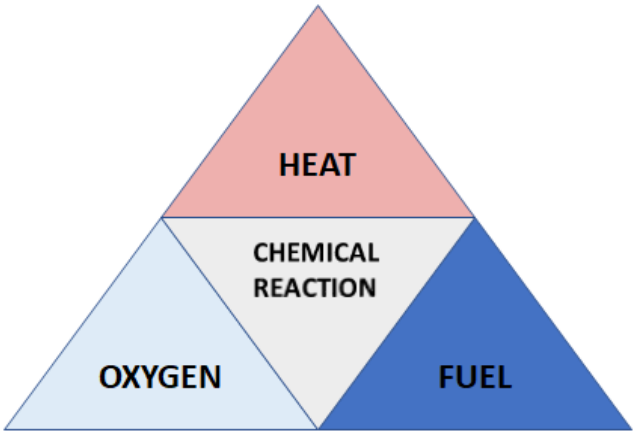


Figure 1.1: Fire tetrahedron. O'Connor (2022)

Comprehending the complex interactions among these four elements is crucial in the context of fire suppression. It forms the core of effective fire prevention and suppression strategies, underpinning safety measures. Moreover, this comprehension is instrumental in the advancement of innovative fire suppression methods.

In fire safety, fires are classified into several classes, including Class A, Class B, Class C, Class D, and Class K fires, depending on the type of fuel involved. Understanding fire classification is essential for determining the appropriate extinguishing agents and techniques for each type of fire, ensuring effective fire safety measures Della-Giustina (2014).

The International Maritime Organisation (IMO) has identified two standards that describe the various classes of fires: the International Standards Organization (ISO) Standard and the NFPA Standard. Regarding NFPA and according to Voelkert (2009) and Cote (2004), fire classification is illustrated as follows:

Class A fires involve solid materials that leave ash or have a burning ember. The most effective way to extinguish Class A fires is by absorbing the heat. Water is the most commonly used agent, but other agents such as halon, halogenated agents, and foam can also be used effectively.

Class B fires involve flammable liquids or gases, such as gasoline, oil, propane, and natural gas. Extinguishing Class B fires requires agents like foam, dry powder, or carbon dioxide (CO_2) to cool the fuel and displace oxygen Hurley et al. (2015).

Class C fires entail live electrical equipment, necessitating the use of extinguishing agents like CO_2 or dry chemical powder, which do not conduct electricity back to firefighters. These agents work by smothering the flames and depriving them of oxygen Hurley et al.

(2015), Voelkert (2009).

Class D fires involve combustible metals such as titanium, potassium, sodium, and magnesium. Specialised dry powder extinguishing agents like graphite powder, sodium chloride, or sand are recommended for these fires Della-Giustina (2014).

Class K fires are specific to cooking oils and fats. These fires require specialized wet chemical extinguishing agents and suppression systems Della-Giustina (2014).

In fire suppression, both organic and inorganic substances can inhibit combustion processes. Halogenated hydrocarbons and inert gases are two common examples. Inert gases suppress fires through physical mechanisms like cooling and dilution, while halogenated hydrocarbons typically interfere chemically with combustion. Notably, inorganic salts, especially alkali metal salts, can also inhibit combustion. Physical fire suppression mechanisms include processes like smothering, cooling, and dilution, while chemical suppression methods break the chain reactions that propagate flames Pitts et al. (1991). Recent advances in fire suppression have led to the development of innovative agents and systems, including halocarbon and inert gaseous agents, water mist systems, compressed air foam systems, and aerosol fire extinguishing systems. Aerosol fire extinguishing technology, initially developed during the Soviet Soyuz rocket program over two decades ago, has gained attention. Aerosol agents consist of small particles, approximately 10 μm in diameter, capable of remaining suspended in the air for a limited duration, providing effective fire protection. Research has shown an inverse relationship between particle size and suppression efficiency Babushok et al. (2017), Ewing et al. (1989, 1992), Rosser Jr et al. (1963). Particulate aerosols are primarily pyrotechnically generated aerosols (PGA), although non-pyrotechnically generated particle aerosols are under investigation. Generators containing aerosol-forming compounds can serve as handheld fire extinguishers or remotely fitted systems for spaces of varying volumes. Although the effectiveness of aerosol agents is reasonably well understood due to their ability to suppress fires similar to larger dry chemical particle systems, the precise suppression mechanism remains unexplained Sheehan (2013).

Potassium-containing compounds have demonstrated fire suppression capabilities compared to gas or foam systems in numerous applications. Scientific literature supports the effectiveness of compounds containing alkali metals, such as potassium (K) and sodium (Na), as experimental flame retardants Birchall (1970), Chatrathi & Going (2000), Hastie (1973), Reed et al. (1997). These compounds have effectively reduced the burning velocity Rosser Jr et al. (1963). However, the technology is relatively new and requires the overcomement of various challenges to become a robust commercial product Rohilla et al. (2019). One such challenge is the kinetic study of the inhibitory mechanism.

In the typical mechanism of hydrocarbon combustion, small reactive radicals, such as hydroxide (OH), hydrogen atom (H), and oxygen (O), rapidly consume fuel molecules, producing more radicals of the same kind in the process. This chain reaction leads to an increase in temperature as a result of thermodynamics, accelerating the reaction and

producing even more radicals. Consequently, fuel consumption occurs rapidly, resulting in the production of carbon dioxide (CO_2) and water (H_2O).
Potassium-containing compounds can disrupt these chain reactions by absorbing free radicals, effectively quenching flames. This thesis investigates the inhibition mechanism using the Chemkin package with thermochemical and transport properties from the database compiled by Kee et al. Kee et al. (1985), a package widely validated with experimental data and employed by different studies for accurately estimating laminar burning velocities and other properties of the combustion process.

Currently, there is a lack of a well-established correlation that can reliably predict the effectiveness of potassium species in suppressing gas flames. Previous research, such as the study conducted by Babushok et al. (2017), suggested the use of potassium bicarbonate ($KHCO_3$) as an aerosol agent to inhibit methane (CH_4)/air flames. However, it's essential to note that the numerical simulations employed in such studies rely on empirical data, and the numerical method is not clearly defined.

To ensure safe and effective use of potassium-containing compounds, such as aerosol agents KO_2, $KHCO_3$, and KCO_3, a more precise understanding of their reaction kinetics and mechanisms concerning interaction with flame propagation radicals in various gas mixtures is required. This specific aspect remains inadequately comprehended. The Gas Research Institute Mechanism (GRI-Mech) Smith et al. (1999) is suggested as a framework, incorporating potassium reactions. This research contributes information on the quantitative analysis of the kinetic inhibition effect achieved by incorporating potassium species into the reaction mechanisms. To address this, GRI-Mech will be utilised to investigate the numerical correlation between the concentration of suppressant agents and the laminar burning velocity in various gas mixtures, as well as to analyse the reaction pathways.

1.2 Research Approach and Objectives

1.2.1 Research Approach

The approach involves a chemical kinetic analysis. Initial tests were carried out using a box rig to investigate the effects of releasing the K_2O fire suppression agent on small fires, clearly demonstrating its impact on flames. Data collection on the kinetic reactions of potassium species and their thermodynamic and transport data is required.

Kinetics modeling and analysis are utilised to determine the flame speed of H_2/air mixture and CH_4/air mixture, as well as the reduction of mole fraction of hydroxyl radical with the addition of KO_2, $KHCO_3$, or KCO_3 at different equivalence ratios and inhibitor mole fractions. The numerically determined flame speed and hydroxyl radical mole fraction are then used to evaluate the effects of KO_2, $KHCO_3$, and KCO_3 on H_2 and CH_4 flames.

Furthermore, based on the impact of potassium species, some combustion properties, including reaction pathways, will be estimated for more investigations.

Kinetic simulations are divided into different parts:

Develop a strategy by the Chemical Kinetic Mechanism of the H_2/air mixture based on the GRI-Mech mechanism and Reduced mechanism

The H_2/O_2 combustion system is selected for this study because it is well described by a relatively simple reaction mechanism. This choice facilitates a kinetic understanding of the inhibition mechanism of KO_2, $KHCO_3$, and KCO_3 before their application to more complex fuels. In addition, the inhibition and suppression of H_2 fires have historically faced significant challenges. The Chemkin library has adopted the GRI-Mech mechanism version 3.0, and kinetically stoichiometric H_2 flame is tested based on this mechanism by predicting the adiabatic flame temperature (AFT), flame speed, flammability limit, and analysing the pathway reactions. The results are validated with the values in the literature reviews. On the other hand, the reduced mechanism of H_2 combustion by Hadi is used to develop the kinetic simulation of stoichiometric H_2 flame, and the results are compared with the H_2 flame simulations developed by the GRI-Mech mechanism.

Investigating the Impact of Merging Kinetic Reaction Mechanisms for K-species/H_2/air Mixtures Based on GRI-Mech and Reduced Mechanisms

This study involves integrating individual kinetics from a master mechanism (GRI-Mech or Reduced mechanism) with a donor mechanism that contains potassium species reactions, using the mechanism utilities in Chemkin software. When a species in the donor mechanism exists in the master mechanism but varies in thermodynamic or transport data, the data from the master mechanism are retained and those from the donor mechanism are disregarded. Similarly, if a reaction in the donor mechanism shares the same formula as a reaction in the master mechanism but has different Arrhenius coefficients, the reaction in the master mechanism takes precedence, and the reaction in the donor mechanism is excluded.

A relative tolerance of 10% is established for comparing species and reaction data, enabling the consideration of species and reactions with minor differences in thermodynamic, transport, and rate data as equivalent. To thoroughly evaluate all merged reactions, the mechanisms are investigated by studying the kinetic numerical estimations of AFT, the flame speed, the flammability limit, and analysing the pathway of stoichiometric H_2/air mixtures. This examination extends to stoichiometric potassium/air mixtures.

Investigating the Inhibition Effect of KO_2, $KHCO_3$, and KCO_3 on H_2 and CH_4 Flames

This section aims to demonstrate the inhibition effect of KO_2, $KHCO_3$, and KCO_3 on H_2 flames and $KHCO_3$ and KCO_3 on CH_4 flames. The demonstration includes predicting flame speed and OH free radical reduction at equivalence ratios of 0.9, 1, and 1.1, with varying mole fractions of the fire suppression agent.

These simulations identify the effective agent for both the H_2 and CH_4 flames. Additionally, the effect of $KHCO_3$ on CH_4 flames is illustrated for comparison purposes.

1.2.2 Objectives

Numerically, this thesis aimed at establishing the effect of KO_2, $KHCO_3$, and KCO_3 on H_2/air mixture and CH_4/air mixture by developing a gas-phase kinetic model for inhibiting flames with these potassium compounds.

The objectives of the study:

1. Create a gas-phase kinetic model to describe the inhibition of flames by potassium compounds. This model will account for the intricate chemical reactions involved in flame suppressions.

2. Validate the gas-phase kinetic model's accuracy and reliability in describing the inhibition of flames by potassium compounds (KO_2, $KHCO_3$, and KCO_3). This validation will involve comparing the numerical results obtained from the developed model with existing data and empirical findings that consider the kinetic model without the reactions of potassium species.

3. Numerically assess the effectiveness of KO_2, $KHCO_3$, and KCO_3 in inhibiting the combustion of H_2 and CH_4 when mixed with air. This assessment will provide insights into the potential of these compounds as flame suppressants.

4. Establish a correlation between the concentration of KO_2, $KHCO_3$, and KCO_3 and their impact on the S_L and reduction of OH radicals in H_2-CH_4 flames.

5. Determine the influence of varying concentrations of selected potassium compounds on the adiabatic flame temperature of H_2-CH_4 flames.

6. Investigate the detailed reaction mechanisms involved in flame inhibition by potassium species. Understanding of how these compounds interact with radicals and intermediates in the combustion process.

1.3 Thesis Layout

This thesis is divided into eight chapters, each of which contributes a part to the thesis's overall objective. Below is a brief description of each chapter.

Chapter 1 presents the research background and the knowledge gap. The aim and the methodology associated with the objectives are pointed out in this thesis.

Chapter 2 is dedicated to presenting the principles of fire suppression, which include various aspects such as fire suppression agents, the mechanisms involved in fire suppression, and the evaluation parameters for fire suppression agents. In addition, this chapter provides the key reaction mechanisms that form the basis of this thesis.

Chapter 3 describes a test conducted to study the effects of releasing (K_2O) aerosol on hydrocarbon flames.

Chapter 4 outlines a strategy for studying the effect of potassium species on flames, using a hydrogen-air mixture under stoichiometric conditions.

Chapter 5 discusses the combination of potassium species reactions with the GRI-Mech and Reduced mechanisms using Chemkin.

Chapter 6 investigates the inhibitory effects of KO_2, $KHCO_3$, and KCO_3 on H_2 flames based on incorporating the potassium species reactions into the GRI-Mech model.

Chapter 7 is based on the incorporation of potassium species reactions into the GRI-Mech model, delves into the inhibition effect of KO_2, $KHCO_3$ and KCO_3 on CH_4 flames.

Chapter 8 showcases test results depicting the interaction of K_2O with hydrocarbon flames and describes the numerical analysis strategy used to assess the effectiveness of KO_2, $KHCO_3$, and KCO_3 in both H_2 and CH_4 flames. In addition, it proposes directions for future research in this field.

Chapter 2

Literature Review on the Principle of Fire Suppression

This review of the literature examines key aspects of fire suppression, focussing on the application of potassium-containing compounds as fire suppression agents.

In this chapter, previous studies on the inhibition of flame by potassium species are illustrated. Considerations such as laminar burning velocity, flammability limits, and pathway reactions are discussed to assess the efficacy of suppression agents. In addition, detailed illustrations of the reaction kinetics and mechanisms for hydrogen and methane are included. Moreover, the reactions of potassium-containing species with the species of the hydrocarbon system, along with their thermodynamic and transport data, provide essential steps for the kinetic model.

2.1 Fire Suppression principles

Fire extinguishment stands as the frontline defense when prevention measures fall short. There are four fire suppression principles that exist, these are as mentioned below:

Controlling the fuel, this concept involves two methods. Firstly, physically remove or separate the fuel from the fire. For example, close a valve that feeds a gas or flammable liquid fire. Secondly, the fuel can be chemically affected by diluting it. Della-Giustina (2014). The concept of controlling the fuel is often used as a fire prevention measure rather than as a means of suppressing or extinguishing a fire. By controlling the fuel, the likelihood of a fire starting or spreading is reduced. However, if a fire has already started, the primary goal is typically to remove one or more of the other elements of the fire triangle (oxygen, heat, or chemical chain reactions) in order to extinguish the fire.

Oxygen reduction is a commonly used mechanism for fire suppression. This method involves limiting the amount of oxygen available to the fire, which in turn reduces the fire's intensity and may eventually extinguish it. This can be accomplished by smothering the fire with materials such as foam or powder, or by displacing O_2 with an inert gas such as CO_2 or nitrogen (N_2) ABS (2015).

Temperature reduction is another effective method of fire suppression. This method involves absorbing heat from the fire, which can be accomplished by using water, foam, or other cooling agents. By reducing the temperature of the fire, the reaction rate can be slowed or stopped, ultimately leading to extinguishment.

Chemical interruption of the fire reaction chain involves interrupting the chemical reactions that take place during a fire, which can be achieved by using chemical suppressants such as halon, halocarbons, and dry chemicals. These agents work by interfering with the chemical reactions that sustain the fire, ultimately leading to extinguishment ABS (2015).

2.2 Fire Suppression Agents

Fire suppression agents are substances that are used to control or extinguish fires. These agents can be water, foam, dry chemical powder, carbon dioxide, and many other substances, depending on the type of fire and the fire suppression system being used. Fire suppression systems are designed to control or extinguish fires automatically or manually. There are various types of fire suppression systems, such as fire sprinklers, fire alarms, and portable fire extinguishers. Each system is designed to respond to specific types of fires and is equipped with the appropriate fire suppression agents. The most commonly used fire suppression agents include water, foam, dry chemicals, and carbon dioxide.

2.2.1 Water-Based Suppression

Water-based suppression is a common type of fire suppression method that involves using water or water-based solutions to extinguish fires. This method works by cooling the fuel source below its ignition temperature, removing heat from the fire, and thereby suppressing it. Water-based suppression systems are widely used in many different types of buildings and industries, including residential, commercial, and industrial settings. The use of water-based suppression systems is generally considered safe and effective, and they are often required by local fire codes and regulations.

Water

It is one of the most used fire suppression mechanisms. It is effective for extinguishing fires that involve ordinary combustibles, such as wood, paper, and cloth. According to NFPA, water should not be used on Class B fires involving flammable liquids or gases, as it can spread the fire and make it more dangerous.

In addition to its effectiveness in suppressing Class A fires, water has limitations and should not be used for certain types of fires. For example, water should not be used for

Class D fires, which involve combustible metals, as it can cause violent reactions Conroy (2003).

Water mist

It is a type of water-based fire suppression system that uses fine water droplets to extinguish fires. It works by absorbing heat, cooling the fuel and surrounding area, and reducing the concentration of oxygen available to the fire. Water mist systems have several advantages over traditional water-based systems, including less water usage, reduced damage to property, and less clean-up after a fire Kraus-Namroży & Brzezińska (2022).
Water mist fire suppression systems utilise a fine water spray that contains water droplets of less than 1000 microns, with 99% of the water dispersed being made up of these small droplets. The increased surface area of these smaller droplets allows them to be easily drawn into the fire plume compared to standard spray sprinkler droplets. Once drawn into the fire plume, the droplets rapidly evaporate into steam, leading to both oxygen displacement and heat absorption, as discussed earlier. The primary mechanism responsible for the gas-phase extinguishment of flames due to water mist application is the rapid absorption of heat during the droplets' phase change process, while the secondary effects of oxygen displacement and prewetting contribute to a lesser extent toward fire suppression and extinguishment.

An advantage of water mist systems is their ability to extinguish fires with minimal water usage. The fine water droplets generated by the system can cover a larger surface area, requiring less water to achieve the same level of fire suppression as traditional sprinkler systems. This can result in less water damage to the protected area, which can be especially beneficial in environments such as data centres, museums, and historical buildings

Another advantage of water mist systems is their ability to be tailored to specific fire risks. The size of the water droplets can be adjusted to optimize the system's effectiveness for different types of fires, such as Class A, B, and C fires. In addition, the water mist can be combined with other agents, such as foams or gels, to increase the system's effectiveness for specific fire hazards Zhang et al. (2017). In addition, according to Kraus-Namroży & Brzezińska (2022), the use of water mist can reduce the amount of smoke produced during a fire, which can improve visibility and increase the chances of safe evacuation.

Farrell et al. (2023) discusses various issues and challenges associated with water mist fire suppression systems. The authors highlight that water mist systems are effective in suppressing fires by cooling and smothering the flames, as well as reducing the

concentration of oxygen available to the fire. They also note that water mist systems can be more effective than traditional water-based systems in certain situations, such as in confined spaces or with certain types of fuel.

However, the authors also discussed several challenges associated with the implementation of water mist systems, such as the need for proper design and installation to ensure optimal performance, as well as the potential for corrosion and clogging of the system's components. Moreover, the effectiveness of water mist systems can be influenced by various factors, including the size and type of fire, the location and layout of the space, and the presence of other materials that can interfere with the mist's ability to reach the flames.

2.2.2 Foam-Based Suppression

Foam-based suppression is a specialised fire suppression method that involves the use of a foam solution to extinguish fires. This method works by forming a foam layer on the fuel source, which helps to smother the fire and prevent the release of flammable vapors. Foam-based suppression systems are commonly used in industrial settings where flammable liquids and gases are present, as well as in aircraft hangars, oil refineries, and other high-risk environments. Foam-based suppression systems are designed to be highly effective and can quickly extinguish fires, helping to minimize damage and protect property and lives. These include:

Foam

It is commonly used for flammable liquid fires. Ferguson & Janicak (2005) discuss the use of foam in fire suppression and its effectiveness in controlling fires. They note that foam-based fire suppression systems are particularly effective in controlling fires involving flammable liquids, as the foam can create a barrier between the fuel and the air, preventing the fire from spreading. The authors also discuss the different types of foam, including aqueous film-forming foam (AFFF) and protein foam, and their applications. AFFF is commonly used in industrial and commercial settings because of its versatility and effectiveness, while protein foam is often used in high-risk applications such as aircraft hangars and petrochemical facilities. Ferguson & Janicak (2005) also highlights the importance of proper proportion and application of foam, as well as regular maintenance and testing of foam-based fire suppression systems. They note that inadequate foam proportioning or application can result in reduced effectiveness or even failure of the fire suppression system.

Foam extinguishers have some disadvantages and limitations that need to be taken into account when selecting a fire suppression method. As noted by Ferguson & Janicak (2005), foam extinguishers may not be suitable for use in fires caused by electrical equipment or combustible cooking oils, as well as class B fires involving pressurised fuels.

Additionally, foam extinguishing agents may not be effective at freezing temperatures, which can limit their use in cold environments. It is important to note that while foam extinguishers may have limitations, they can still be a highly effective fire suppression method in many situations, particularly those involving flammable liquids or gases. However, it is important to select the appropriate fire suppression method based on the specific circumstances and potential hazards present.

Compressed Air-Foam Systems (CAFS)

CAFS is used to create a foam solution that is dispensed through a nozzle or monitor to extinguish a fire. The foam consists of small bubbles that cover the fuel surface, separate it from the air, and suppress the fire. CAFS can be used with water or other extinguishing agents to increase their effectiveness. This system is particularly useful for fighting Class A fires that involve solid fuels such as wood, paper, or cloth. CAFS also has the advantage of using less water than traditional fire suppression systems, reducing water damage and runoff Rie et al. (2016). However, CAFS requires specialised equipment and training for proper use and may not be suitable for all fire scenarios.

2.2.3 Gas-Based Suppression

Some fires, such as those involving electrical equipment or sensitive materials, cannot be extinguished using water or foam. In these cases, gas-based suppression systems are used. Gas-based suppression systems use inert gases or chemical agents to suppress fires by reducing the oxygen concentration in the air surrounding the fire. This can effectively extinguish the flames without leaving behind any residue or causing significant damage to property. These systems use gases, such as carbon dioxide, argon, or halon, to displace oxygen and suppress fire O'Connor (2022).

Carbon Dioxide (CO_2)

CO_2 is a common gas used in gas-based suppression systems due to its ability to quickly displace oxygen in the air and extinguish fires. When discharged from a CO_2 extinguisher, the gas immediately smothers the fire by reducing the oxygen concentration in the surrounding air below the level required to sustain combustion. This effectively starves the fire of the oxygen it needs to continue burning.

According to Conroy (2003), CO_2 extinguishers are typically used for Class B and Class C fires, which involve flammable liquids and electrical equipment, respectively. These extinguishers are often found in industrial and commercial settings, such as manufacturing facilities and server rooms, where water or other traditional fire suppression methods could cause significant damage to equipment and property. It

is important to note, however, that the use of CO_2 extinguishers can also have some drawbacks. Due to oxygen displacement, the use of CO_2 extinguishers can create a hazardous environment for anyone in the affected area, as reduced oxygen levels can cause dizziness, disorientation, and even unconsciousness. Additionally, the use of CO_2 can be ineffective for fires involving solid materials, such as wood or paper, as the gas CO_2 does not cool the burning material or remove the fuel source.

Inert Gas Agents

Clean agent fire suppression systems use environmentally friendly inert gases, such as nitrogen, argon, and helium, which have zero ozone depletion potential and no global warming potential. These gases do not produce harmful by-products when used to extinguish fires.

The suppression mechanism of inert gas systems involves reducing the oxygen concentration in the air surrounding the fire, which effectively extinguishes the flames. There are three commonly used types of inert gas system: Argonite (IG-55), Inergen (IG-541), and Argon (IG-01). Argonite consists of 50% nitrogen and 50% argon, Inergen contains 52% nitrogen, 40% argon, and 8% carbon dioxide, and Argon contains 100% argon Kim (2001) .

It is important to note that unlike CO_2, inert gases are non-toxic to humans at low concentrations. However, low oxygen levels can still pose a concern, and special precautions must be taken to ensure safe use. Inert gases suppress fires by reducing the oxygen concentration and flame temperature below the level required for combustion, leading to fire extinguishment. However, they are not as effective as halocarbon agents and require a larger quantity of agent to be dispersed to extinguish fire.

Despite their effectiveness, inert gas agents do have some limitations. For example, they require special storage cylinders, as they are stored as high-pressure gases, and their discharge can result in a significant reduction in the oxygen level in the space, which may pose a risk to human occupants Kim (2001).

Halocarbon Gases

Halons were a family of gas-based suppression systems that were widely used in fire protection applications. They were composed of halogenated hydrocarbons that contained bromine, fluorine, or chlorine atoms. Halons were a type of gaseous or volatile liquid chemical used for fire and explosion protection, the most widely used types being Halon 1301, which is used primarily as a total flood agent, and Halon 1211, which is typically used in streaming applications Speitel & Lyon (2009). However, because of their harmful

impact on the environment, halons are no longer used in most fire protection applications.

Halon extinguishing agents are highly sought after in the industry as they rapidly vaporise during a fire and do not leave behind any corrosive or abrasive residue. Furthermore, due to their non-damaging effect on electrical components (unlike dry-chemical agents), they have gained widespread popularity. Although Halon 1301, and 1211 have proven to be highly effective as extinguishing agents, they were identified as ozone depleting substances in the Montreal Protocol on Substances that Deplete the Ozone Layer. Halons are bromated chlorofluorocarbons and are potent destroyers of the earth's ozone layer. As a result, their use is being phased out Ferguson & Janicak (2005).

2.2.4 Powder-based suppression

These suppression agents are commonly used for fire suppression and are effective against Class A, B, and C fires. These agents work by separating the fuel source from the oxygen, thus preventing the combustion process. There are several types of powder-based suppression agents, including dry chemical, inert powder, and hybrid powder agents.

Dry Chemical Agents

Dry chemical agents are the most common type of powder-based suppression agent and are composed of a fine powder made up of a mixture of chemicals. According to NFPA17 (1980), dry chemical agents are "especially effective for fires involving flammable liquids and gases, electrical hazards, and small fires, in general".

Inert powder agents

These are composed of nonreactive materials such as sand, limestone, or graphite. They work by suffocating the fire and reducing the concentration of oxygen around the fuel source. Inert powder agents are recommended for use in areas where electronics, computers, and other sensitive equipment is present.

Hybrid Powder Agents

hybrid powder agents are designed to provide more effective suppression capability than single agent powders by combining two or more different types of suppression agents, typically a dry chemical and an inert powder. This allows a wider range of fire types to be effectively suppressed.

Hybrid powder agents such as the ABC multipurpose dry chemical, combine monoammonium phosphate and ammonium sulfate to create a dual-agent powder. This type of hybrid powder can be used for class A, B, and C fires, and is commonly used in portable fire extinguishers and fixed suppression systems ABS (2015).

2.2.5 Aerosol-Based Suppression Agents

Aerosol-based suppression agents are a type of fire suppression technology that uses a fine mist or aerosol of solid particles to suppress fires. There are different types of aerosol fire suppression agents, including condensed aerosols and hybrid aerosols. Condensed aerosols, such as those based on potassium compounds or metal oxides, and hybrid aerosols combine the benefits of both types and are used in a variety of applications, including industrial settings and transportation systems. Some types of aerosol fire suppression agents are shown below:

Pyrogen

It is an aerosol-based fire suppression agent that uses a solid particulate aerosol to suppress fires. The particles are made of potassium compounds that inhibit the chemical chain reactions that occur during a fire, effectively extinguishing the flames. Pyrogen is effective in class A, B, C, E, and F fires.

Pyrogen employs a distinctive extinguishing mechanism in which a specially designed solid chemical, when ignited either electrically or thermally, generates combustion products in the form of micron-sized dry chemical particles and gases. The dry chemical particles, primarily consisting of potassium carbonates, and the gaseous mixture, composed mainly of carbon dioxide, nitrogen, and water vapor, combine to form a uniform fire extinguishing aerosol. Prior to release into a protected area, the hot aerosol propels itself through a unique solid chemical coolant, which undergoes decomposition, absorbing significant amounts of heat. This ensures a flameless discharge and uniform distribution of the cool aerosol within the designated area. The rapid discharge rate of the aerosol contributes to a powerful knockdown effect. The micron-sized aerosol particles exhibit gas-like three-dimensional properties, facilitating swift distribution throughout the enclosure, reaching even the most concealed and shielded locations. Achieving homogeneous distribution takes just seconds, and the extended holding times play a crucial role in preventing fire re-ignition Berezovsky (n.d.).

Stat-X

It is an example of a hybrid aerosol system from Fireaway Inc. Stat-X uses a proprietary mixture of potassium-based solid aerosol particles and inert gases to suppress fires.

The system releases a condensed aerosol that quickly fills the protected space, extinguishing the fire by interrupting the chemical chain reaction. The system is designed to be compact and easy to install, making it suitable for a wide range of applications Fireaway (2013).

This thesis focuses on the investigation of particular fire suppression agents in the

form of condensed aerosols, specifically those based on potassium compounds such as KO_2, $KHCO_3$, and KCO_3.

2.3 Potassium Containing Compound Based Condensed Aerosol Fire Suppression Agent

According to NFPA (2010), the condensed aerosol is defined as an extinguishing medium consisting of finely divided solid particles, generally less than 10 microns in diameter, generated by a thermal decomposition process of a solid aerosol-forming compound, without the need for a separate gas carrier. The diameter of potassium-containing compound-based aerosol particles used for explosion suppression can vary depending on the specific product and application. Generally, these aerosols are produced as dry powders and then dispersed in the air using specialised equipment. The size of the particles in the aerosol can affect their behaviour and effectiveness.

Research has shown that potassium species particles in the range of 1 to 10 micrometers in diameter are most effective for explosion suppression. Particles in this range are small enough to remain suspended in the air for an extended period, allowing them to reach and interact with flames or explosions, while they are large enough to settle out of the air quickly once the suppression process is complete Dolan & Dempster (1955), Rosser Jr et al. (1963), and Fischer & Leonard (1995).

2.3.1 Ingredients for Condensed Aerosol-Based Potassium Species Generation

The composition of ingredients to generate condensed aerosol-based potassium species can vary depending on the specific product or system used. However, generally, it involves a solid fuel tablet made up of a mixture of potassium-based compounds, which is thermally decomposed to generate the aerosol.

The solid fuel tablet typically consists of a mixture of potassium salts, such as potassium carbonate, potassium sulphate, and potassium nitrate, as well as other ingredients, such as a binder, a fuel source, and a combustion catalyst. The binder is used to hold the ingredients together and help with the combustion process, while the fuel source provides the energy needed for the thermal decomposition to occur. The combustion catalyst helps promote the decomposition of the fuel. Other additives or binders may also be included in the tablet to help with combustion and aerosol production. These may include materials such as silica, alumina, and calcium carbonate, which can improve the flowability and handling of the tablet and enhance the aerosol properties Rohilla et al. (2019).

The exact composition and formulation of these ingredients may be proprietary and not publicly disclosed by the manufacturer, as it is often considered confidential information. However, the general makeup of the ingredients is known to be crucial

in producing a condensed aerosol-based potassium species that can effectively suppress fires.

2.3.2 Aerosol Suppression Generation

There are typically three methods for delivering the aerosol suppression agent to the fire compartment:

- Piping in and dispersing prefabricated micron particles using a powerful ventilator such as a compressed inert gas system. This method is known as a powder aerosol system.
- Discharging, pulverizing, and propelling prefabricated micron particles through a nozzle by an impulse generated from a small pyrotechnic charge. This method is referred to as a propelled aerosol system. However, producing micrometer-sized particles of the potassium-based agent can be expensive and the particles may agglomerate in their storage canisters over time, reducing the reliability of the systems.
- Generating condensed micrometre particles in place through the thermal decomposition of a solid fuel tablet. This method is known as a pyrotechnically generated aerosol, or condensed aerosol system. Pyrotechnic aerosol suppression agents produce a large amount of heat during the thermal decomposition of the solid fuelRohilla et al. (2019). Fireless units used in this investigation are based on pyrotechnically generated aerosols, and these units have been used to test the potassium oxide-based suppression agent in Chapter 3.

2.3.3 Potassium Containing Compounds as Suppression Agents

Potassium-containing compounds have been identified as effective flame inhibitors in different studies, Dewitte et al. (1964), Birchall (1970), Mitani & Niioka (1984), Williams & Fleming (1999),Tapscott et al. (2001), Taveau et al. (2015), Zhou et al. (2019), Liu et al. (2020).

The study by Roosendans et al. (2017) presents experimental findings that indicate a notable suppression of CH_4/air explosions with the addition of potassium metal salt suppressants.

The study conducted by Babushok et al. (2017) is introduced, emphasising their investigation of the impact of $KHCO_3$ addition on burning velocity and temperature of combustion in premixed flames CH_4 / air. The observed decrease in burning velocity is attributed to reductions in radical concentrations, influenced by the thermal effects of the added agent.

Additionally, Wang et al. (2023) is referenced for their visualisation of the inhibition effects of $KHCO_3$ and KH_2PO_4 on the explosion process of ethylene. The study

reveals that $KHCO_3$ addition leads to a decrease in explosion pressure, showing superior inhibition effects compared to KH_2PO_4 at similar concentrations. The better physical inhibition of flame/explosion of $KHCO_3$ is explained by its lower initial pyrolysis temperature and higher heat absorption. Furthermore, the chemical inhibition characteristics are superior due to the greater production of KOH from rapid $KHCO_3$ pyrolysis.

To evaluate the effectiveness of potassium-containing aerosols, different methods have been proposed, including laboratory-scale experiments, full-scale fire tests, and computer modelling simulations Quintiere (2016). These methods help determine the efficiency of extinguishing, concentration distribution, and environmental impact of potassium-containing aerosols, which are important factors in evaluating the performance of agents.

2.3.4 Previous Studies of Flame Inhibition by Potassium-Species-Based Aerosol

The specific topic of flame inhibition by condensed aerosols based on potassium species has limited studies compared to other fire suppression agents. Although there is research on the use of potassium compounds in general as flame inhibitors, the specific focus on the kinetic study of KO_2, $KHCO_3$, and KCO_3 on the H_2 and CH_4 do not have a body of literature as extensive.

The available research is concentrated on specific applications or scenarios. The development and investigation of condensed aerosols based on potassium species as fire suppression agents are relatively recent or still an emerging field of research.

Previous studies have investigated the potential of potassium-species-based aerosols for flame inhibition and fire suppression. These studies have explored both experimental approaches and numerical modelling to assess the effectiveness of these aerosols. An overview of previous research in this area is shown below.

Experimental Studies

Flame Suppression Experiment

Experimental setups have been designed to examine the flame inhibition capabilities of aerosols based on potassium species. These experiments involve introducing the aerosols into controlled flame environments and measuring the resulting changes in flame behavior. Parameters such as flame temperature, flame size, heat release rate, and combustion products are analyzed to evaluate the suppression effects of the aerosols. Kuang et al. (2011) investigated the effectiveness of superfine potassium bicarbonate powder in suppressing small-scale fires.

The study used a cone calorimeter to generate a controlled fire and compared the suppression performance of the superfine potassium bicarbonate powder to that of a conventional potassium bicarbonate powder and a commercially available dry chemical

powder. The results showed that the superfine potassium bicarbonate powder was more effective in suppressing fire than the conventional potassium bicarbonate powder and the dry chemical powder. The authors suggested that the improved performance of the superfine potassium bicarbonate powder was due to its finer particle size, which enabled it to better penetrate the flame and form a more effective barrier against heat and combustion gases.

Flame Propagation and Extinction Tests

Experimental investigations have focused on studying the impact of potassium-species-based aerosols on flame propagation and extinction. These tests involve exposing fuel/air mixtures to aerosols and analysing the changes in flame propagation speed, flame front geometry, and the ability of the flame to self-extinguish in the presence of aerosols. Kwon & Kim (2013) investigated the extinction effectiveness of pyrogenic condensed aerosols in a fire extinguishing system.

The thermal characteristics of the solid aerosols as extinguishing agents were analysed using thermogravimetry (TG) and differential thermal analysis (DTA). The results indicated that the addition of resin to the main component of Potassium Nitrate (PN) effectively mitigated the exothermic reaction of the pyrogenic condensed-aerosol extinguishant. To ensure the safety of the extinguisher, the study also conducted the modified closed pressure vessel test (MCPVT) and measured the conductivity of the solid aerosol extinguisher.

The results obtained from the maximum height test demonstrated the extinguishing capability of the pyrogenic condensed aerosol extinguishing agent in a gaseous fire extinguishing system.

Particle Characterization

Experimental studies have also aimed to characterize the physical properties of potassium-species-based aerosols. The particle size distribution, concentration, morphology, and chemical composition of the aerosols are analysed using techniques such as particle size analysers, microscopy, and spectroscopy. These characterisations provide insights into the aerosol's behaviour, dispersion, and interaction with flames.

Increasing the particle size of solid particles used for flame suppression can indeed reduce their effectiveness. This is because the surface area of the particles plays a crucial role in the suppression of the fire. By reducing the size of the solid particles, the surface area increases, allowing for better coverage of the fire area and enhancing the suppression effect Fleming et al. (1998). Supporting this notion, Babushok et al. (2017) found from previous studies, Rosser Jr et al. (1963), Ewing et al. (1989), Ewing et al. (1992) that solid particles with particle sizes in the range of 5-25μm exhibited a higher inhibition effect on flames. These smaller particles provide a larger surface area for interaction with the flame,

allowing for more effective suppression. On the other hand, larger particles may have a lower effect on flame suppression due to their reduced surface area and potentially limited interaction with the fire Zhou et al. (2019), Fischer & Leonard (1995).

Numerical Simulations

Reaction Kinetics Modeling: Researchers have developed reaction kinetics models to study the chemical reactions that occur between aerosols based on potassium species and combustion products. These models consider the complex reactions and species interactions involved in flame inhibition. By incorporating experimental data and kinetic parameters, these models help to understand the underlying mechanisms responsible for flame suppression.

One of the studies conducted by Babushok et al. (2017) focused on examining the effectiveness of $KHCO_3$ (potassium bicarbonate) in CH_4 (methane) flames. The researchers developed a comprehensive kinetic model to investigate the impact of potassium-containing compounds on hydrocarbon-air flames. The results of the study showed that $KHCO_3$ had a noticeable effect on the burning velocity of premixed CH_4/air flames. Specifically, the presence of $KHCO_3$ led to a reduction in the burning velocity of the flames.

Furthermore, the study found that $KHCO_3$ influenced the consumption of free radicals by potassium (K) and potassium hydroxide (KOH) atoms. This suggests that the presence of $KHCO_3$ affected the reaction pathways and the kinetics of the flame.

Additionally, the inhibition effectiveness of $KHCO_3$was observed to be higher in lean mixtures (lower fuel-to-air ratio) compared to rich fuel mixtures (higher fuel-to-air ratio). This indicates that $KHCO_3$ exhibited greater flame suppression properties in fuel-lean environments. Another study published by Babushok & Tsang (2000) provides the relative effectiveness of different inhibitors for suppressing alkane combustion. The findings contribute to the understanding of flame inhibition mechanisms.

The study involves the development of a detailed kinetic model to assess the inhibition capabilities of different compounds in alkane flames. The researchers compared the performance of various inhibitors by analysing their impact on the burning velocity and ignition delay of alkane-air mixtures. The results of the study provide rankings for the inhibitors on the basis of their effectiveness in inhibiting alkane combustion. The inhibitors were assessed in terms of their ability to reduce the burning velocity and delay the ignition of alkane flames.

According Zhou et al. (2019), the numerical findings revealed a reduction in the maximum mol fractions and equilibrium mol fractions of H and OH radicals during the chain reaction processes with the inclusion of $KHCO_3$. The presence of $KHCO_3$ particles facilitated a catalytic cycling mechanism, as indicated by the reactions KOH + H = K + H_2O and K+ OH + M =KOH + M. This cycling process promoted the combination of H

and OH radicals, ultimately leading to the production of stable H_2O.

The combination of experimental studies and numerical simulations provides a comprehensive understanding of the flame-inhibition capabilities of potassium-species-based aerosols. These investigations contribute to the development of effective fire suppression strategies and the optimization of aerosol-based suppression systems.

2.4 Numerical Evaluation of Aerosol Inhibition Effects

To evaluate the inhibition effect of aerosols numerically, various software tools can be used. These software tools provide capabilities for modelling and simulating the behaviour of aerosols in combustion systems. Some widely used software tools for this purpose include:

2.4.1 Computational Fluid Dynamics, CFD

in CFD, the intricate interplay of fluid flow, combustion, and chemical reactions is mathematically described and solved through computer-based processes. Computational fluid dynamics has become an essential tool for understanding and predicting the intricate behavior of reacting flows. These flows represent inherently complex systems, characterized by the intricate interplay between chemical kinetics and fluid mechanics Muhammad et al. (2022).

2.4.2 Chemkin

Chemkin is a software package designed to facilitate the formulation, solution, and interpretation of problems related to elementary gas-phase chemical kinetics. It serves as a versatile and powerful tool for integrating complex chemical kinetics into simulations of fluid dynamics. The package comprises two key software components: an Interpreter and a Gas-Phase Subroutine Library. The Interpreter is a program that interprets a symbolic description of a user-defined elementary chemical reaction mechanism. One output from the Interpreter is a data file that establishes a connection to the Gas-Phase Subroutine Library. This library encompasses approximately 100 highly modular Fortran subroutines that can be invoked to retrieve information on the equation of state and thermodynamic properties Kee et al. (1989).

Chemkin-Pro offers various reactor models, catering to different scenarios. These reactors can be open, allowing species to flow in and out of the reactor boundaries. Alternatively, they can be closed, resembling a batch reaction setup where no additional species can enter or exit the reactor. Reactions can occur in homogeneous or partially stirred environments. Additionally, there are specialised models, such as one-dimensional reactors ANSYS (2019).

Thermodynamic Data

The initial data input for Chemkin-Pro pertains to the thermodynamic properties of all the species involved in the simulation. These properties include the specific heat capacity (C_{pk}), specific enthalpy (H_k), and specific entropy (S_k) Coltrin et al. (1996). These thermodynamic parameters are computed within the programme using various constants, which are sourced from Chemkin-Pro's native thermodynamic property database or alternative references such as JANAF tables. In the equations provided, the subscript "T" represents the temperature and "R" denotes the ideal gas constant Design (2015), Coltrin et al. (1996)

$$\frac{C_{pk}}{R} = a_{1k} + a_{2k} \cdot T + a_{3k} \cdot T^2 + a_{4k} \cdot T^3 + a_{5k} \cdot T^4 \tag{2.1}$$

$$\frac{H_k}{RT} = a_{1K} + \frac{a_{2k}}{2} \cdot T + \frac{a_{3k}}{3} \cdot T^2 + \frac{a_{4k}}{4} \cdot T^3 + \frac{a_{5k}}{5} \cdot T^4 + \frac{a_{6k}}{T} \tag{2.2}$$

$$\frac{S_k}{R} = a_{1k} \ln(T) + a_{2k} T + \frac{a_{3k}}{2} T^2 + \frac{a_{4k}}{3} T^3 + \frac{a_{5k}}{4} T^4 + a_{7K} \tag{2.3}$$

The numerical coefficients, denoted as $a_1, a_2, \ldots, a_6$ and a_7, are provided in the NASA or JANAF thermodynamic files. These equations and parameters enable the program to calculate and utilize essential thermodynamic data for the species, facilitating accurate and comprehensive simulations within Chemkin-Pro.

The next essential requirement for Chemkin-Pro pertains to the provision of kinetic data encompassing both gas-phase and surface reactions. Typically, the widely adopted approach for specifying kinetic rates is the straightforward Arrhenius form (more details in Subsection 2.6.1), where the reaction rates are based on the reaction rate constant, denoted as K, Hubbard et al. (2020).

Chemical Reaction Rate Expression

The chemical rate expressions in Chemkin are constructed based on thermodynamic considerations. The reaction rates are influenced by the composition of the species, the temperature, and the pressure. Specifically, in Chemkin, the production rate of the k-th species is expressed as the sum of the rate of progress variables for all reactions, including those involving the k-th species. The equation representing this relationship is as follows:

$$r_k = \sum_{i=1}^{I} v_{ki} q_i \quad (k = 1, \ldots, K) \tag{2.4}$$

Where r_k is the production rate of the k-th species, v_{ki} represents the stoichiometric coefficient, and q_i is the rate of progress variable for the reaction. q_i is obtained by the

difference between the forward and reverse rates, as shown below Coltrin et al. (1996):

$$q_i = k_{f_i} \prod_{k=1}^{K} X^{(v_{ki'})} - k_{r_i} \prod_{k=1}^{K} X^{(v_{ki''})} \tag{2.5}$$

where:

- q_i is the rate of progress variable for reaction i,
- k_{f_i} is the forward rate constant for reaction i,
- k_{r_i} is the reverse rate constant for reaction i,
- X represents the concentration of the species involved in the reaction,
- $v_{ki'}$ and $v_{ki''}$ are the stoichiometric coefficients of the reactant and product species, respectively, in reaction i,

In Chemkin, the temperature dependence of the forward rate constant for a reaction is assumed based on the modified Arrhenius equation, as shown in 2.16. The reverse rate constant k_{r_i} is linked to the forward rate constant through the equilibrium constant Kee et al. (2003). This relationship is expressed below:

$$k_{r_i} = \frac{k_{f_i}}{K_{c_i}} \tag{2.6}$$

The thermodynamic properties are used to calculate the equilibrium constant, denoted as k_{c_i} according to the following expression:

$$k_{ci} = k_{pi} \left(\frac{P_{\text{atm}}}{RT} \right)^{\sum_{k=1}^{n} v_{ki}} \tag{2.7}$$

and

$$k_{pi} = \exp \left(\frac{\Delta S_i}{R} - \frac{\Delta H_i}{RT} \right) \tag{2.8}$$

In the context of chemical reactions, the subscript i represents the specific reaction under consideration. The symbols S° and H° denote the standard entropy and standard enthalpy, respectively. The term Δ signifies the alteration observed during the transition from reactants to products in the ith reaction Coltrin et al. (1996). The change in the standard-state molar enthalpy and entropy is shown as below:

$$\frac{\Delta H_i^\circ}{R} = \sum_{k=1}^{n} v_{ki} \frac{H_i^\circ}{RT} \tag{2.9}$$

$$\frac{\Delta S_i^\circ}{R} = \sum_{k=1}^{n} v_{ki} \frac{S_i^\circ}{RT} \tag{2.10}$$

where k_i^v is calculated by subtracting the forward stoichiometric coefficients from the reverse stoichiometric coefficients for the k-th species in the i-th reaction.

Transport Properties

Much like the application of thermodynamic data, the inclusion of transport data in a numerical model stands as a crucial step in accurately simulating chemical kinetics and fluid dynamics.

Transport parameters are a foundational element of any kinetic mechanism and are indispensable for simulating non-uniform processes, such as flame propagation. It has been recognized for many years that transport properties are just as vital in flame modeling as the rate constants of chemical reactions. In addition, a shared database was established, originally created by Sandia National Laboratories, which gained popularity, especially in conjunction with the widely used Chemkin software package Konnov (2019).

To apply transport data in a numerical model, one must first collect the necessary transport coefficients for the chemical species involved in the system. These coefficients are typically temperature-dependent and can be acquired from various sources.

However, it is important to note that for some chemical compounds, complete transport data may be missing. In such cases, assumptions or estimations regarding their transport properties to proceed with modeling are required. These assumptions are essential to fill data gaps and ensure that the numerical model can accurately represent the behaviour of all species in the system. Once the transport data are available, they are integrated into the numerical model using the relevant transport equations. The transport properties, such as viscosity and thermal conductivity, impact the flow behaviour and energy transfer within the system. Accurate modelling of these properties is essential for predicting phenomena like flame propagation and chemical reactions. The table 2.1 provides an example of the transport properties for potassium Design (2015):

Table 2.1: Transport Data File of the K-species

Species	Geometry	ε/kB	σ	μ	α	Zrot	Refrence
K	0	850	4.25	0.000	0.000	1.000	Kee et al. (1986)

”The ’Species’ column lists the chemical species for which transport data is provided, each identified by its chemical formula.

In the ’Geometry’ column, an index categorizes the molecule’s geometric configuration as monatomic, linear, or nonlinear. A value of 0 denotes a single-atom molecule, while a value of 1 represents a linear configuration, and 2 indicates a non-linear configuration.

ε/kB: This column represents the well depth parameter, divided by the Boltzmann constant. The well depth parameter describes the depth of the potential energy well

between two molecules and is an indicator of the strength of intermolecular forces. A higher ε/kB indicates stronger interactions.

σ: This column typically repeats the collision diameter value, providing the actual numerical value for σ.

μ: This column represents the dynamic viscosity of the species. Dynamic viscosity is a measure of a fluid's resistance to shearing flows and is important for understanding the fluid's behavior in response to shear forces.

α: This column often represents the polarizability of the species. Polarisability is a measure of the ease with which the electron distribution within a molecule can be distorted by an external electric field.

Zrot: This column indicates the rotational relaxation collision number. It provides information on the rate at which the species can rotate or tumble when it collides with other molecules in a gas.

These properties play a role in understanding the collisional behaviour of molecules, energy transfer, and interactions between species at a molecular level Design (2015).

In Chemkin, transport properties, such as dynamic viscosity (η), thermal conductivity (λ), and binary diffusion coefficients (D_{ij}), are typically provided in the form of polynomial fits. To utilize these transport data in the necessary calculations, it's essential to apply the polynomial fits to obtain the transport properties at a given temperature. The equations for using these fits are as follows Design (2015):

For dynamic viscosity (η), the equation takes the form:

$$\ln \eta = \sum_{n=1}^{N} a_{n,k} \, (lnT)^{n-1} \tag{2.11}$$

Similarly, for thermal conductivity (λ), the equation is as follows:

$$\ln \lambda = \sum_{n-1}^{N} b_{n,k} \, (lnT)^{n-1} \tag{2.12}$$

The equation for binary diffusion coefficients (D_{ij}) follows the same pattern:

$$\ln D_{ij} = \sum_{n-1}^{N} d_{n,jk} \, (lnT)^{n-1} \tag{2.13}$$

Where:

N: is the number of coefficients in the polynomial fit.

an: These coefficients are associated with dynamic viscosity, and they are part of a polynomial fit that models how viscosity changes with temperature based on thermodynamic data.

bn: These coefficients are linked to thermal conductivity and they are used in a

polynomial fit to describe how thermal conductivity varies with temperature, relying on thermodynamic data.

dn: These coefficients are used for binary diffusion coefficients, and they are involved in a polynomial fit to capture the temperature-dependent behaviour of binary diffusion coefficients based on thermodynamic data.

In the Chemkin reactor physical properties icon, there are four selections available to determine how transport properties are solved. These options include:

Use Mixture Averaged Transport: This option calculates transport properties using a mixture-averaged approach, considering the average properties of all species in the mixture to determine the species' ordinary diffusion coefficients and fluxes. Chemkin employs its internal algorithms to calculate the mixture-averaged transport properties. These internal algorithms consider the interactions and behavior of all the species in the mixture to determine the overall transport properties, without relying on the specific properties you might have set for individual species in the chemistry database.

Use Multicompound Transport: This selection employs a multicompound transport model, which accounts for interactions between different species in the mixture.

Use Lewis Number: Use the Lewis number to define the ratio of thermal to mass diffusion, providing an additional dimension to characterize species transport. **User Defined mixture average transport properties**: Transport properties, in this case, will be calculated based on the fundamental transport properties that are provided in the chemistry set ANSYS, Inc. (2023).

2.5 Combustion Properties

When evaluating the effectiveness of fire suppression agents, it is crucial to identify key parameters that accurately assess their performance. These parameters serve as metrics for gauging the agents' ability to control and extinguish fires efficiently.

A significant parameter in the evaluation of fire suppression agents is laminar burning velocity, S_L. It refers to the speed with which a laminar flame front propagates through a fuel-air mixture under specified conditions. S_L represents the intrinsic ability of a flame to spread and sustain itself. It is influenced by factors such as fuel composition, mixture concentration, temperature, and pressure. The measurement and analysis of laminar burning velocity could provide valuable insights into the performance of fire suppression agents. Evaluating the impact of suppression agents on the reduction or alteration of S_L indicates their ability to slow or inhibit the combustion process, leading to flame suppression and fire control Xu et al. (2017).

Numerical simulations and experimental techniques are commonly employed to evaluate S_L and its interaction with fire suppression agents. These methods allow researchers to quantify the effectiveness of fire suppression agents in terms of their ability to suppress flame propagation. This information enables the development of more

efficient suppression agents and the optimization of fire safety strategies.

Several studies have investigated the relationship between S_L and fire suppression agents. For example, researchers have examined the effects of various chemical agents, such as halon and water mist, on the burning velocity of combustible mixtures. The results have shown that these agents can effectively reduce the burning velocity, thus slowing the propagation of the flame Linteris & Truett (1996), and Yoshida et al. (2015). There are other parameters that are important for evaluating the effectiveness of fire suppression agents. Some of these parameters include the heat release rate which measures the amount of heat released per unit of time during a fire and the flammability limit.

2.5.1 Laminar Burning Velocity

Laminar flames play a crucial role in understanding the fundamental principles of flame theory and are essential for comprehending complex combustion phenomena, such as flame front instabilities, extinction, and turbulence. The S_L is described as the velocity at which a flame front propagates through a combustible mixture in the absence of turbulence. The chemistry of flames exhibits similarities in various hydrocarbon fuels and is predominantly influenced by reactions involving small molecules and radicals that contain oxygen (O), hydrogen (H), and a single carbon (C) atom. Flame propagation can be understood as a delicate balance between the production and consumption of reactive radicals. An increased pool of radicals improves reactivity, which in turn affects the velocity of laminar burning Law (2010).

The S_L is found to be directly proportional to the flame temperature. Higher flame temperatures promote dissociation reactions, leading to the generation of more free radicals within the flame. This, in turn, accelerates the overall combustion reaction rate and increases the burning velocity. The S_L can be expressed as follows:

$$S_L = \frac{1}{A_C \rho} \frac{dm}{dt} \tag{2.14}$$

Here, A_C is the cross-sectional area of the flame front, ρ is the density of the unburned gas adjacent to the flame front, and $\frac{dm}{dt}$ represents the mass flow rate of the unburned gas into the flame front Rallis & Garforth (1980).

In a conduit containing a premixed mixture of fuel and oxidiser, it can be seen that after ignition, a flame progresses to the unburned mixture, as depicted in Figure 2.1. The lower portion of the illustration provides a closer look at the structure of the flame. The combustion reaction zone, commonly referred to as the ”flame,” is typically quite thin, usually spanning just a few millimetres, particularly in ambient conditions when dealing with hydrocarbon fuels. Within the preheat zone, there is a gradual increase in

the temperature of the reactants as they transition from the temperature of the unburned mixture to an elevated temperature near the reaction zone. As the temperature of the reactants approaches the ignition temperature of the fuel, chemical reactions become more rapid, marking the front of the combustion reaction zone, which is the flame itself. Inside the flame, the reaction rate increases and then begins to decrease as the fuel and oxidiser are consumed, and products are generated. Due to the concentration gradient of species, reactants diffuse toward the reaction zone, and their concentrations in the preheat zone decrease as they draw closer to the reaction zone. The temperature of the products closely approximates the adiabatic flame temperature McAllister et al. (2011).

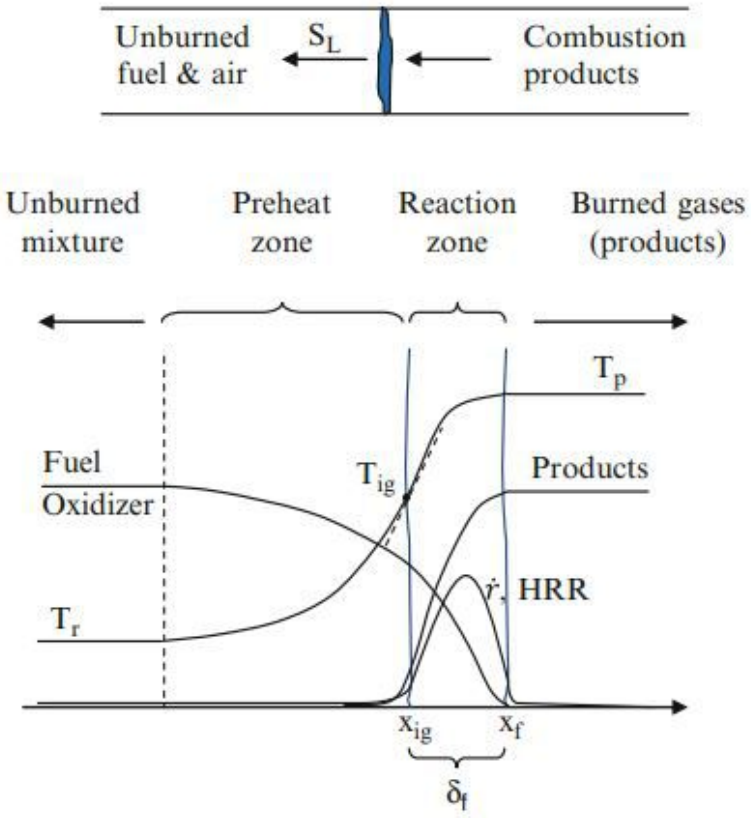


Figure 2.1: Sketch of a premixed flame propagating in a duct from right to left.

Where: δ is the thickness of the reaction zone.
^{r} is the average magnitude of fuel consumption rate over the entire flame $(mol/cm^3.sec)$.
Tig is the ignition temperature.
Tr is the temperature of the reactant mixture.
Tp is the temperature of the combustion products.
The propagation of the flame through the unburned mixture depends on a sequence of two consecutive processes. Initially, the heat generated within the reaction zone is conveyed in the opposite direction, raising the temperature of the incoming unburned mixture until it reaches the ignition temperature. Subsequently, the reactants, which have been preheated, undergo chemical reactions within the reaction zone.

Both processes have equal significance, and as a result it is reasonable to anticipate that the speed of the flame will depend on a combination of transport and chemical reaction properties McAllister et al. (2011).

Various methods are employed to determine S_L, including experimental and numerical modelling techniques. In numerical methods, S_L is meaningful when related to a planar flame front that occurs in a one-dimensional flow system. (Di Sarli & Di Benedetto (2007) have utilized the Chemkin package to numerically simulate one-dimensional S_L.

The Laminar Burning Velocity of Hydrocarbon Mixture

To accurately predict and analyse S_L, researchers use chemical reaction mechanisms that describe the complex kinetics of hydrocarbon combustion. Several widely used mechanisms have been developed for different hydrocarbons. One notable mechanism is the Warnatz mechanism Warnatz (1985), which provides a detailed description of the oxidation reactions involved in the combustion of hydrocarbons such as methane, ethane, propane, and higher hydrocarbons. To determine the S_L of a hydrocarbon mixture, detailed reaction mechanisms such as GRI-Mech 3.0 Smith et al. (1999) are commonly employed. GRI-Mech 3.0 includes a comprehensive set of chemical reactions that describe the combustion process of different hydrocarbon species. By simulating the reaction kinetics and considering the transport properties of the mixture, the laminar burning velocity can be calculated.

The range of laminar burning velocities for different hydrocarbons is significant. For example, methane typically exhibits laminar burning velocities in the range of 30-40 cm/s, while higher hydrocarbons such as propane and butane may have laminar burning velocities ranging from 50-70 cm/s. It is important to note that these values are approximate and can be influenced by experimental conditions and the specific composition of the fuel mixture.

Studying the effect of potassium species as a suppression agent on the laminar burning velocity of hydrocarbon mixtures is an area of interest in fire suppression research. Potassium-containing compounds have been investigated for their ability to inhibit combustion reactions and suppress flames. Evaluating their impact on laminar burning velocity provides information on their effectiveness as fire suppression agents.

In order to comprehensively understand the S_L of hydrocarbon mixtures and its relationship with the suppression effect of potassium species, researchers employ a combination of experimental techniques, numerical simulations, and chemical kinetic models. These approaches allow the evaluation of S_L under different conditions and the investigation of the inhibitory effects of potassium species on flame propagation.

The Laminar Burning Velocity of H_2/air Mixture

The laminar burning velocity of H_2/air is an important property in combustion studies, as it describes the velocity at which a premixed hydrogen-air flame propagates in a quiescent mixture. S_L has been extensively studied using a variety of experimental techniques and methodologies, and the resulting data provide insights into the fundamental combustion behaviour of H_2. The S_L of H_2/air has been extensively studied and measured the S_L of H_2 / air using various experimental techniques and numerical simulations. Several studies, including Dowdy et al. (1991), Sun et al. (1999) and Milton & Keck (1984), have reported measurements of the S_L of H_2-air mixtures. Dowdy et al. (1991) used a spherical combustion chamber and measured S_L of H_2 / air mixtures in various equivalence ratios. Liu & MacFarlane (1983) used a constant velocity nozzle burner as a function of the temperature and composition of the unburned gases. Ilbas et al. (2006) used a cylindrical combustion chamber at various equivalence ratios. Milton & Keck (1984) used a spherical combustion bomb and measured the laminar burning velocity of H_2/air mixtures at various pressures and temperatures ranging from 0.5 to 7 atm and 300 to 550K, respectively. Numerical simulations of the S_L of H_2/air mixtures have also been conducted by researchers, including Williams & Grcar (2009). These simulations use complex mathematical models to predict the S_L of H_2/air mixtures based on various input parameters, such as temperature, pressure, and equivalence ratio. One review article by Hu et al. (2009) provides experimental and numerical studies on premixed H_2/air flames at elevated pressures and temperatures as well as a discussion of the key factors that influence S_L, such as pressure, temperature, equivalence ratio, and mixture composition. The authors point out that S_L increases with increasing initial temperature and decreases with increasing initial pressure. In addition, the determination of S_L is significantly influenced by the competition between chain branching reactions and chain termination reactions. Chain branching reactions, which are temperature-sensitive and two-body reactions, and chain termination reactions, which are temperature-insensitive and three-body reactions, play pivotal roles in this competition. Furthermore, the suppression or enhancement of the overall chemical reaction is directly associated with changes in initial pressure or temperature. This phenomenon arises from the decrease or increase in the mol fractions of H and OH within the flames. Notably, there exists a strong correlation between S_L and the maximum concentrations of H and OH radicals in the reaction zone of premixed flames. Higher S_L aligns with elevated radical concentrations in the reaction zone. The S_L for H_2/air mixtures over a range of equivalence ratios increased with increasing equivalence ratio up to a certain point, after which it decreased due to the onset of cellular instabilities Pareja et al. (2010).

Previous studies on the S_L of H_2/air have reported varying values for this important combustion property. A comparison of these values can provide insights into the accuracy and consistency of different experimental techniques and methodologies, as well as

the effects of various experimental parameters on S_L. One study by Pareja et al. (2010) compared the S_L data reported in several previous studies forH_2/air mixtures at atmospheric pressure and room temperature. The authors found that the reported values varied widely, ranging from approximately 30 cm/s to 350 cm/s, depending on the experimental technique and conditions used. At an equivalence ratio of 1, S_L of H_2 / air flames have been measured to be in the range of 210-280 cm/s in various studies such as Ilbas et al. (2006), Liu & MacFarlane (1983), Günther & Janisch (1972) and Wu & Law (1985). This range of values is due to differences in the experimental conditions and measurement techniques used in each study. The S_L of H_2/air mixtures in equivalence ratio less than 1 generally decreases as the equivalence ratio decreases below the stoichiometric ratio (ϕ = 1). The exact range of burning velocity values can vary depending on the experimental conditions, However, the S_L range for H_2/air mixtures in the ϕ = 0.4 to 0.9 range is approximately 40 cm/s to 170 cm/s (Tse, 2000) Hermanns (2007), These ranges suggest that the burning velocity decreases as the equivalence ratio decreases below 1.

2.5.2 Flammability Limit

The flammability limits have been extensively used as a key indicator to perform quantitative risk assessments of explosion hazards. They define the boundaries within which a fire can occur and are crucial for assessing the effectiveness of fire suppression agents Miao et al. (2011). There are two important limits to consider:

The LFL represents the minimum concentration of fuel vapour or gas in the air required for combustion to be sustained, while the UFL represents the maximum concentration beyond which the mixture becomes too rich to support combustion Turns et al. (2012). The flammability limits of different hydrocarbons can vary significantly depending on their chemical structure, molecular weight, and vapour pressure. The flammability limit plays a crucial role in ensuring safety during industrial processes. While there is existing data on the flammability limits of pure hydrocarbons available in the literature, challenges arise in industrial applications due to the presence of various combinations of fuels under standard and non-standard conditions. In these scenarios, data on flammability limits can be scarce or even unavailable, making it essential to conduct comprehensive studies and gather relevant information to address potential safety concerns Zhao (2010). The flammability limit of H_2 is a critical parameter that governs the range of concentrations within which H_2 can form a flammable mixture with air. It is essential to understand these limits to ensure safety when handling, storing, or using hydrogen gas, which is highly flammable and can lead to explosive situations if not managed properly. In the case of H_2/ air mixtures, the flammability limits are commonly expressed as 4.1% (lower limit) and 74% (upper limit) H_2. However, these figures do not provide a complete picture, as the limits significantly vary depending on factors such as

temperature and pressure. The actual flammability range differs if the mixture is at room temperature or above and if it is at atmospheric pressure Shapiro & Moffette (1957).

When evaluating fire suppression agents, it is essential to consider their impact on the limits of flammability. Effective suppression agents should be capable of reducing the flammability range, particularly by increasing the LFL and decreasing the UFL. By modifying the flammability limits, suppression agents can help prevent the initiation and spread of fires.

The evaluation of the flammability limit can be carried out through experimental testing and numerical simulations. Experimental methods involve conducting tests to determine the concentration range at which combustion can occur and assessing how suppression agents influence these limits. Numerical simulations, such as Chemkin models, can also provide insights into the impact of suppression agents on the flammability limits. Table 2.2 shows the flammability limit for different gases McAllister et al. (2011).

Table 2.2: Flammability Limits (% fuel/air by volume)

Gas	**Lower flammability limit**	**Upper flammability limit**
Hydrogen	4.0	75.0
Methane	5.0	15.0
Butane	1.8	8.4
Ethane	3	12
Gasoline	1.4	7.6

2.5.3 Pathway Analysis

Pathway Analysis of H_2

This pathway outlines the primary reactions involved in the combustion of H_2 leading to the formation of H_2O as the final products. It also includes intermediate species and reactions along the way Tsang & Hampson (1986):

1. Initiation: H_2 oxidation process begins with the initiation of the reaction. One common initiation step involves the dissociation of (H_2) into two (H) through homolytic cleavage: $H_2 \rightarrow 2H$.

2. Propagation: Once the (H) are formed, they react with molecular oxygen (O_2) in a series of chain propagation reactions. These reactions involve the production of (OH) and the formation of (O or H) Glassman et al. (2014):

$H + O_2 \rightarrow OH + O$

$O + H_2 \rightarrow OH + H$

The (OH) generated in these reactions can further react with H_2 to form H_2O:

$OH + H_2 \rightarrow H_2O + H$

This process continues in a chain until the available reactants are consumed.

3. Termination: Chain propagation reactions can be terminated in several ways. One common termination step is the recombination of two hydroxyl radicals to form hydrogen peroxide (H_2O_2):
$2\,OH \rightarrow H_2O_2$
Another termination step involves the reaction of two hydrogen atoms to produce (H_2):
$2\,H \rightarrow H_2$.

4. Overall reaction: The overall reaction of H_2 oxidation to H_2O can be represented as follows:
$2\,H_2 + O_2 \rightarrow 2\,H_2O$
This pathway outlines the primary reactions involved in the oxidation of (H_2) to (H_2O), including the formation of intermediate species such as (OH) and (H_2O_2).

Pathway Analysis of Hydrocarbon

Initiation reactions are the first steps in the combustion of hydrocarbons. They involve breaking the chemical bonds within the hydrocarbon molecules to produce highly reactive species, such as radicals, that can initiate the combustion process. Two common initiation reactions are:

1. **Homolytic Cleavage (Initiation by Heat or Light)**

In this process, a molecule of the hydrocarbon CH_4 absorbs energy, often in the form of heat or light. This energy causes a chemical bond, typically a carbon-hydrogen (C-H) bond, to break homolytically (i.e., each atom retains one electron). This results in the formation of highly reactive radicals: $CH_4 \rightarrow CH_3 + H$
Here, CH_3 represents the methyl radical, and H is a H_2 radical. These radicals are highly reactive and serve as the initial species that participate in subsequent reactions, initiating the combustion process.

2. **Initiation by Oxygen Radicals**

Another initiation mechanism involves the reaction of hydrocarbons with oxygen radicals, often produced by a heat or light source. For example, the reaction of CH_4 with oxygen radicals can lead to the initiation of combustion: $CH_4 + O \rightarrow CH_3 + OH$
In this case, CH_3 is the methyl radical, and OH is the hydroxyl radical. Like in the previous example, these radicals are highly reactive and play a crucial role in initiating combustion.

Propagating Reactions: Once the combustion process is initiated, it follows a sequence of propagating reactions. These reactions sustain the flame through a chain reaction mechanism that involves radicals. Two primary types of propagating reactions are crucial for flame propagation:

1. **Chain Initiation**

The chain initiation phase commences when radicals generated during initiation reactions react with O_2, producing more radicals and initiating a chain reaction. For instance, CH_3 reacts with molecular oxygen:

$CH_3 + O_2 \rightarrow CH_3O_2$
or $CH_3 + O_2 \rightarrow CH_3O + O$
The resulting CH_3O_2 or CH_3O radicals can continue the cycle by reacting with other species, thus generating more radicals and perpetuating the combustion chain.

2. **Chain Propagation**
The chain propagation phase involves radicals interacting with the original hydrocarbon molecules, giving rise to additional radicals. For instance, the methyl radical (CH_3) can react with CH_4 to form CH_3 and OH:
$CH_4 + O \rightarrow CH_3 + OH$
This reaction generates both CH_3 and OH. Both of these radicals can indeed participate in subsequent reactions, contributing to the propagation of the combustion chain.

Termination Reactions:
Termination reactions bring the fiery spectacle to a close. These reactions occur when radicals combine with each other or with stable molecules to form non-radical, stable compounds. There are several types of termination reactions in hydrocarbon combustion,

1. **Radical Combination (Bimolecular Termination)**
Two radicals collide and react to form a stable molecule. In the combustion of CH_4, one of the termination reactions involves the combination of two CH_3 to form an ethane molecule (C_2H_6):
$2CH_3 \rightarrow C_2H_6$
2. **Radical Combination with Stable Molecules**
Radicals can also combine with stable molecules present in the combustion environment. For example, CH_3 can combine with OH to produce methanol (CH_3OH):
$CH_3 + OH \rightarrow CH_3OH$
Some termination reactions involve the conversion of radicals into different species. For example, the reaction of $2CH_3$ can lead to the formation of CH_4 and C_2H_6, Tsang & Hampson (1986):
$2CH_3 \rightarrow C_2H_6$
Termination reactions are essential to control the duration and intensity of the flame. As radicals are consumed through termination reactions, the chain reactions that sustain the flame gradually slow down and eventually cease, leading to the extinguishment of the flame.

2.6 Chemical Reaction Kinetics and Reaction Mechanism

understanding the reaction kinetics and reaction mechanism is crucial for conducting numerical simulations to investigate the effect of fire suppression agents based on KO_2, $KHCO_3$, and KCO_3 on H_2 and CH_4 flames. Reaction kinetics refers to the study of the rate and mechanism of chemical reactions, including identification of intermediate species

and determination of the rate constants. The reaction mechanism refers to the series of elementary steps by which a reaction occurs.

In the case of H_2 and CH_4 flames, the reaction mechanism for their combustion involves several steps. Initially, the fuel reacts with oxygen to produce free radicals, such as H and OH. These radicals then react with each other or with the fuel to produce other species, such as H_2O and CO_2. The kinetics of these reactions depend on various factors, such as temperature, pressure, and the concentrations of the reactants.

2.6.1 Reaction Kinetics

Chemical reaction kinetics is the study of how chemical reactions occur, including the rate of reaction and the factors that affect that rate. A fundamental understanding of chemical reaction kinetics requires understanding of several key concepts, including reaction rate, reaction order, activation energy, and the effect of catalysts.

The rate of a chemical reaction is determined by the frequency of successful collisions between reactant molecules and the energy of those collisions. This rate can be described using a rate law, which relates the rate of the reaction to the concentrations of the reactants and any catalysts present. The rate law equation can be determined experimentally through methods such as initial rate analysis, integrated rate law analysis, and graphical methods.

The order of a reaction describes how the rate of the reaction is affected by changes in the concentration of the reactants. For example, a reaction may be first order with respect to one reactant and second order with respect to another. The overall order of the reaction is the sum of the orders of each reactant. The order of a reaction can be determined experimentally through methods such as the initial rate method or the integrated rate method.

Activation energy is the energy required to initiate a chemical reaction. This energy barrier must be overcome before reactant molecules can form products. The Arrhenius equation describes the relationship between activation energy, temperature, and reaction rate. Understanding the activation energy of a reaction can provide insight into the mechanism of the reaction (Atkins 2010). The Arrhenius equation illustrates the relationship between rate constant (k) and temperature (T) and it is given below:

$$k = Ae^{-\frac{E_a}{RT}} \tag{2.15}$$

Similar to A and E_a, A is a temperature-independent constant. The A and E_a could be estimated from experiments or calculations in statistical mechanics. They depend on the nature of the elementary reaction.

Where: E_a is the activation energy (kJ/mol), R is the gas constant (8.314×10^{-3} kJ mol^{-1} K^{-1}), A is the pre-exponential factor or frequency factor, k is the rate constant for the reaction, and T is the absolute temperature (K).

In the modified Arrhenius equation,

$$k = A \cdot T^n \cdot e^{-\frac{E_a}{RT}} \tag{2.16}$$

AT^n represents the collision frequency, while the exponential factor indicates the fraction of collisions that have energy levels greater than the activation energy. Both the Arrhenius equation and this modified Arrhenius equation are expressions based on experimental data Turns et al. (2000).

2.6.2 Reaction Mechanism

Understanding the reaction mechanism is important when studying the inhibition effect of potassium-containing compounds because it can provide information on how the inhibitor interacts with the reactive species in the process. This knowledge can be used to design and optimize the aerosol agent for maximum effectiveness.

Inhibition of chemical reactions typically involves the interaction of the inhibitor with the reactants, intermediates, or products of the reaction. The mechanism of the reaction determines which species are most reactive and which steps are rate-limiting. By understanding the mechanism, researchers can identify the most important species to target with the inhibitor.

Reaction mechanisms describe the sequence of elementary steps involved in a chemical reaction, including the breaking and formation of chemical bonds and the rates of individual steps Westbrook & Dryer (1984). At the molecular level, chemical reactions involve the rearrangement or combination of molecular species. These reactions can occur through various pathways, each involving a different set of intermediates and transition states. Understanding the reaction mechanism is essential to predict the outcome of chemical reactions accurately, optimize reaction conditions, and design new reactions or products Heghes (2007).

Reaction mechanisms can range from a single elementary reaction to hundreds or even thousands of reactions in a network. The complexity of the mechanism depends on the system's size, the available experimental or computational resources, and the required accuracy. In the literature, terms like "detailed," "skeletal," and "reduced" are used to describe the level of complexity of a mechanism Zettervall et al. (2021).

During a chemical reaction, numerous intermediate species are formed, which are often difficult to observe as they occur only briefly. These intermediate species vary depending on the type of reaction. One type of intermediate species is the formation of free radicals, which are important radicals in flames. Free radicals are highly reactive and play a critical role in combustion processes. The unstable species can be referred to as transitional chemical species. Depending on their effects, there are different elementary reaction types, such as chain initiation steps that create radicals from stable compounds. When these radicals react with other stable species, new radicals are formed.

This step is known as chain propagation, where one new radical is formed, or chain branching, where more than one radical is formed. On the other hand, chain-propagating reactions are responsible for producing new radicals by consuming other radicals. In the chain termination step, all the intermediate reactions come to a halt. Branch chain propagation reactions result in an increase in the concentration of H and OH radicals. This increase in the number of chain carriers (reactive species H, OH, O) could lead to chain branch explosions and thermal explosions, which means that the rate of reaction increases without limit Simic (1981).

To avoid system explosion, it requires removing free radicals as fast as they are formed. Even branching of the 1% chain in the H_2 /O_2 reaction would cause an explosion.

2.7 Reaction Mechanism of Hydrocarbon Combustion

Reaction mechanisms for hydrocarbon combustion are complex and involve multiple steps and intermediates. These mechanisms are used to predict and understand the behavior of combustion systems, including engine performance, pollutant emissions, and fire safety.

One of the earliest studies of the mechanisms of hydrocarbon reactions was conducted by Irving Langmuir in the early 1900s. Langmuir proposed that the reaction between hydrocarbons and oxygen proceeds through a chain mechanism that involves the formation of free radicals.

Curran et al. (1998) and Curran et al. (2002). established kinetic mechanisms for complex hydrocarbons by categorising reactions into specific classes and utilising a modular approach to construct the mechanisms.

Various experimental and computational studies have been conducted to investigate the combustion mechanism of hydrocarbons, as exemplified in the work of Warnatz (1985). This investigation has resulted in a multitude of completed or reduced mechanisms for hydrocarbon combustion.

For instance, the most comprehensive methane combustion mechanism, GRI-Mech 3.0 developed by Smith et al. (1999), comprises over 325 elementary reactions and more than 50 species. Similarly, Jachimowski (1984) developed a propane combustion mechanism consisting of 83 elementary reactions and 27 chemical species.

Furthermore, Heghes (2007) developed a relatively comprehensive C_1-C_4 hydrocarbon oxidation mechanism that included H_2 oxidation. This mechanism comprised 20 elementary reactions and 9 species for the hydrogen oxidation process.

One widely used mechanism for hydrocarbon combustion is the GRI-Mech mechanism developed by the Gas Research Institute (GRI) Smith et al. (1999). The GRI-Mech mechanism includes detailed reaction pathways for methane, ethane, propane, and

butane combustion, as well as simplified pathways for higher hydrocarbons. The mechanism includes hundreds of elementary reactions and thousands of species, making it computationally intensive but highly accurate.

Another widely used mechanism is the LLNL mechanism developed by Lawrence Livermore National Laboratory Westbrook et al. (2009). The LLNL mechanism includes detailed reaction pathways for a wide range of hydrocarbons, including alkanes, alkenes, and aromatics, as well as oxygenated compounds such as alcohols and ethers. The mechanism includes thousands of elementary reactions and hundreds of species and has been used to study a wide range of combustion systems.

The combustion of a hydrocarbon fuel consists primarily of the sequential fragmentation of the initial fuel molecule into smaller intermediate species, which are ultimately converted to final products, usually dominated by H_2O and CO_2. In many cases, these intermediate species can be fuels themselves. Carbon monoxide (CO) and hydrogen (H_2) are common species that are observed during the oxidation of all hydrocarbons Westbrook & Dryer (1984).

In hydrocarbon oxidation, the radical species H, O, OH, CH_3, and HO_2 are the chain carriers Westbrook (2000). In addition, these radical species are common to all hydrocarbon combustion, where OH is one of the most important radicals involved in the oxidation of hydrocarbons in the atmosphere. OH is highly reactive and can react with a wide range of organic compounds, including hydrocarbons.

The reaction between OH and a hydrocarbon produces a hydroxylated radical, which can then undergo further reactions to produce a variety of oxidized products, H can be formed during the reaction between OH and a hydrocarbon and can also be involved in chain reactions that lead to the production of additional radicals. H is highly reactive and can react with other molecules to form new radicals, O is another highly reactive species that can participate in the oxidation of hydrocarbons. Atomic oxygen can react with a hydrocarbon molecule to form a carbonyl oxide radical, which can then react with other molecules to produce additional radicals, and CH_3 is a radical that is often formed during the oxidation of methane and other hydrocarbons. Like other radicals, CH_3 is highly reactive and can undergo a wide range of reactions, including reactions with other radicals to produce additional oxidized products Atkinson & Arey (2003).

2.8 Reaction Mechanism of H_2/air Oxidation

The mechanism and kinetics of combustion H_2 are relatively simpler compared to the combustion of hydrocarbons. However, the combustion kinetics of H_2 is important in studying the inhibition effect of fire suppression agents such as KO_2, $KHCO_3$, and KCO_3 on flames.

The reaction mechanism of H_2/air oxidation has been extensively studied over the years using a variety of experimental and computational approaches Mueller et al. (1999), Aung et al. (1997), Aung et al. (1998),Wang et al. (2003), and Kwon & Faeth (2001). After conducting experiments, the obtained results were compared with simulations with the GRI-Mech 2.1, 3.0. models by different studies such as Konnov (2000).

Since the pioneering work by Kassel (1937) which was later updated by Von Elbe & Lewis (1942), several other researchers have contributed to the development of the mechanism to improve its accuracy and predictive capability Tse et al. (2000), Hughes et al. (2001), Ó Conaire et al. (2004), and Burke et al. (2012).

The branching elementary reactions occur in the gas phase. Ignition occurs when the rate of branching is higher than that of breaking Kassel (1937). The reaction mechanism of H_2/air oxidation is a complex process that involves multiple intermediate species and reaction steps. Specifically, for O_2 combustion, the branching of the reaction takes place during collisions between H and O_2 and breaking by H + O_2 + M = HO_2 + M or O +H_2 + M = H_2O +M Kassel & Storch (1935). Furthermore, Elbe & Lewis (1937) have pointed out the effective slow chain step to be H + $O_2 \rightarrow$ OH + O, which is crucial in the ignition region for hydrogen combustion. Therefore, the complete mechanism for H_2-air oxidation involves the following elementary reactions:

$H + O_2 \rightarrow O + OH$

$OH + H_2 \rightarrow H_2O + H$

$H_2 + O \rightarrow OH + H$

$H + O_2 + M \rightarrow HO_2 + M$

$HO_2 + H_2 \rightarrow H_2O_2 + H$

These five reactions are the key steps in the chain reaction that drives the combustion process Kassel (1937). The first reaction is the initiation step, which produces the reactive hydroxyl OH radical that drives the chain reaction. The second and third reactions represent the branching reactions, where the chain reaction branches out to produce additional OH and HO_2 radicals. The fourth reaction is the termination step, which occurs when two radicals react and no longer participate in the chain reaction. The fifth reaction is the formation of hydrogen peroxide H_2O_2, which can also participate in the chain reaction and contribute to the combustion process. This reaction mechanism provides a comprehensive understanding of the various steps involved in the H_2/air oxidation process, which is important to optimise industrial processes that depend on the combustion of hydrogen Turns et al. (2000).

The mechanism for kinetics modelling of hydrogen combustion can vary depending on the specific application and conditions of the combustion process. However, a commonly used mechanism for hydrogen combustion is the GRI-Mech 3.0 mechanism, which was developed by the Gas Research Institute (GRI) Smith et al. (1999). It has been extensively

validated against experimental data and is widely used in combustion simulations and modelling.

The GRI-Mech 3.0 mechanism includes over 53 reactions and 21 species, including H_2,O_2, H, OH, O, HO_2, H_2O, and CO_2, among others. This mechanism includes the primary steps in the combustion of hydrogen with air, as well as additional reactions that describe the formation and oxidation of intermediate species.

Other commonly used mechanisms for hydrogen combustion include the JetSurF 2.0 mechanism and the San Diego mechanism, among others. These mechanisms include a similar number of reactions and species and are also widely used in combustion simulations and modeling. The JetSurF 2.0 is a comprehensive reaction mechanism that models the combustion and decomposition of hydrogen.

The mechanism includes more than 2000 reactions involving 348 species and it is based on fundamental principles of physical chemistry and thermodynamics. It has been validated against a wide range of experimental data, including laminar flame speeds, ignition delay times, and shock tube experiments. The mechanism is available in various formats, including Chemkin, and Cantera, and it can be easily incorporated into CFD codes and other simulation tools. The San Diego mechanism is a commonly used reaction mechanism for the combustion of hydrogen. It was developed at the University of California, San Diego in the 1990s and includes more than 268 reactions involving 57 chemical species.

Li et al. (2004) conducted a comprehensive study in 2004 to update the H_2/O_2 reaction mechanism developed by Mueller et al. (1999). The authors introduced 19 elementary reactions, including $H+O_2+M–HO_2+M$ and $H_2+OH–H_2O+H$, into the updated mechanism. Through their study, Li et al. demonstrated that the importance of the elementary reactions varies according to the temperature range. They also found that the H_2+OH $–H_2O+H$ reaction is significant in observing flame propagation at high pressure.

Gonçalves et al. (2010). used the Chemkin transport package to achieve flame propagation model performance, similar to the simulation conducted by Li et al. The competition between chain branching and recombination reactions during flame propagation can increase or reduce the laminar burning velocity, as stated by Hu et al. in their study. Li et al. indicated that primary chain branching reactions in hydrogen oxidation mechanisms include $H+O_2<=>O+OH$, $O+H_2<=>H+OH$, $H_2<=>H+H_2O$, and $OH+H<=>OH+OH$. These reactions increase the concentration of H, O, and OH radicals and enhance the reactions. Overall, the work of these authors contributes to a better understanding of combustion mechanisms and the factors that affect them.

Konnov (2004) updated the detailed reaction mechanism for small hydrocarbon combustion by updating the H_2O_2 reactions scheme and compared its performance with an extended set of experimental data from the literature. The study aimed to improve the precision of the mechanism used to model H_2/air combustion. In the present work, the

GRI-Mech 3.0 mechanism and the Reduced mechanism developed by Hadi from Konnov for H_2/air combustion were considered.

2.9 Potassium-Containing Compounds Data

The reaction mechanisms integrated hydrocarbons and potassium-containing species are relatively rare in the reaction mechanisms. There are two mechanisms considered in the equilibrium simulation of reaction kinetics these are GRI-Mech 3.0 Smith et al. (1999) and the reduced mechanism 0.5 by Hadi based on the Konnov mechanism. Both have been used for kinetic modelling and analysis. GRI-Mech has been used in many studies for the modelling of hydrogen, methane, ethane, propane, and natural gas combustion reaction kinetics. However, Konnov developed a comprehensive mechanism that includes C_1-C_3 hydrocarbon species and detailed N-H-O chemistry to accurately predict the formation of NOx. Initially based on methane combustion, the Konnov mechanism was later expanded to encompass other compounds such as methanol, acetaldehyde, ethanol, and ethylene oxide. The current version of the mechanism, known as Konnov 0.5, consists of 1200 reactions and 125 species. To ensure its reliability, the mechanism underwent validation through various experimental techniques, including shock tube experiments, laminar flame speed measurements (up to 10 atm at near stoichiometric equivalence ratio), and flow reactors. Compared to GRI-Mech, both mechanisms exhibit a relatively comprehensive reaction scheme for H_2 oxidation.

Three different files were created for potassium-containing species; these files contain reactions of potassium species, thermodynamics, and transport data. Table 2.3 shows the reactions of potassium-containing species with the species of the hydrocarbon system. The reactions of potassium-containing species, consisting of 85 reactions of 12 species (K, KH, KO, KO_2, KO_3, K_2O, K_2O_2, KOH, $(KOH)_2$, K_2CO_3, KCO_3, and $KHCO_3$). Presenting the thermochemistry of K-containing species relevant to the combustion environment, all data are from the literature review.

Table 2.3: Kinetic model for potassium-containing species, A units mol-cm-sec-K, E units cal/mol

N	**Reactions**	**A**	**n**	**Ea**	Reference
R326	$K+O_2=KO_2$(no third body)	3.60E+14	0.0	0.0	Glarborg & Marshall (2005)
R327	K+OH=HKO (no third body)	2.18E+21	-1.0	0.0	Babushok et al. (2017)
R328	K+H=HK (no third body)	3.00E+17	-1.0	0.0	Hindiyarti et al. (2006)
R329	K+O=KO (no third body)	1.50E+21	-1.5	0.0	Glarborg & Marshall (2005)

R330	K+HCO=HK+CO	3.00E+13	0.0	3496	Williams & Fleming (1999), Babushok et al. (2017)
R331	$K+HO_2=HK+O_2$	2.00E+13	0.0	13991	Babushok et al. (2017)
R332	$K+HO_2=HKO+O$	7.00E+12	0.0	7494	Babushok et al. (2017)
R333	$K+H_2O_2=HKO+OH$	2.50E+13	0.0	0.0	Babushok et al. (2017)
R334	$K+H_2O_2=KO+H_2O$	1.60E+13	0.0	0.0	Babushok et al. (2017)
R335	KO+H=K+OH	2.00E+14	0.0	1499	Babushok et al. (2017)
R336	$KO+O=K+O_2$	1.20E+14	0.0	238.84	Babushok et al. (2017)
R337	KO+OH=HKO+O	2.00E+13	0.0	0.0	Glarborg & Marshall (2005), Williams & Fleming (1999)
R338	$KO+OH=K+HO_2$	3.00E+13	0.0	9993	Babushok et al. (2017)
R339	$KO+HO_2=HKO+O_2$	5.00E+13	0.0	0.0	Glarborg & Marshall (2005), Williams & Fleming (1999)
R340	$KO+HO_2=KO_2+OH$	3.00E+12	0.0	3998	Babushok et al. (2017)
R341	$KO+H_2=HKO+H$	1.60E+13	0.0	0.0	Glarborg & Marshall (2005)
R342	$KO+H_2=K+H_2O$	3.10E+12	0.0	0.0	Glarborg & Marshall (2005)
R343	$KO+H_2O=HKO+OH$	6.00E+11	0.5	0.0	Slack et al. (1989), Babushok et al. (2017)
R344	$KO+CO=K+CO_2$	1.00E+14	0.0	0.0	Babushok et al. (2017)

R345	KO+HCO=HKO+CO	3.00E+13	0.0	0.0	Babushok et al. (2017)
R346	KO+CH_4=HKO+CH_3	1.20E+12	0.0	3496	Babushok et al. (2017)
R347	KO+CH_2O=HKO+HCO	1.20E+13	0.0	3998	Babushok et al. (2017)
R348	KO+KO=KO_2+K	1.00E+13	0.0	0.0	Babushok et al. (2017)
R349	KO+H=HKO (no third body)	3.60E+22	-2.0	0.0	Babushok et al. (2017)
R350	KO+O=KO_2 (no third body)	1.45E+19	-1.0	0.0	Babushok et al. (2017)
R351	KO+CH_3=K+CH_3O	2.30E+13	0.0	5995	Babushok et al. (2017)
R352	KO+C_2H_6=HKO+C_2H_5	1.20E+13	0.0	5995	Babushok et al. (2017)
R353	KO+C_2H_4=HKO+C_2H_3	1.50E+13	0.0	7994	Babushok et al. (2017)
R354	KO+C_2H_2=HKO + C_2H	2.00E+13	0.0	8994	Babushok et al. (2017)
R355	KO+C_3H_8=HKO+C_3H_7	1.50E+13	0.0	4996	Babushok et al. (2017)
R356	KO_2+H=K+HO_2	1.90E+12	0.0	0.0	Babushok et al. (2017)
R357	KO_2+H=HKO+O	1.00E+13	0.0	0.0	Babushok et al. (2017)
R358	KO_2+H=KO+OH	5.00E+13	0.0	6995	Babushok et al. (2017)
R359	KO_2+O=KO+O_2	1.30E+13	0.0	0.0	Glarborg & Marshall (2005)
R360	KO_2+CO=KO+CO_2	6.00E+13	0.0	22984	Babushok et al. (2017)
R361	KO_2+OH=HKO+O_2	1.20E+13	0.0	0.0	Babushok et al. (2017)
R362	KO_2+H_2=HKO+OH	1.80E+12	0.0	19857	Babushok et al. (2017)
R363	KO_2+HCO=HKO+CO_2	6.00E+12	0.0	0.0	Babushok et al. (2017)

R364	$KO_2+CH_3=HKO+CH_2O$	6.00E+12	0.0	0.0	Babushok et al. (2017)
R365	$HKO+H=K+H_2O$	2.20E+12	0.5	0.0	Slack et al. (1989)
R366	$HKO+CH_3=K+CH_3OH$	3.50E+12	0.0	9993	Babushok et al. (2017)
R367	$HKO+HO_2=KO_2+H_2O$	6.00E+12	0.0	5297	Babushok et al. (2017)
R368	$HKO+HKO=K_2H_2O_2$	8.00E+13	0.0	0.0	Glarborg & Marshall (2005)
R369	$HK+H=K+H_2$	1.00E+14	0.0	0.0	Hindiyarti et al. (2006)
R470	HK+O=K+OH	5.00E+13	0.0	0.0	Hindiyarti et al. (2006)
R371	HK+O=KO+H	6.00E+12	0.0	6995	Babushok et al. (2017)
R372	$HK+OH=K+H_2O$	1.00E+14	0.0	0.0	Babushok et al. (2017)
R373	HK+OH=HKO+H	1.00E+13	0.0	0.0	Babushok et al. (2017)
R374	$HK+HCO=K+CH_2O$	2.00E+13	0.0	0.0	Babushok et al. (2017)
R375	$HK+CH_3=CH_4+K$	1.00E+14	0.0	0.0	Babushok et al. (2017)
R376	$HK+CH_3O=K+CH_3OH$	2.00E+13	0.0	0.0	Babushok et al. (2017)
R377	HK+KO=K+HKO	1.00E+14	0.0	0.0	Babushok et al. (2017)
R378	$KO+K=K_2O$(w/o M)	1.00E+16	0.0	0.0	Babushok et al. (2017)
R379	$K_2O+H=K+HKO$	5.00E+12	0.0	2997	Babushok et al. (2017)
R380	$K_2O+O=K_2O_2$	1.00E+14	0.0	0.0	Babushok et al. (2017)
R381	$K_2O+O=KO+KO$	1.00E+13	0.0	9993	Babushok et al. (2017)
R382	$K_2O+OH=KO+HKO$	1.00E+13	0.0	4996	Babushok et al. (2017)

R383	$KO+KO=K_2O_2$	1.00E+14	0.0	0.0	Babushok et al. (2017)
R384	$K_2O_2+H=HKO+KO$	1.50E+13	0.0	998	Babushok et al. (2017)
R385	$K_2O_2+O=KO_2+KO$	1.00E+13	0.0	7994	Babushok et al. (2017)
R386	$K_2O_2+OH=HKO+KO_2$	1.00E+13	0.0	2997	Babushok et al. (2017)
R387	$K_2CO_3=K_2O+CO_2$(w/o M)	5.00E+16	0.0	80944	Babushok et al. (2017)
R388	$K_2CO_3+O=K_2O_2+CO_2$	3.00E+14	0.0	6995	Babushok et al. (2017)
R389	$KO_2+O=KO_3$ (no third body)	1.45E+19	-1.0	0.0	Babushok et al. (2017)
R390	$H+KO_3=KO_2+OH$	2.00E+13	0.0	0.0	Babushok et al. (2017)
R391	$O+KO_3=KO_2+O_2$	2.00E+13	0.0	0.0	Babushok et al. (2017)
R392	$OH+KO_3=KO_2+HO_2$	1.00E+13	0.0	8994.9	Babushok et al. (2017)
R393	$CH_3+KO_3=CH_3O+KO_2$	1.00E+13	0.0	4996	Babushok et al. (2017)
R394	$KO+O_2=KO_3$ (no third body)	3.40E+14	0.0	0.0	Babushok et al. (2017)
R395	$HKO+CO_2=KHCO_3$(no third body)	4.09E+14	0.0	0.0	Babushok et al. (2017)
R396	$KO+CO_2=KCO_3$(w/o M)	3.90E+14	0.0	0.0	Babushok et al. (2017)
R397	$KCO_3+H=KHCO_3$ (no third body)	2.00E+16	0.0	0.0	Babushok et al. (2017)
R398	$KO_2+CO=KCO_3$(no third body)	3.00E+16	0.0	0.0	Babushok et al. (2017)
R399	$K+KCO_3=K_2CO_3$(no third body)	2.00E+18	0.0	0.0	Babushok et al. (2017)
R400	$KHCO_3+H=K+CO_2+H_2O$	2.70E+13	0.0	7124	Babushok et al. (2017)
R401	$KHCO_3+H=KCO_3+H_2$	1.50E+13	0.0	9993	Babushok et al. (2017)

R402	$KHCO_3$+O=KCO_3+OH	1.00E+13	0.0	12491	Babushok et al. (2017)
R403	$KHCO_3$+OH=KCO_3+H_2O	2.00E+13	0.0	7494.98	Babushok et al. (2017)
R404	KCO_3+H=HKO+CO_2	3.00E+12	0.0	3998	Babushok et al. (2017)
R405	KCO_3+O=KO_2+CO_2	5.00E+12	0.0	2997	Babushok et al. (2017)
R406	$KHCO_3$+KO=K_2CO_3+OH	6.00E+12	0.0	6995	Babushok et al. (2017)
R407	$KHCO_3$+HKO=K_2CO_3+H_2O	3.00E+12	0.0	8994	Babushok et al. (2017)
R408	KCO_3+KO=K_2CO_3+O	7.00E+12	0.0	4996	Babushok et al. (2017)
R409	KCO_3+KO_2=K_2CO_3+O_2	1.00E+13	0.0	2997	Babushok et al. (2017)
R410	K_2CO_3+OH=KCO_3+HKO	3.00E+14	0.0	10991	Babushok et al. (2017)

Note:

- The notation ”(no third body)” indicates that third-body have been excluded from the specified reactions. By removing third-body reactions, the focus is on achieving computational stability while retaining essential reactions related to potassium chemistry.
- In the table, ’N’ refers to the number of the reaction, serving as a identifier for each reaction in the combined kinetic model, (GRI-Mech mechanism/K-species mechanism).

The kinetic mechanism for the behavior of potassium-containing species was analyzed in several works for different environments (Benilov et al. (1994); Glarborg & Marshall (2005); Hastie (1973); Hastie et al. (1986); Hindiyarti et al. (2006); Jensen et al. (1979); Plane et al. (2014); Slack et al. (1989)).

2.9.1 Apply Thermodynamic Data into Numerical Model

In Chemkin, thermodynamic properties are represented using polynomial fits as functions of temperature. These polynomials describe the behavior of gas-phase species and are based on the assumption that the gas is thermally perfect. Each species is associated with a set of polynomial coefficients, which include 7 coefficients for the upper-temperature range and 7 coefficients for the lower-temperature range.

Alongside these polynomial coefficients, the thermodynamic data also provide additional essential information for each species, including the species name, its elemental composition, the range of the temperature, and the phase (e.g., gas or solid). This comprehensive data set allows Chemkin to accurately model and predict the thermodynamic properties of various chemical species under different temperature conditions. Specific heat, formation enthalpy, and formation entropy, associated with A, n, and E (Arrhenius equation parameters), are crucial parameters used in the calculation of equilibrium constants, specifically k_c (the equilibrium constant at constant pressure). These parameters are employed to model the temperature-dependent thermodynamic properties of chemical species within the Chemkin thermodynamic database, often using NASA polynomials or the JANAF thermodynamic data.

In the context of Chemkin, the JANAF thermodynamic data can be used as an alternative or in addition to NASA polynomials to describe the thermodynamic properties of chemical species. Instead of NASA polynomials, which are a specific form of representation of thermodynamic properties, Chemkin can use JANAF data to provide the same information. The key difference between the two is the representation format.

NASA polynomials provide a concise mathematical expression for thermodynamic properties as a function of temperature, making them suitable for numerical simulations.

On the contrary, the JANAF tables provide tabulated data at specific temperature points, which can be used to interpolate or approximate thermodynamic properties for various temperatures.

It's important to acknowledge that not all chemical species have their polynomial coefficients available in databases. Some species, including certain potassium species, have no polynomial coefficients such as $KHCO_3$, KO_3, and KCO_3. The thermodynamic data for K-species was collected from the literature when available, including sources such as Janaf and NASA databases.

The corresponding thermodynamic properties were collected using different references as shown in Table 2.4.

Table 2.4: Thermodynamic database for potassium-containing species (kcal, cal, mol, K)

Species	**H(298K)**	**S(298K)**	**Cp (298K)**	**Reference**
K	21.312	38.299	4.972	Stull (1965)
HK	29.402	47.304	7.418	Stull (1965)
KO	17.0012	56.8600	8.61828	Stull (1965)
KO_2(s)	-68.000	29.280	18.486	Babushok et al. (2017)
K_2O(s)	-86.803	22.5155	20.109669	Stull (1965)
K_2O_2(s)	-118.500	37.1700	23.969	Stull (1965)
$K_2H_2O_2$	-156.500	78.3700	19.4813	Stull (1965)
K_2CO_3(s)	-274.900	37.1700	27.276	Babushok et al. (2017)
HKO	-55.5700	56.4700	11.603	Stull (1965), Babushok et al. (2017), Glarborg & Marshall (2005)
KO_3	-18.39	68.26	15.38	Vasiliu et al. (2010), Babushok et al. (2017)
$KHCO_3$(s)	-230	27.58	21.28	Meng et al. (1995), Babushok et al. (2017)
KCO_3	-124.900	74.300	16.384	Babushok et al. (2017)

2.9.2 Apply Transport Data of Potassium species into Numerical Model

Table 2.5 shows the transport properties provided in the Chemkin chemical set.

Table 2.5: Transport Database of the K-species

Species	Geometry	ε/kB	σ	μ	α	Zrot	Refrence
K	0	850	4.25	0.000	0.000	1.000	Kee et al. (1986)
KO	1	383	3.812	0.000	0.000	1.000	Kee et al. (1986)
HKO	2	1213	4.52	0.000	0.000	1.000	Kee et al. (1986)
KO_2	2	1213	4.69	0.000	0.000	1.000	Kee et al. (1986)
HK	1	93.3	3.542	0.000	0.000	1.000	Kee et al. (1986)
K_2O	2	1213	4.69	0.000	0.000	1.000	Assumed
K_2O_2	2	1213	4.69	0.000	0.000	1.000	Assumed
K_2CO_3	2	1213	4.69	0.000	0.000	1.000	Assumed
$K_2H_2O_2$	2	1213	4.69	0.000	0.000	1.000	Assumed
KO_3	2	1213	4.69	0.000	0.000	1.000	Assumed
$KHCO_3$	2	1213	4.69	0.000	0.000	1.000	Assumed
KCO_3	2	1213	4.69	0.000	0.000	1.000	Assumed

Note:

- In the kinetic model, 'HK' is equivalent to 'KH,' and 'HKO' is equivalent to 'KOH.
- In the transport properties data, $K_2O, K_2O_2, K_2CO_3, K_2H_2O_2, KO_3, KHCO_3, KCO_3$ has been assumed to have properties equivalent to KO_2 for the simplicity of the modelling.

In the absence of available data, assumptions are made regarding polynomial coefficients and transport data. In this study, the assumption of uniform transport data and polynomial coefficients is applied to specific potassium-containing species, which include K_2O, $KHCO_3$, K_2O_2, K_2CO_3, KO_3, $K_2H_2O_2$, and KCO_3. Additionally, the polynomial coefficients of K_2CO_3 are used for $KHCO_3$ and KCO_3, and the polynomial coefficients of KO_2 for KO_3. These assumptions are grounded in several key considerations:

Similar Chemical Families: These potassium-containing species belong to analogous chemical families, demonstrating structural resemblances. It is common for species within the same chemical family to exhibit similar transport properties, owing to shared characteristics in molecular size, shape, and interactions with surrounding molecules.

Modelling Simplification: The assumption of uniform transport properties and polynomial coefficients serves the purpose of streamlining the modelling process. Therefore, in the complex chemical systems, assuming similarities among these potassium-containing species simplifies and expedites the modelling efforts.

The thermodynamic and transport data files for Potassium-containing compounds with the species of the hydrocarbon system are presented in Appendix (C).

2.10 Summary

- Fire suppression mechanisms are essential tools for preventing and controlling fires.
- Laminar burning velocity is a vital parameter in the development of effective fire suppression strategies. It offers valuable insights into the factors that sustain a flame and helps identify potential targets for suppression. It serves as a critical metric for evaluating the effectiveness of fire suppression agents.
- KO_2, $KHCO_3$, KCO_3 are the potassium species that are used to verify their chemical kinetic on H_2, and CH_4 flames.
- A relatively comprehensive combustion mechanism covering H_2 was GRI-Mech and reduced mechanism from Konnove. The important chain branching reactions in H_2 oxidation mechanism are included in the mechanism.
- A brief introduction to numerical reaction kinetics modelling emphasises the importance of using the Arrhenius equation for chemical kinetics simulations.
- In the context of the Arrhenius equation, the thermodynamic data, such as enthalpy of formation and specific heat is necessary for the accurate calculation of the rate constant and reaction rate.
- Species enthalpy and entropy are required for computing the equilibrium constant (K_c) and forward rate constant (k_f) to determine production rates and species concentrations.
- Transport properties will not be calculated based on the fundamental transport properties provided in the chemistry set in Chemkin.
- Examining the performance of one of the potassium species on different types of small fires will be covered in the next chapter.

Chapter 3

Demonstration Testing of Potassium Oxide Fire Suppression Agent on Hydrocarbon Flames

In recent years, both the private and public sectors have embarked on a quest to develop innovative classes of fire suppressants that redefine firefighting strategies. Among these pioneering agents, solid particulate condensed aerosol agents have emerged as a promising avenue. Their distinct advantages include superior volumetric efficiency, affordability with low initial and life-cycle costs, minimal toxicity, negligible negative environmental impact, and adaptability in a diverse spectrum of applications Kibert & Dierdorf (1994).

A program of test design has been initiated with the primary objective of investigating the effectiveness of potassium oxide (K_2O) as a fire suppression agent, especially in addressing small-scale fires. This research aims to provide an initial insight into the performance characteristics of K_2O as a potential fire suppressant.

This chapter introduces the test method and test rig. Detailed explanations are provided for the types of fires and the fire suppression generation. The calculation procedures for determining the size of the tested fires are outlined. Moreover, this chapter presents a clear demonstration of the test procedures, along with a discussion of the results.

3.1 Tests Programme

The core objective of the testing program lies in the evaluation of K_2O as a fire suppression agent in the context of both wood fires and flammable liquid fires. These represent two crucial scenarios that are frequently encountered in fire emergencies. Through carefully designed experiments, the program seeks to quantify the extinguishing capabilities and provide empirical evidence of its efficacy.

3.1.1 Test Method and Test Rig

In the context of fire safety and research, a specialised bin box (chamber) was designed and constructed to facilitate a series of fire extinguishing tests.

The bin box with dimensions, at 1000 mm in height, extending 500 mm in width,

and measuring 600 mm in length, thus offering a volumetric capacity of approximately 0.3 cubic metres. Constructed from robust sheet steel, the bin box was engineered to withstand the demanding conditions of fire testing as shown in Figure 3.1. There was a single-sided ventilation. This ventilation design allowed controlled airflow during the tests, ensuring that the experimental conditions closely mirrored the real world scenarios. The front facing side of the bin box was fabricated using transparent glass. This design choice served a dual purpose: it allowed researchers to closely observe and document the fire extinguishing tests from a safe vantage point while ensuring that the tests could be conducted with the benefit of natural light. Despite the outdoor environment where the fire extinguishing tests took place, the bin box's controlled and monitored conditions made it an ideal setting for conducting experiments of this nature. The exterior conditions could be closely monitored while the internal variables were controlled.

Within this prepared experimental chamber, a tray with dimensions measuring 410 mm in length, 410 mm in width, and 30 mm in height. This tray, with a volume of approximately 0.0053 cubic metres, was placed in the centre of the bin box. To ensure the most realistic representation of the fire scenarios, the tray was placed on a layer of cotton.

To capture data during the tests, five wire sensors were installed within the bin box. These sensors were dedicated to measuring temperature fluctuations at various critical points within the chamber. Their placement and configuration are detailed and visually depicted in Figure 3.2, providing a clear reference for data collection points. These included measurements at the fire source, the middle of the chamber, in close proximity to the suppression sensor, and above the fire source. These thermosensitive lines were carefully connected to a sophisticated measurement device that continuously monitored temperature variations inside the bin box.

For documentation and visual evaluation of the experiments, a commercial digital camera was incorporated into the setup, as illustrated in Figure 3.3. This camera provided a visual record of the experimental rig, ensuring a complete overview of the testing environment and conditions.



(a) Front view of the fire area



(b) Side view of the fire area



(c) Interior view of the fire area

Figure 3.1: Bin box as a fire test area.

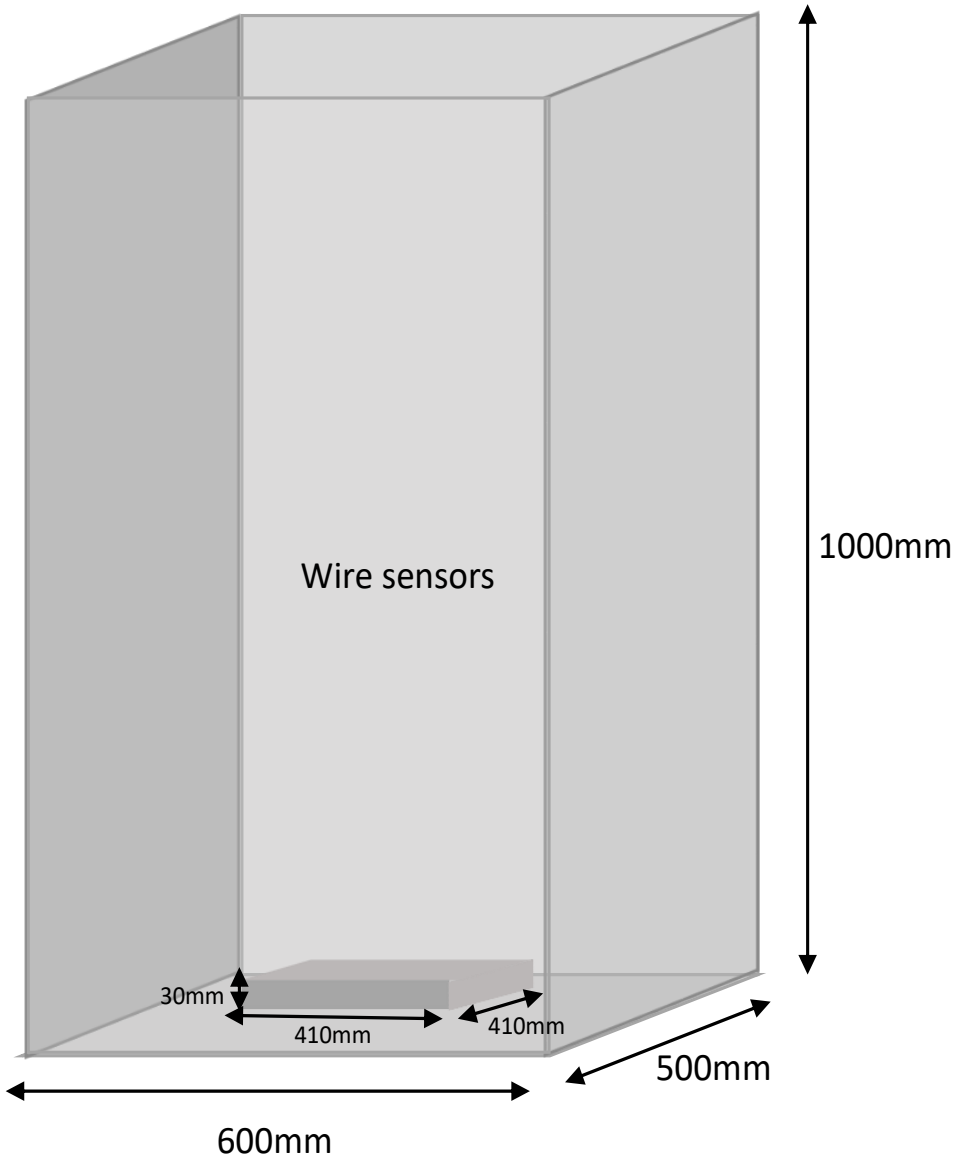


Figure 3.2: Setup of the bin box.

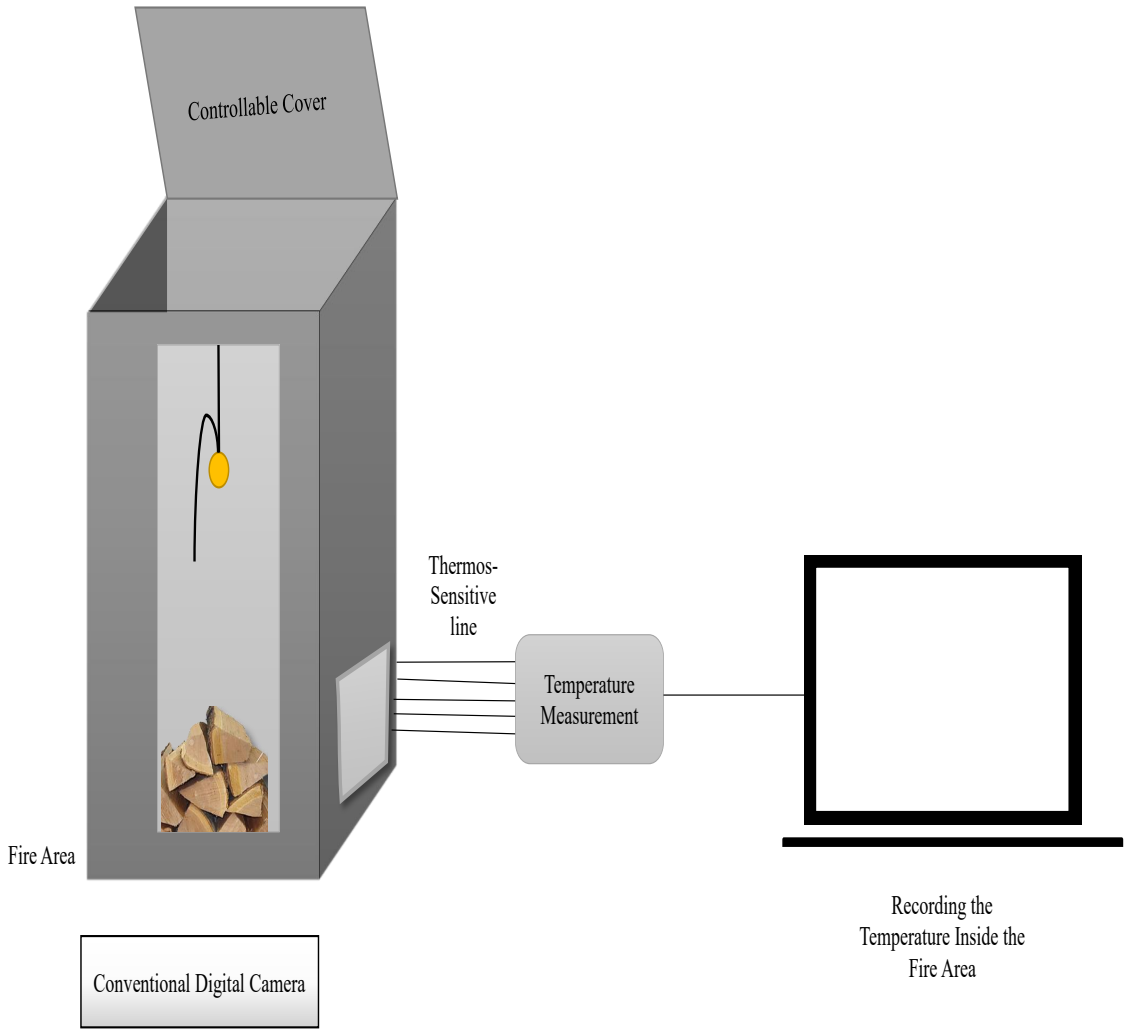


Figure 3.3: Arrangement and configuration of the bin box.

The Fireless 0.3 Pyrotechnic Aerosol Unit

The Fireless 0.3 pyrotechnic aerosol unit, a specialised apparatus designed to generate and disperse condensed aerosols for fire suppression purposes. The choice of this particular unit was underpinned by its demonstrated efficacy and applicability to suppress fires within the confines of a bin box, a key requirement for the experimental setup.

The specifications of the Fireless 0.3 unit were gathered from the manufacturer's publications, offering a comprehensive overview of its capabilities. These specifications, outlined in Table 3.1.

The Fireless 0.3 pyrotechnic aerosol unit primary features and specifications include:

Aerosol Generation: The unit is adept at swiftly generating condensed aerosols, making it well-suited for rapid fire suppression responses.

Size Compatibility: Its design and dimensions align seamlessly with the requirements of a bin box, ensuring an efficient and tailored approach to fire suppression within the designated testing environment.

Table 3.1: The Specifications of the Fireless 0.3 unit.

Characteristics	Fireless 0.3
Active Substance	Potassium K
Type of potassium	Potassium Oxide (K_2O)
Discharging Time	2-3 sec
Diameter	< 1 µm
Weight	75 g
Protected Volume	0.3 m^3
Storage Life	10 years

3.1.2 Types of Flames Tested

In the fire suppression test, two different types of fuels were selected for examination. The design of the fuel loads was instrumental in creating a fully developed fire environment, essential to achieving repeatable and reliable results in fire suppression experiments. The chosen fuels for the two main fire scenarios were dried wood and paraffin oil.

1. **Dried Wood Fuel Load**

The dried wood fuel load was prepared, incorporating small pieces of fuel to ensure optimal ignition conditions. The ignition of this fuel source was initiated using a spark. During the pre-burn phase, the dried wood logs were arranged and centred within a square burn tray, positioned in the middle of the bin box. Importantly, note that the contribution of the ignition source (spark) to the overall heat generated by dried wood is considered negligible.

2. **Paraffin Oil Fuel Load**

The second fuel load involved the use of flammable liquid, specifically paraffin oil. The paraffin oil was applied to the fuel tray and then ignited to create the desired fire scenario.

3.1.3 Calculating the Size of the Fire

The rationale for selecting the fuel loadings is based on the size of the fireless unit and the fire area used in the tests, ensuring controlled and reproducible conditions for evaluating the performance of the suppression agents. The heat capacity of the fuel will be used to calculate the fire size, which will then determine the appropriate amount of fuel to load.

To calculate the size of the fire for 2 kg of dry wood and a volume of flammable liquid equal to 0.0053 m^3, it is required to determine the heat output for each of these scenarios. According to Incropera et al. (1996) the heat output can be calculated using the formula

below:

$$Q = m \times c \times \Delta T \tag{3.1}$$

Where:

Q is the heat output in joules (J).

m is the mass of the fuel in kilograms (kg).

c is the specific heat capacity of the fuel in (J/kg°C).

ΔT is the temperature rise of the fuel in degrees Celsius (°C).

Scenario 1: Dry Wood (2 kg)
Assumption:

Dry wood has an approximate specific heat capacity of around 1600 J/kg°C (Qing-xian (2000)).

A conservative temperature rise of 500 °C during combustion is assumed, based on test results.

Q = 2 × 1600 × 500 = 1600000 J = 1600 kJ

So, For the combustion of 2 kg of dry wood, the estimated heat output is approximately 1600 kJ.

Scenario 2: Flammable Liquid (Volume = 0.0053 m³)
Assumptions:

The specific heat capacity for Kerosene is typically around 2470 J/kg°C Kern & Kern (1950)
The density of 807 kg/m³ for Kerosene Staffell (2011).

The temperature rise (ΔT) = 200 °C

Calculating Mass (m) of Kerosene:

$$m = V \times \rho \tag{3.2}$$

Where: m is the mass measured by kg, V is the volume measured by (m³), and ρ is the density measured by (kg/m³).

m = 0.0053 × 807 = 4.3 kg

The Heat Output can be calculated using 3.1.

Q = 4.3 × 2470 × 200 = 2124200J = 2124 kJ

3.2 Release of K_2O in Hydrocarbon Flames

Two planned tests were conducted to investigate the release of K_2O within hydrocarbon flames, aiming to understand its behavior in such an environment.

3.2.1 First Test: Dry Wood

In the first test, a fire fuelled by approximately 1600 kJ of dry wood was ignited. Two kilograms of dry wood were used. The procedure for this test was as follows:

- The fireless aerosol extinguisher, a crucial component of the test, was positioned as depicted in Figure 3.4.
- Sensors were placed inside the bin box to ensure comprehensive data capture.
- After igniting the fuel, consisting of dry wood, the fire was allowed to grow for 30 seconds. At the designated moment, the chamber window was closed, and the activation of the aerosol extinguisher was awaited, as shown in Figure 3.5.
- The tests observed and recorded fluctuations in the fire's temperature as the aerosol extinguisher began its operation within the chamber.

3.2.2 Second Test: Paraffin Liquid (Kerosene)

In the second test, a fire with an estimated energy of 2124 kJ focused on a different fuel: paraffin liquid (kerosene). This flammable liquid was subjected to two fireless apparatuses: the fireless 0.3 unit and handheld equipment.

Fireless 0.3 Unit:

- The fireless generator was installed, and sensors were placed within the chamber.
- The flammable liquid awaited ignition, initiated through the chamber window.
- As the flames grew, the release of K_2O was monitored.
- The fire was allowed to grow, reflecting changes following the release of K_2O.
- Close attention was paid to the fire's temperature, with every change systematically recorded and analysed, providing data on the interaction between K_2O and the kerosene flame.

Handheld Equipment:

- Sensors were installed within the chamber, and the flammable liquid was prepared.
- Ignition of the flammable liquid occurred through the chamber window.
- The handheld fire suppression equipment was activated as the flame grew to assess its effectiveness in suppressing the fire and managing K_2O release.
- Any changes in the fire's temperature were recorded and analysed.



(a) Fuel centered in tray inside the bin box



(b) Install the fireless generator inside the bin box



(c) Ignite the fuel

Figure 3.4: Fuel ignition setup instructions.



(a) The moment of closing the window.



(b) Pre-burning for 4 seconds.



(c) Pre-burning for 7 seconds.



(d) Pre-burning for 9 seconds.



(e) Pre-burning for 10 minutes.



(f) The moment of activating the fireless generator.



(g) seconds after releasing the agent.



(h) 30 seconds after releasing the agent.



(i) 9 minutes after releasing the agent.



(j) Re-ignition after 1 hour.

Figure 3.5: Fire growing at different stages.

3.3 Results and Discussion

The data obtained from testing the K_2O agent was analysed and graphically represented using the Microsoft Excel program. In this section, the key findings and observations derived from the analysis of these graphical representations are discussed.

Figure 3.6 represents the relationship between the fire temperature within the test chamber, generated by solid fires, and the reaction time of the K_2O agent. This graph illustrates a significant trend, illustrating how the introduction of the K_2O agent promptly mitigates the fire's temperature. The drop in temperature is indicative of the rapid and efficient action of the agent in suppressing solid fires.

In addition, Figures 3.7 and 3.8 provide further clarification regarding the K_2O agent's

performance, particularly in situations involving flammable liquids. These graphs show changes in temperature within the test chamber. Graphic representations illustrate that the K_2O agent demonstrates its efficacy in reducing the temperature within the chamber when faced with liquid fires. Moreover, Figure 3.8 provides K_2O's ability to rapidly extinguish flames upon release toward the fire. However, using handheld equipment is more dangerous than using fixed equipment.

The activation temperatures of the fire suppression sensor at 210 °C and 300 °C, depending on the location of the generator, play an important role in controlling the fire. Activating the generator leads to a gradual reduction in temperature, ultimately achieving a stable, non-combustible environment.

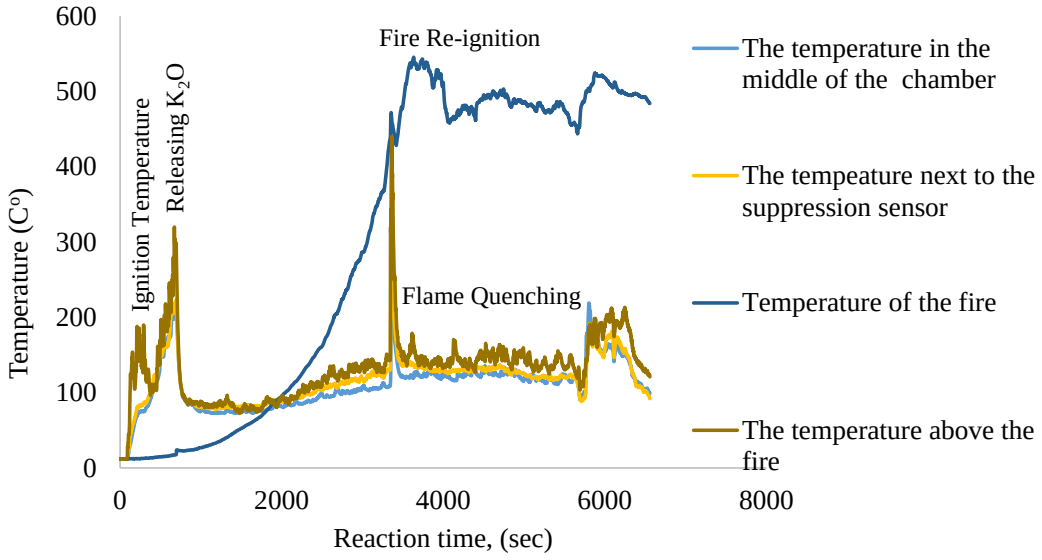


Figure 3.6: Testing wood fire suppression using a 0.3 fireless generation.

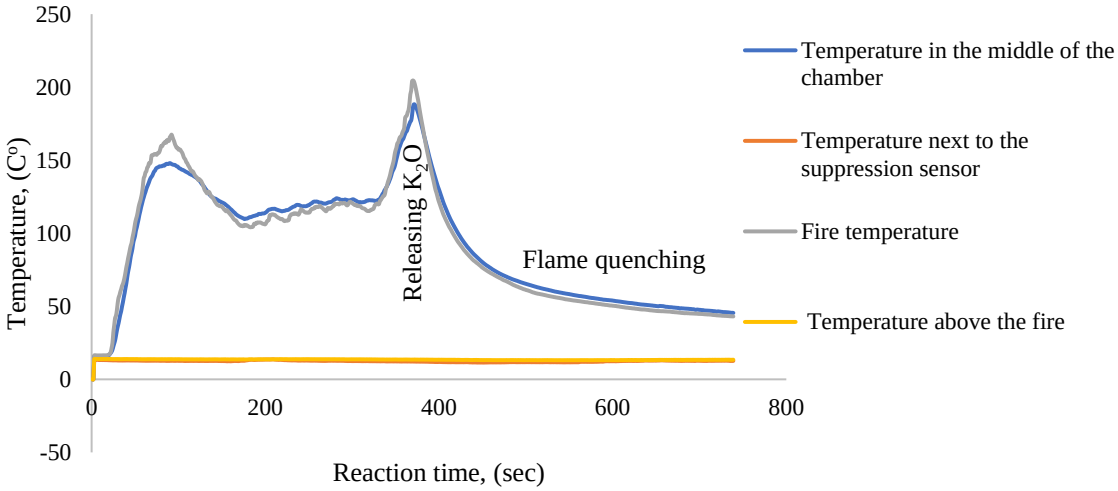


Figure 3.7: Testing pool fire suppression using a 0.3 fireless generation.

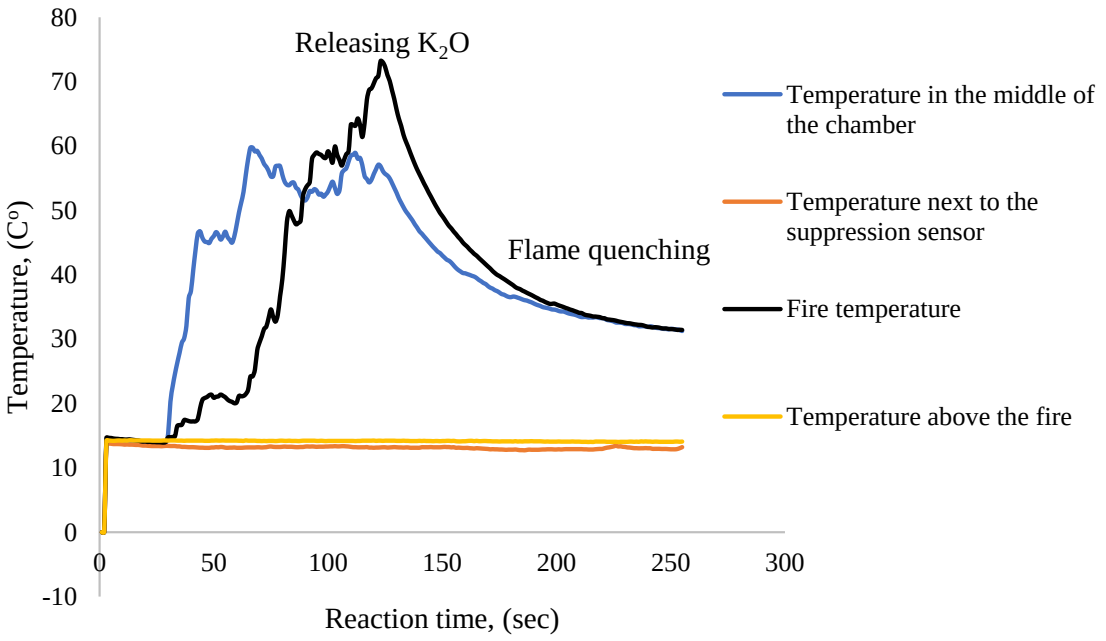


Figure 3.8: Temperature profile of oil fire in bin box with application of handheld.

From above Figures, the performance of K_2O in every stage is as shown below:

Ignition Stage: The first stage captures the inception of the fire, marking the point at which flames begin to emerge and grow. This initial phase continues until the sensor of the condensed aerosol generator is activated. During this time, the fire intensifies, posing a significant hazard.

Quenching Stage: The second stage reveals a critical moment in fire suppression as K_2O is released towards the flames. This action leads to the rapid quenching of the fire. The extinguishing effect of K_2O is demonstrated during this stage.

Re-ignition Stage: The third stage, where fires may re-ignite after initial suppression. This phase underscores the need for sustained monitoring to ensure the flames do not reignite, especially when dealing with deep-seated fuel sources.

Temperature Reduction Stage: The final stage illustrates the gradual reduction in temperature.

3.4 Real-World Implications and Applications

The tests were carried out inside a closed bin box, which played a crucial role in containing the fire and ensuring the effective operation of the tireless unit. The confined environment within the bin box allowed the fireless generation to efficiently suppress the fire. It is important to note that the size of the fireless generator used in these experiments

was optimized to match the relatively small scale of the fire within the bin box. This suggests that for larger areas, a proportionally larger fireless generator system would be necessary to achieve the same level of fire suppression.

If the bin box were open, the fire could potentially re-ignite due to the introduction of oxygen, which underscores the importance of maintaining a closed environment for the K_2O agent to work effectively. This highlights the critical role of containment in fire suppression, as the closed environment ensures that the fire is deprived of oxygen, thereby preventing reignition and ensuring complete extinguishment.

The findings from this study have significant implications for the practical application of K_2O as a fire suppression agent. The ability of K_2O to rapidly reduce fire temperatures and extinguish flames makes it a promising candidate for use in various fire-prone environments. However, the study also emphasizes the need for further research on the effectiveness of different potassium species on various flammable liquids or gases, as their impact on flame properties may vary. In particular, while K_2O proved effective against kerosene fires, other potassium-based agents might require additional testing to determine their suitability for other types of fires.

Additionally, the findings underscore the importance of strategic placement and activation of fire suppression systems. The variation in activation temperatures (210 °C and 300 °C) depending on the generator's location indicates that these systems can be fine-tuned to respond to different fire scenarios, enhancing safety in complex environments. For example, K-species-based fire suppression systems could be integrated into the safety infrastructure of high-risk areas such as oil refineries, storage facilities for hazardous materials, and even in aviation, where rapid-fire suppression is critical.

Furthermore, while the use of handheld fire suppression equipment presents higher risks due to proximity to the fire, fixed K-species-based fire suppression systems could be employed in automatic or remote controlled configurations, ensuring safety while effectively managing fire outbreaks.

3.5 Summary

- The tests demonstrate that potassium-containing compounds, (specifically K_2O), have the potential to suppress various types of fires effectively.
- Thermocouples were used to monitor temperature changes inside the bin box during the tests, indicating a focus on understanding thermal behaviour in fire suppression scenarios.
- The estimated heat output from a wood fire is approximately 1600 kJ.
- The estimated heat output from flammable liquid (Kerosene) fire is approximately 2124 kJ.

- K_2O shows a fast reaction time in quenching hydrocarbon flames.
- Although K_2O can control gas flames, it may not completely extinguish deep-seated fires, suggesting certain limitations in its application.
- The findings from the analysis of the K_2O agent's performance in suppressing solid and liquid fires provide valuable insights into its potential real-world applications. The significant drop in fire temperature observed upon the introduction of the K_2O agent highlights its rapid and effective action in mitigating solid and flammable liquid fires. This suggests that the agent based on the K species could be used for fire suppression in environments where solid materials such as wood or flammable liquids (Kerosene) are the primary fuel source, such as industrial facilities, warehouses, and residential buildings.
- The thermal sensors were installed at random locations within the test chamber, rather than at predefined and controlled points. This random placement could result in uneven spatial coverage and sampling bias, affecting the accuracy and reliability of the temperature measurements recorded. The data obtained from the tests will not be used in the simulation study conducted as part of the thesis, suggesting a clear distinction in the research approach.
- The data regarding fireless generation will be used to estimate the primary potassium species released during the tests. This numerical simulation aims to identify the specific potassium species, which will then be studied for their effects on H_2 and CH_4 flames.
- An initial study of H_2 flames using two different combustion mechanisms will be presented in the next chapter. This study will serve as a foundation for developing gas-phase kinetic reactions involving combustion mechanisms integrated with the reactions of K-species mechanisms.

Chapter 4

Comparisonal Study of Hydrogen Flame Based on GRI-Mech and Reduced Mechanisms

This chapter presents an analysis of the numerical simulation of the reaction kinetics of H_2 oxidation using both GRI-Mech-3.0 and Reduced mechanisms of H_2 combustion. The results of the kinetic simulation are compared with previous studies in the literature review.

Moreover, this chapter identifies the sensitivity and pathway reactions of the H_2 flame modelled by various mechanisms.

The simulations aim to test two sets of various mechanisms, laying the foundation for further research in this field. H_2 can be used as a model fuel in inhibition studies to develop strategies to inhibit flames, and these strategies can then be applied to other types of flames as well. Once a strategy has been identified in H_2 flame inhibition studies, it can be tested on other fuels, such as CH_4 or C_3H_8, to determine its broader applicability.

Detailed information regarding the GRI-Mech mechanism 3.0, the Reduced reaction mechanism for H_2 combustion from Hadi's work from Konnov, and their respective files containing thermodynamics and transport data are available in Appendices (A) and (B).

The use of H_2 as a model fuel in inhibition studies has several advantages, as mentioned in Chapter 1 Subsection 1.2.1.

4.1 Computational Simulation Method

Chemical reaction kinetics are simulated using the Chemkin package. The simulation covers the entire duration of the reaction, starting from the initial conditions and continuing until the system reaches a state where chemical reactions have reached equilibrium. The reaction of the mixture H_2/air is under stoichiometric conditions. Four types of reactors have been employed in the simulations. The first reactor is a closed equilibrium reactor used to predict the AFT, the second is a one-dimensional flame speed reactor (open reactor) used to calculate the S_L, and the third reactor is perfectly stirred, (PSR) used to predict the flammability limit as an open reactor, the last reactor is a Batch reactor to illustrate the behavior of the primary species.

In these simulations, it is assumed that all gas species are thermally perfect and uniformly mixed in the reactor, maintaining a constant pressure of 1 atm. The initial temperature is determined based on prediction parameters. For predicting the AFT, the initial temperature was set at 300 K. However, in the context of S_L calculations, two different initial temperatures are required: 298 K and 673 K. These values are chosen based on the specific mechanisms utilised in the simulations. In addition, the initial gas temperature for predicting the flammability limit is 1700 K. Arrhenius parameters used in the Arrhenius equitation were supplied by the detailed reaction mechanism, in which each elementary reaction was associated with the value of the Arrhenius parameters. The reaction mechanisms developed by the GRI-Mech and Reduced mechanism were used to supply the Arrhenius parameters, A, n, and E, the GRI-Mech 3.0 mechanism utilised in this study was adopted from Chemkin software, which is widely recognised as a valuable resource for modelling complex chemical kinetic systems. It was originally adopted from Smith et al. (1999). On the other hand, the Reduced mechanism for H_2 combustion employed in this study was obtained from Hadi's work from Konnov Nozari & Karabeyoğlu (2015).

4.2 Reactor Models in Chemkin

Chemkin offers various reactor models to simulate and analyse chemical reactions and combustion processes. Each model serves specific purposes and can be employed to study different scenarios. Below are detailed explanations of some of the reactor models commonly used in Chemkin:

4.2.1 One-Dimensional Flame Speed Reactor

A flame is created by a chemical reaction that continues by itself and is often seen because the gases it burns give off light. Associated with a flame is a flame front, in which gas that hasn't yet burned gets hot and turns into intermediate radicals or products. The flame front serves as an indicator of the propagation of the flame. The study conducted by Rallis & Garforth (1980), delved into the structure of the flame front. The author's findings demonstrated that at the flame front, the unburned gas undergoes heating and transforms into intermediate radicals or products. The flame front serves as a pivotal indicator of the flame's progression. The flame front is typically considered to comprise two distinct regions, commonly known as the preheat and reaction zones. The preheat zone and reaction zone occupy the space between the cold boundary, which corresponds to the temperature of the unburned gas, and the hot boundary, where the temperature nears the flame temperature (equilibrium temperature). Within this area, the temperature of the unburnt gas primarily elevates due to heat conduction, accompanied by a degree of convection from the adjacent reaction zone. The temperature undergoes a concave ascent as it enters the reaction zone, where the reaction rate is relatively fast in this region.

As the temperature continually rises and approaches the equilibrium flame temperature, both temperature and concentration gradients gradually stabilise. Ideally, the thickness of a flame front extends between the cold boundary and the hot boundary. Hence, it is essential that the specified flame temperature remains slightly higher than the inlet flame temperature yet significantly lower than the equilibrium temperature. Given that the flame's position is constant within the coordinate system, and the S_L represents the relative velocity between the flame front and the unburned gas, the solution for the S_L corresponds to the velocity at a point where both temperature and species molar fractions closely resemble those of the unburned gas. Furthermore, it is imperative for the temperature and species gradients to approach zero at the hot boundary, ensuring the prevention of heat loss across the boundary. Consequently, the solution for the S_L must meet the requirement of temperature and species gradients approaching zero at both the cold and hot boundaries.

The one-dimensional flame speed reactor in Chemkin investigates chemical reaction behavior in a simplified, one-dimensional domain. It is designed to calculate essential parameters, including species and temperature profiles, along with the laminar flame speed, for one-dimensional, steady, and freely propagating premixed laminar flames. This model provides a comprehensive means of analyzing combustion processes in a controlled and simplified environment, making it particularly useful for studying phenomena like laminar flame propagation, where a flame front continuously advances in a single direction. The solution for the laminar flame speed is associated with the velocity at which the entire unburned mass flow enters the reactor, supplying fuel and oxidiser to the flame front located at a reference point (x = 0). The ultimate solution for the laminar flame speed is achieved when there is a zero gradient in temperature and species concentration at the flame front. Since mass and energy are conserved across the flame, from continuity: Equation (4.1):

$$m_{\text{flame}} = \rho v = \rho_u v_u = \rho_b v_b \tag{4.1}$$

where m_{flame} is the constant mass flux, or laminar burning flux; ρ is the gas density, v is the gas velocity, and the subscripts u and b denote the unburned and burned regions, respectively.

Chemkin is supplied with the specified air/fuel mixture, initial pressure, and temperature. A critical factor influencing flame speed calculation is the temperature distribution within the domain. The computation of laminar flame speed entails solving for the heat and chemical species transport across the flame width, using thermodynamic properties data files, as well as transport properties and chemical kinetics mechanisms.

The premixed flame models in Chemkin employ implicit finite difference methods and a combination of steady-state and time-dependent techniques to solve a set of governing partial differential equations. The solver algorithm automates grid refinement, ranging from coarse to fine, to improve convergence properties and ensure optimal mesh

placement Kumar (2020).

For the calculation of the flame speed, a 1-dimensional flow with uniform inlet conditions is used, simplifying the governing equations to:

Continuity

Continuity equation:

$$\dot{M} = \rho u A \tag{4.2}$$

Energy

Energy equation:

$$\frac{d}{dx}\left(\dot{M}\frac{dT}{dx} - \frac{1}{C_p}\lambda A\frac{dT}{dx}\right) + A\sum\left(\rho Y_k V_k C_{p,k}\frac{dT}{dx}\right) + A\sum\left(\dot{w}_k h_k W_k\right) = 0 \tag{4.3}$$

Species

Species equation:

$$\dot{M}\frac{dY_k}{dx} + \frac{d}{dx}(\rho A Y_k V_k) - A\dot{w}_k' W_k = 0 \quad (k = 1, \ldots, K_g) \tag{4.4}$$

Equation of State

Equation of State:

$$\rho = \frac{PW}{RT} \tag{4.5}$$

Where: x represents the spatial coordinate; $\dot{M}$ is the mass flow rate; T is the temperature; Y_k is the mass fraction of the kth species; P is the pressure; u is the velocity of the fluid mixture; ρ is the mass density; W_k is the molecular weight of the kth species; W' is the mean molecular weight of the mixture; R is the universal gas constant; λ is the thermal conductivity of the mixture; C_p is the constant pressure heat capacity of the mixture; C_{p_k} is the constant pressure heat capacity of the kth species; w_k is the molar rate of production by chemical reaction of the kth species per unit volume; h_k is the specific enthalpy of the kth species; V_k is the diffusion velocity of the kth species; $\dot{Q}_{\text{rad}}$ is the heat loss due to gas and particle radiation; A is the cross-sectional area of the stream tube encompassing the flame normalised by the burner area Design (2015).

Boundary Conditions For freely propagating flames, the boundary conditions are deduced. The location of the flame is constrained by fixing temperature at one point so that temperature and species gradients vanish at the cold boundary, so that the solution of

the flame speed eigenvalue $\dot{M}$ is achieved. At the cold boundary:

$$\epsilon_k, 1 - Y_{k,1} - \frac{\rho A Y_k V_k \dot{M}}{2} = 0 \quad \text{and} \quad T_1 - T_b = 0 \tag{4.6}$$

where: $\epsilon_k, 1$ - inlet reactant fraction of the kth species T_b - Specified burner temperature

At the hot boundary:

$$Y_{k,J} - Y_{k,J-1} = 0 \quad \text{and} \quad \frac{T_J - T_{J-1}}{X_J - X_{J-1}} = 0 \tag{4.7}$$

Design (2015)

4.2.2 Equilibrium Reactor

This reactor is employed to determine the chemical state of a mixture under equilibrium conditions. It accommodates any number of gas-phase or condensed species, enabling the analysis of composition and phase equilibrium. The outcomes are solely influenced by the thermodynamic properties of the selected species in the chemistry set, along with the initial composition and specified conditions. The initial composition defines the relative proportions of chemical elements in the system. In cases where two equilibrium states are possible, an initial estimate of the equilibrium temperature can be useful for distinguishing between a ”burned” and an ”unburned” equilibrium state. In its current implementation, the equilibrium program assumes that the gas phase is a mixture of ideal gases, while condensed phases are treated as ideal solutions. Users have the flexibility to define atomic populations by specifying initial species and their fractions in each phase, as well as the state parameters.

State parameters can be specified in various ways, including:
Temperature and pressure.
Pressure and entropy.
Enthalpy and pressure.
Volume and entropy.
Species composition can be either ”frozen” during a calculation or determined as part of the equilibrium analysis. Furthermore, calculations can be interconnected through continuations, allowing conditions from a prior equilibrium case to serve as the starting point for subsequent cases with different constraints. This feature enables users to employ the Equilibrium Reactor Model to analyze stages in a thermodynamic cycle. The Equilibrium Reactor Model is frequently used to determine adiabatic flame temperatures for combustible gas mixtures. This involves specifying an initial reagent gas mixture and constraining equilibrium under conditions of constant enthalpy (adiabatic) or constant pressure. Alternatively, the calculation can be conducted with constant internal energy or constant volume. Accurate adiabatic flame temperature calculations require the inclusion

of all radical species potentially present in the flame, in addition to stable reactants and products. Typically, an initial guess for the equilibrium temperature of approximately 1000 K or higher is necessary to guide the equilibrium solver toward the burned-gas solution Design (2015).

4.2.3 0-D Closed (Batch Reactor)

In Chemkin, the 0-dimensional closed batch reactor model enables the examination of chemical reactions within a closed system. The simulation provides information on the transformation of reactants into products over time. This model is particularly useful for studying reaction kinetics, equilibrium conditions, and overall reaction behavior in a controlled environment. Closed batch reactors have no inlets or outlets for flow during the period of interest, although there may or may not be heat flow to the external environment. Such batch systems are inherently transient, where the chemical state changes as the production and destruction of species progress through chemical reactions Design (2015). The key steps involved in solving the transformation reactions inside the batch reactor include:

Initialisation: Set the initial conditions, including the initial concentrations of reactants, temperature, and pressure.

Integration: Use numerical methods to integrate the system of ordinary differential equations over time. This involves solving for the changes in species concentrations, temperature, and other variables at each time step.

Time Stepping: Iteratively advance the simulation in small time increments, updating the concentrations and other parameters based on the calculated rates of reaction.

Convergence: Ensure that the solution converges to a stable state, indicating that the system has reached equilibrium or a steady state.

Perfectly Stirred Reactor (Continuous Stirred Tank Reactor - CSTR)

In a Continuous Stirred-Tank Reactor (CSTR), reactants continuously enter through the feed stream, and products consistently exit through the effluent stream. With the exception of start-up and shut-down phases, the reactor is maintained in a steady state, where the contents remain constant over time.

The CSTR is frequently employed to investigate the correlation between equivalence ratio and temperature in combustion systems. In a CSTR, reactants undergo thorough mixing, and the reactor operates with a uniform composition and temperature. This configuration allows for the exploration of how changes in the equivalence ratio—representing the ratio of the actual fuel-to-oxidiser ratio to the stoichiometric fuel-to-oxidiser ratio—affect the overall temperature within the reactor. Additional details

about the model applied are provided in Section 4.4.3.

4.3 Equivalence Ratio (ϕ) in Combustion Analysis

(ϕ) is a dimensionless parameter that quantifies the mixture conditions of a combustion process. It describes the relationship between the actual fuel-to-oxidiser ratio in a mixture and the stoichiometric (ideal) fuel-to-oxidiser ratio required for complete combustion. It is calculated by comparing the actual mass or mole ratio of fuel to oxidiser to the stoichiometric mass or mole ratio. The equation for (ϕ) is as follows Mishra (2014):

$$\phi = \frac{\text{Actual Fuel-to-Oxidiser Ratio}}{\text{Stoichiometric Fuel-to-Oxidiser Ratio}} \tag{4.8}$$

There are three cases for (ϕ) to present :
($\phi < 1$): Indicates a lean mixture. In a lean mixture, there is excess oxidiser relative to the amount of fuel.

(ϕ)= 1: Represents a stoichiometric mixture. This is the ideal balance of reactants, ensuring complete combustion with no excess of fuel or oxidiser.

($\phi > 1$): Signifies a rich mixture. In a rich mixture, there is an excess of fuel relative to the oxidiser. This can lead to incomplete combustion, producing byproducts such as carbon monoxide (CO).
Alternatively, it is often expressed as the air/fuel ratio or, in the case of the oxidiser / fuel ratio Lee (2005). The equation in the context of oxidiser/fuel is:

$$\phi = \frac{\text{Actual Oxidiser-to-Fuel Ratio}}{\text{Stoichiometric Oxidiser-to-Fuel Ratio}} \tag{4.9}$$

from equation 4.7 when the mixture is rich that means ($\phi < 1$), and the lean mixture means ($\phi > 1$).

4.3.1 Compositions of the Initial Reactants

The present study employs simulations using pure H_2 to anticipate the adiabatic flame temperature, flame speed, sensitivity, and pathway analysis. The outcomes of the predictions and validation experiments provide evidence that various mechanisms, sourced from the Chemkin library or adopted from commonly used sources in kinetic modelling and analysis, can be integrated with K-containing species reactions for recent and future investigations. The stoichiometric equation for H_2 combustion in air utilised in the simulation is presented below:

$$2H_2 + O_2 + 3.76N_2 \rightarrow 2H_2O + 3.76N_2 \tag{4.10}$$

Determination of Mole Fractions of Reactants

In the context of the balanced chemical equation 4.10, the aim is to calculate the mole fractions of the reactants, H_2, O_2, and N_2 within the reaction mixture. To facilitate this, it is assumed that an equal initial mole of each reactant is utilised, allowing for a consistent starting point for the calculations.

Calculation of Total Moles of Reacting Species: Total moles of the reacting species are determined by adding the moles of each reactant.

$$\text{Total moles of reacting species} = \text{Mole of } H_2 + \text{Mole of } O_2 + \text{Mole of } N_2 \tag{4.11}$$

$$= 2 \text{ mole} + 1 \text{ mole} + 3.76 \text{ mole}$$
$$= 6.76 \text{ mole}$$

Determination of Mole Fractions: The mole fraction of each reactant is calculated as follows:

$$\text{Mole fraction of } H_2 = \frac{\text{Mole of } H_2}{\text{Total moles of reacting species}} \tag{4.12}$$

$$= \frac{2 \text{ mole}}{6.76 \text{ mole}}$$
$$\approx 0.295$$

$$\text{Mole fraction of } O_2 = \frac{\text{Mole of } O_2}{\text{Total moles of reacting species}} \tag{4.13}$$

$$= \frac{1 \text{ mole}}{6.76 \text{ mole}}$$
$$\approx 0.1479$$

$$\text{Mole fraction of } N_2 = \frac{\text{Mole of } N_2}{\text{Total moles of reacting species}} \tag{4.14}$$

$$= \frac{3.76 \text{ mole}}{6.76 \text{ mole}}$$
$$\approx 0.556$$

these mole fractions were calculated based on the stoichiometric chemical reaction equation at Equivalence Ratio =1.

Table 4.1: The reactants mole fractions of H_2/air mixture for flame speed and equilibrium models

Reactants	Mole fraction
H_2	0.295
O_2	0.1479
N_2	0.556

4.4 Modelling methods

4.4.1 AFT Modelling Method

One of the most important features of a combustion process is the highest possible temperature of the combustion products. This maximum temperature is reached when there are no heat losses to the surrounding environment, ensuring that all energy released during combustion is used exclusively to heat the products. McAllister et al. (2011). The adiabatic flame temperature is calculated by specifying mole fractions of initial gas mixtures, considering both the initial and equilibrium temperatures. Different initial temperatures (300, 400, 500 K) were tested, with an increase in the initial temperature increasing the equilibrium temperature. For comparison, the results were based on an initial temperature and assuming the equilibrium temperature, as the equilibrium temperature is essential for predicting AFT, where both unburned and burnt solutions are possible. Table 4.1 shows the reactant mole fractions that are used in AFT simulations.

The AFT model was defined for equilibrium calculations at constant pressure and enthalpy. Thermodynamic data were required for the AFT model. In Chemkin, thermodynamic properties are presented as polynomial fits as functions of temperature. The thermodynamic properties database contains specific information about chemical species and their thermodynamic properties (temperature range and coefficients).

In this study for the simulations that required GRI-Mech 3.0 and Reduced mechanism of H_2 combustion, the thermodynamic and transport data of hydrogen and hydrogen species are supplied by different sources (Chemkin and Konnov).

4.4.2 Batch Reactor Modelling Method

The model is used to investigate the transformation of reactant to product over time in a batch reactor. The batch reactor was used to study a homogeneous H_2/air mixture under specific conditions. Solver type is transient. The ending time for transient simulations is set to 0.000173 s, ensuring a clear representation of reactant-to-product conversion. There is no temperature gradient or heat transfer between the gas and the surface.

4.4.3 Equilibrium Temperature as Function of (ϕ) Modelling Method

In this study, the flammability limits for the oxidation mixture H_2 were investigated. This model uses a chemistry set for H_2 combustion and demonstrates the use of

an equivalence ratio to specify the starting gas mixture. Additionally, it employs a continuation method to change the equivalence ratio. Several critical parameters for this simulation are input. In the physical properties of the reactor, the problem type is initially set to solve the gas energy equation and uses a modified Newton iteration method in the case of a steady-state solver. The input parameters on this panel include the residence time (τ) (the average time that a reactant spends inside the reactor before exiting) of the gas in the PSR $(3.0\times10^{-5}sec)$, system pressure 1 atm and volume of the reactor 67.4 cm³. No value is specified for Heat Loss, so the system will be treated as adiabatic. An initial temperature of (1700 K) is provided; however, it is possible to use (1300 K) as the minimum initial temperature. A relatively low initial temperature, such as room temperature, did not yield reaction in the model.

The fuel is composed of 100 % H_2. Similarly, on the oxidiser mix subtab, the oxidiser is defined as 79 % N_2 and 21 % O_2 (air). The use of the form of input equivalence ratio requires the specification of the products of complete combustion for the Fuel and Oxidiser mentioned, which is defined in the Complete-Combustion Products subtab. In this case, the species of products are H_2O and N_2. Eight additional simulations are specified where the equivalence ratio is gradually changed from (0.9 to 1.7). Table 4.1 shows the reactant mole fractions that are used for predicting the flammability limit.

4.4.4 Flame Speed, (S_L) Modelling Method

Numerical modeling of S_L is performed using the one-dimensional flame speed calculation model in Chemkin. The approach employs the boundary value method for calculating adiabatic flame speed. The configuration is utilized to characterize the burning velocity of a specific gaseous mixture under a defined pressure and inlet temperature. The modeling assumes the absence of heat losses. The gas-phase reaction mechanism, thermodynamic files, and transport properties are required to be supplied as inputs. The reaction mechanisms used in the simulation are GRI-mech and Reduced mechanism which contains the essential steps for H_2 oxidation.

The initial gas pressure was set at 1 atm. Heat loss and thermal expansion were not considered in the simulation, so the pressure was constant throughout the calculation. In addition, a temperature profile was automatically estimated.

The study commenced by establishing an initial gas temperature of 298 K. Furthermore, a temperature profile was provided as the initial estimate of the temperature distribution concerning the distance parameter, x. The starting position was located just above the burner, while the final axial position was set at either 10 cm or 0.5 cm, thereby encompassing the reaction zone for H_2 flame. The solution process required an initial input of grid points, which was adjusted within the range of 6-11 depending on the viability of the solution.

In addition to the aforementioned parameters, the mass flow rate of the inlet gaseous

mixture was supplied. However, it is noteworthy that the final solution was not particularly sensitive to the value of the mass flow rate, which would eventually be determined as part of the flame speed solution. Assuming a mass flow rate for flame speed calculations allows the freely propagating flame to remain at fixed coordinates. Additionally, the composition of the reactants was specified as input before running the model, whereas the expected composition of the products and intermediate fractions were not included in the model. The assumption that the axial velocity, as obtained from the Chemkin simulations, is approximately equal to S_L is made for the purpose of simplifying the analysis and interpretation of the combustion process. This assumption is based on the following considerations:

Steady-State Conditions: The combustion process reaches a steady state where the rate at which the unburned gas approaches the flame front becomes closely aligned with the flame's intrinsic speed,S_L.

Simplified Analysis: Treating the axial velocity as equal to the S_L simplifies the analysis and allows for straightforward comparisons with practical applications.

Assumed Balance: The assumption is made under the understanding that the combustion process is in a state where the rate of consumption of reactants by the flame is in balance with the flame's intrinsic speed. This balance is indicative of stable combustion. The present study entails an analysis and discussion of the S_L simulations for pure H_2, employing both the GRI-Mech and Reduced mechanisms. Notably, the impact of the equivalence ratio on S_L of the flame was not considered in the simulations. Fig.4.1 illustrates the rationale behind the development of the H_2 flame with two different initial temperatures. The results indicated that models could be utilised for simulations of the development of mechanisms with reactions of K-species starting from 610 K. The same working initial temperature for reaction mechanisms results in the same axial velocity of H_2 flame. In this simulation, the initial temperature was assumed to predict S_L of stoichiometric H_2/air mixture at 298 K and 673 K and constant pressure.

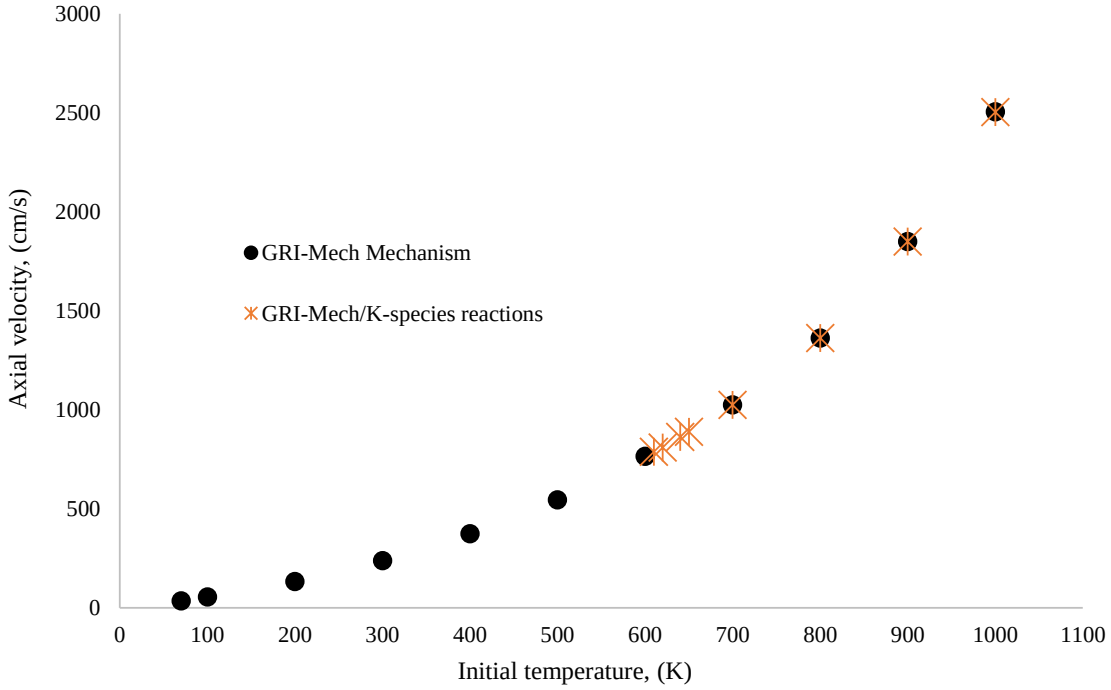


Figure 4.1: The relation between initial temperature and axial velocity of different kinetic reaction mechanisms of H_2/air mixture.

4.4.5 The species Pathway Analysis Modelling Method

Sensitivity analysis is a method used to identify the most important reactions and species involved in a chemical system. In the context of H_2 combustion, sensitivity analysis can be used to identify the reactions and species that have the greatest impact on the combustion behavior and efficiency of H_2/air combustion systems. The sensitivity analysis identifies the most important reactions and species in the combustion mechanism. It also reveals the importance of radical species such as H, OH, and HO_2 in the combustion mechanism.

The H_2/O_2 combustion process yields a significant number of free radicals, which include H, O, OH, and HO_2, as noted by Glassman et al. (2014). These free radicals play crucial roles in initiating and propagating chemical reactions during the combustion process. where H and OH are highly reactive and participate in chain reactions, and O and HO_2 are involved in termination reactions. Kee et al. (2003) in their book "Chemically Reacting Flow" further support this by stating that O, OH, and H are the primary free radicals produced during H_2/O_2 combustion. These free radicals are essential in the combustion process, and their interactions with other species determine the overall behavior of the combustion. Understanding the pathway of these important radicals involved in the reactions, as well as which radicals participate and influence reactant decomposition, is crucial. This knowledge enables the study of the inhibition effect of K-containing compounds on the pathway of the H_2/air mixture. The one-dimensional flame speed model that was used to calculate S_L at 298 K and 673 K was applied to

determine the sensitivity analysis of the H_2/air mixture based on different mechanisms.

4.5 Key Simulation Conditions

This section offers a comprehensive summary of the essential simulation conditions applied throughout the study of stoichiometric H_2/air mixture. Table 4.2 offers a comprehensive overview of the simulation conditions employed in the analysis of the stoichiometric H_2/air mixture. This investigation is conducted using two distinct mechanisms: the GRI-Mech Mechanism and the Reduced Mechanism.

4.5.1 Case 1: Initial Study of Stoichiometric H_2/air Mixture Using the GRI-Mech Mechanism

In this first scenario, the study centers on the stoichiometric H_2/air mixture, employing the GRI-Mech Mechanism to model the reaction. This case serves as the foundation for the exploration, establishing a baseline for subsequent analyses. The conditions and parameters under which this investigation is carried out are crucial in comprehending the behavior of the mixture under ideal stoichiometric conditions.

4.5.2 Case 2: Evaluation of the Stoichiometric H_2/air Mixture Using the Reduced Mechanism

In the second scenario, the study focuses as well as the first scenario on the stoichiometric H_2/air mixture, adopting the Reduced Mechanism from an external source to model the reaction.

Table 4.2: A summary of the simulation conditions used to study the stoichiometric H_2/air mixture at constant pressure based on the GRI-Mech Mechanism or Reduced Mechanism

	Model	Initial Temperature, K	Reaction Mechanism	Mass Flow Rate, g/cm^2s	(ϕ)	Wall Boundary	Data Required	Cases
Flame speed and Perform sensitivity analysis	1-D flame speed	298/673	GRI-Mech	1	1	Adiabatic	Gas-phase Kinetic reactions. Thermodynamic data. Transport data.	Case1
		298/673	Reduce Mechanism	1	1	Adiabatic	Gas-phase Kinetic reactions. Thermodynamic data. Transport data	Case2
AFT	Equilibrium	300	GRI-Mech	N/A	1	Adiabatic	Gas-phase Kinetic reactions. Thermodynamic data	Case1
		300	Reduce Mechanism	N/A	1	Adiabatic	Gas-phase Kinetic reactions. Thermodynamic data	Case2
Species Composition profiles	Closed homogenous reactor (Batch Reactor)	1100	GRI-Mech	N/A	1	Adiabatic	Gas-phase Kinetic reactions. Thermodynamic data.	Case1
		1100	Reduce Mechanism	N/A	1	Adiabatic	Gas-phase Kinetic reactions. Thermodynamic data	Case2
Flammability limit	Perfectly-stirred Reactor (PSR)	1700	GRI-Mech	N/A	1	Adiabatic	Gas-phase Kinetic reactions. Thermodynamic data.	Case1
		1700	Reduce Mechanism	N/A	1	Adiabatic	Gas-phase Kinetic reactions. Thermodynamic data.	Case2

Note:

- N/A in the table signifies that specific values or conditions were considered 'not required' for the model or simulation, as they were deemed unnecessary or irrelevant to the analysis.
- Using 'g/cm^{2}s' as a unit of mass flow in one-dimensional reactor simulations simplifies the representation of mass transport, particularly when calculating the flame speed in combustion studies.
- The temperature profile was automatically estimated from equilibrium.

4.6 Comparsion the Simulations Result of the stoichiometric H_2/air mixture Developed by GRI-Mech and Reduced Mechanisms

A comparison of the simulation results was made for the flame H_2. Specifically, the temperature of the adiabatic flame, S_L, and the flammability limit of oxidation H_2 were modelled using the GRI-Mech and Reduced mechanisms. The findings show a strong agreement between the two mechanisms.

4.6.1 Flame Speed

The flame speed of H_2 flame was modelled using both the GRI-Mech and Reduced mechanisms at constant pressure and the initial temperature firstly at 298, and secondly, 673K. The solutions obtained in the Chemkin output text format are presented in Appendix (D) and (E). These solutions ensure that both temperature and species gradients closely approach zero. At the cold boundary, the axial velocity represents the relative velocity of the unburned gas with respect to the flame front, so that the S_L for H_2/air combustion at 298 K based GRI-Mech and the Reduced mechanism is 236 cm/s and 240 cm/s respectively, Whereas using 673K resulting in S_L to be approximately 950 cm/s based on GRI-Mech mechanism and 970 cm/s developed by Reduced mechanism determined through the simulation. Figures 4.2, Figure 4.3, Figure 4.4 and Figure4.5 show the temperature profile and the characteristics of axial velocity correlated with the distance above the burner.

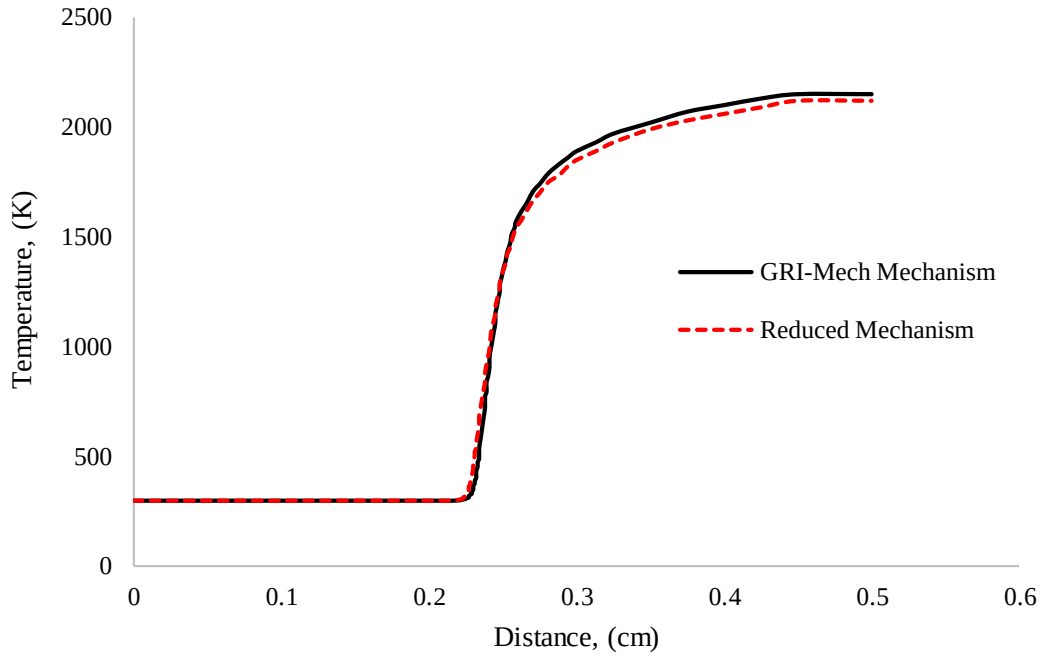


Figure 4.2: The gas temperature above burner for the H_2/air mixture based on GRI-Mech and the Reduced mechanism at 298 K and 1 atm.

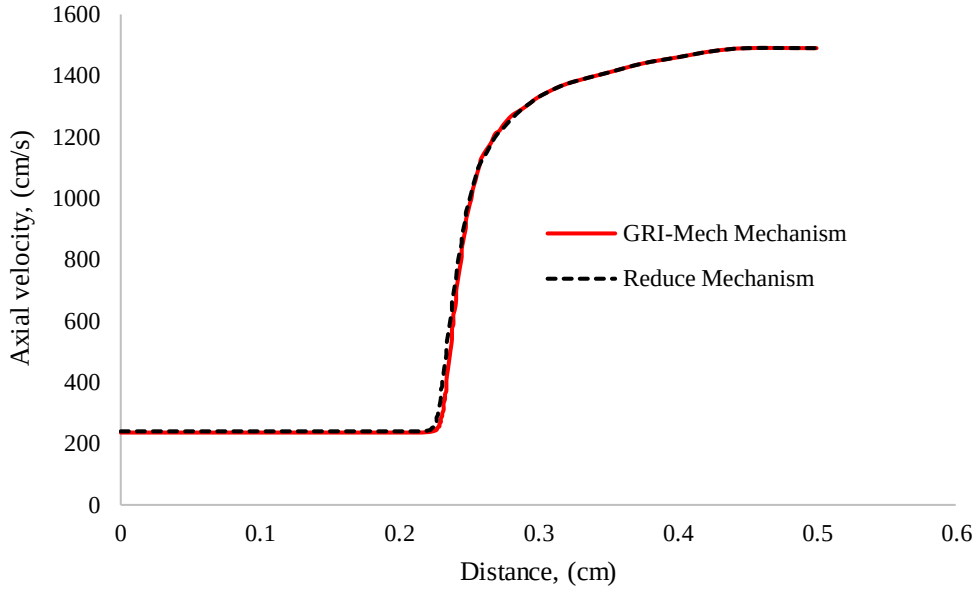


Figure 4.3: The axial velocity profile above burner for the H_2/air flame based on GRI-Mech and Reduced mechanism at 298 K and 1 atm.

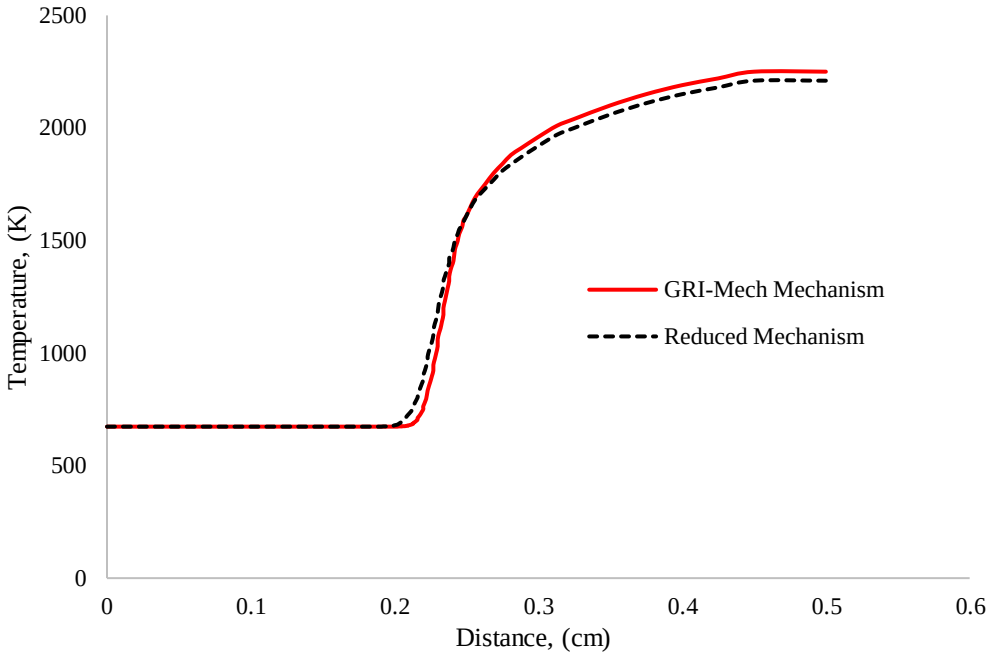


Figure 4.4: The gas temperature above burner for the H_2/air mixture based on GRI-Mech and the Reduced mechanism at 673 K and 1 atm.

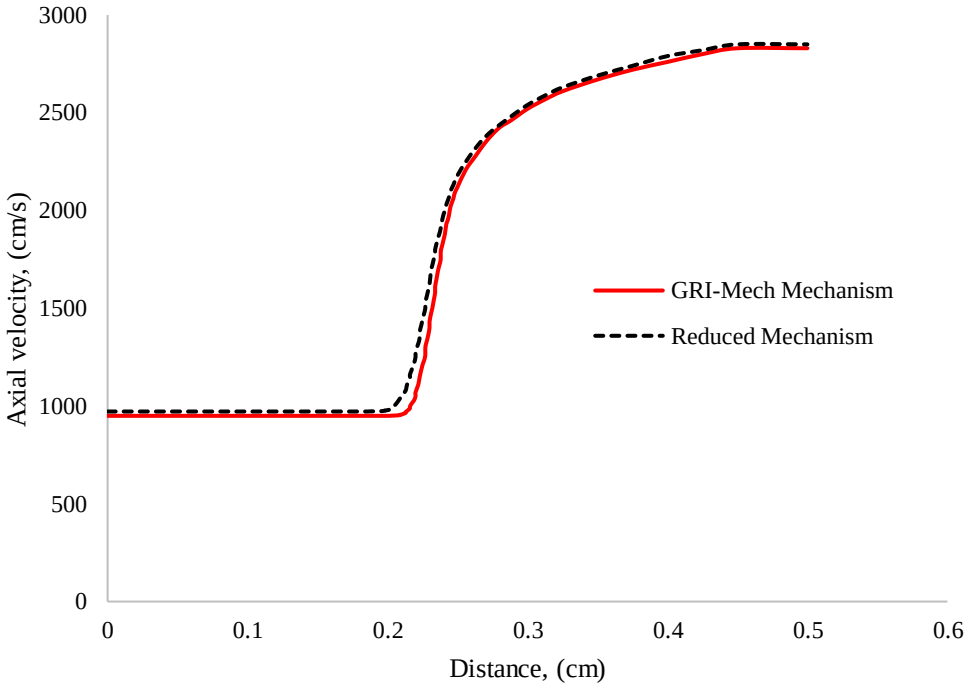


Figure 4.5: The axial velocity profile above burner for the H_2/air flame developed by GRI-Mech and reduced mechanism at 673 K and 1 atm.

Table 4.3: The comparison of laminar burning velocity of the combustion of H_2/air mixture

Temperature (K)	Kinetic Mechanism	S_L, cm/s
298	GRI-Mech mechanism	236
	Reduced Mechanism	240
673	GRI-Mech mechanism	950
	Reduced Mechanism	972

4.6.2 AFT

The adiabatic flame temperature of H_2 oxidation at 300 K and 1 atm was modelled using both the GRI-Mech and Reduced mechanisms. The findings, as depicted in Figure 4.6 show a strong agreement between the two mechanisms. Table 4.7 shows the AFT values.

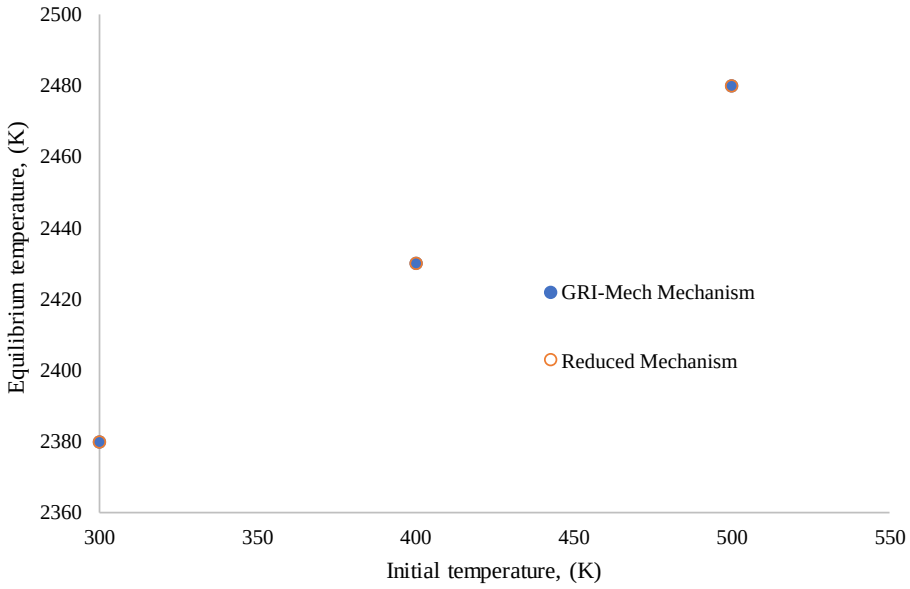


Figure 4.6: The comparison of AFT between GRI-Mech and Reduced mechanism for the oxidation H_2/air mixture of 100% H_2 at 300 K.

Table 4.4: The comparison of AFT of H_2/air mixture modelled by GRI-Mech and Reduced mechanisms

Kinetic Mechanism	AFT of 100% H_2, K
GRI-Mech mechanism	2380
Reduced Mechanism	2380

The behavior of the primary species of H_2/air mixture and time developed by GRI-Mech mechanism, and Reduced mechanism was estimated based on the batch reactor. Figures 4.7 and 4.8 show the simulation result. It can be seen that the mole fraction of H_2 steadily decreases over time. This decrease in the mole fraction of H_2 suggests that H_2 is a reactant in the chemical reaction that takes place. The reduction in H_2 mole fraction

is indicative of its consumption as the reaction progresses. Simultaneously, the mole fractions of other species appear to increase over time. This increase is likely due to the products formed as a result of the reaction.

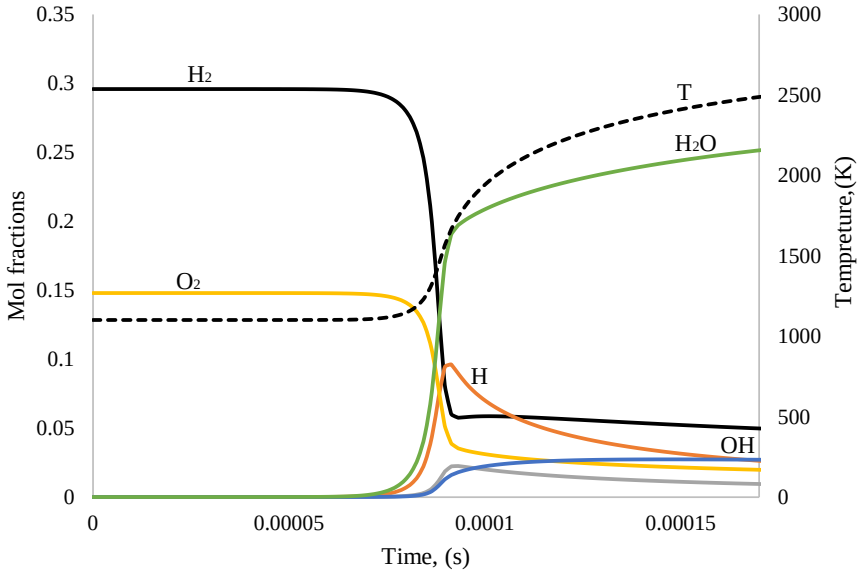


Figure 4.7: The evolution of the main species of H_2/air mixture and temperature in a homogeneous reactor-based GRI-Mech mechanism as obtained for (ϕ) = 1 and P= 1 atm with initial temperature T = 1100 K.

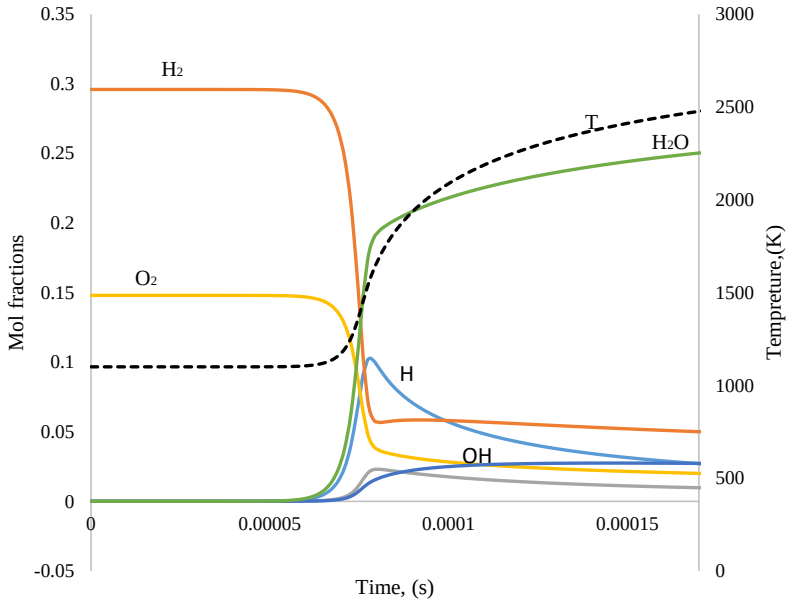


Figure 4.8: The evolution of the main species of H_2/air mixture and temperature in a homogeneous reactor based Reduced mechanism as obtained for (ϕ)= 1 and P= 1 atm with initial temperature T = 1100 K.

4.6.3 Equilibrium Temperature as a Function of Equivalence Ratio

From case 1, the steady-state temperatures for the combusting H_2/air mixture modelled by the GRI-Mech mechanism are shown in Figure 4.9 whereas the steady-state temperatures for the combusting H_2/air mixture modelled by Reduced mechanism is in Figure 4.10.

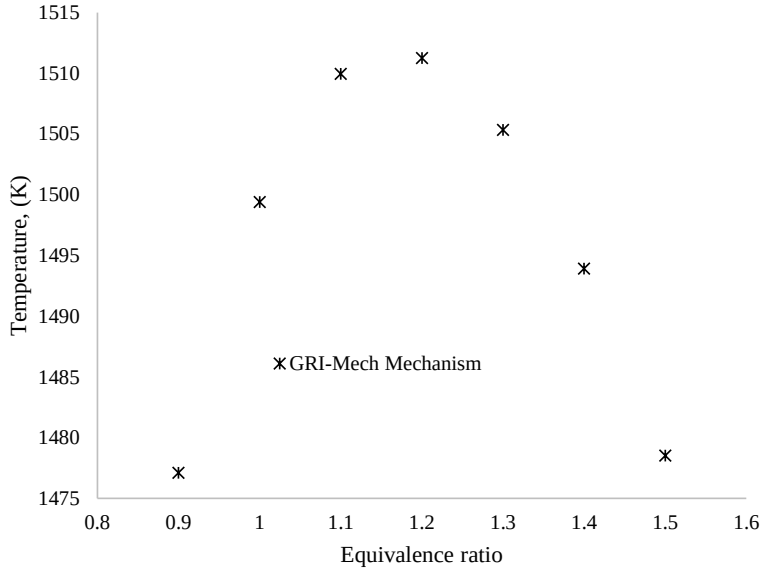


Figure 4.9: Relation between (H_2/air) equivalence ratio and equilibrium temperature before merging the kinetic mechanisms.

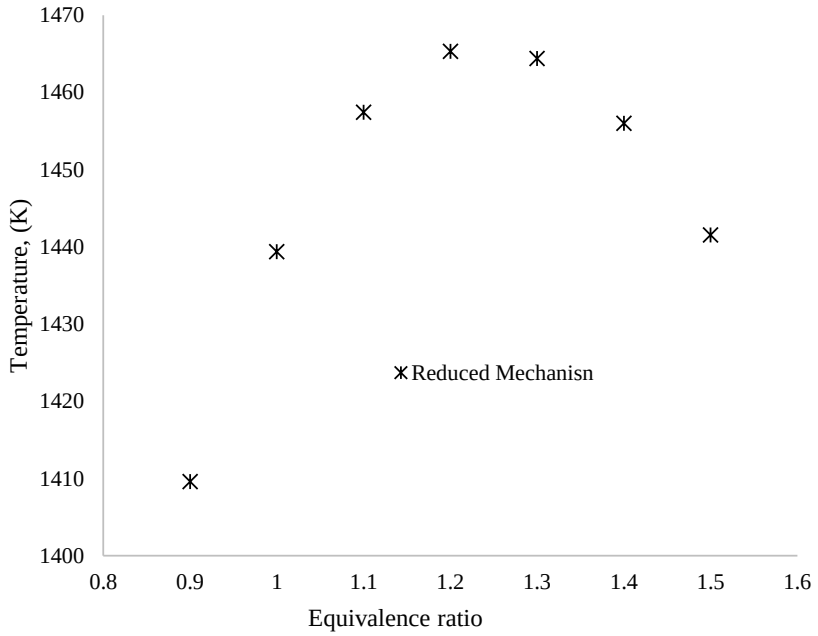


Figure 4.10: Relation between (H_2/air) equivalence ratio and equilibrium temperature before merging the kinetic mechanisms.

The comparison result from case 1 and case 2 is shown in Figure 4.11. In this case, the temperature peaks at a fuel/air equivalence ratio of about 1.2 and 1.3, which means the temperature will be highest in the H_2/air rich. The area between the fuel/air equivalence ratio (0.9 to 1.5) allows the flame to propagate.

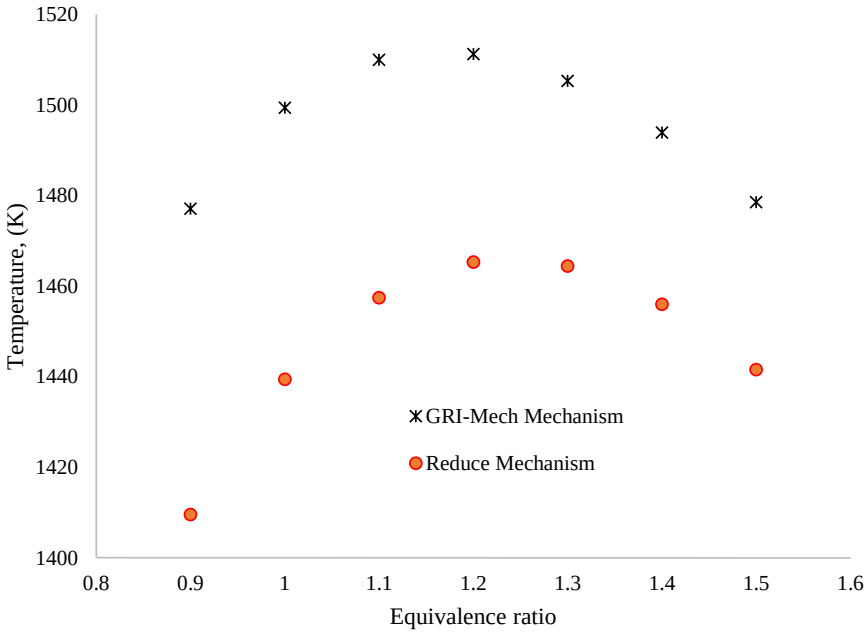


Figure 4.11: Relation between (H_2/air) equivalence ratio and equilibrium temperature before merging the kinetic mechanisms.

4.6.4 The Species Pathway Analysis

Figures 4.12 and 4.13 presented the sensitivity analysis of H_2 oxidation reaction using the GRI-Mech and Reduced mechanisms at 298K, whereas, Figures 4.14 and 4.15 presented the sensitivity analysis of H_2 oxidation reaction using the GRI-Mech and Reduced mechanisms at 673K. In the two cases, consumption of H_2 is predominantly governed by two major paths involving H_2+OH<=>HO_2+H and H_2+O<=>OH+H, in which H and OH radicals are involved. The former reaction is regarded as a chain-carrying reaction, while the latter is a chain-branching reaction. The chain carrier H also plays a crucial role in initiating chain branching reactions by attacking O_2 to form OH+O, which subsequently participates in H_2 consumption reactions, thus forming a cycle.

The primary pathways for the generation of H_2 are H+HO_2<=>O_2+H_2 and 2H+HO_2<=>H_2+HO_2. Decomposition of H_2 oxidation leads to the production of H and OH as major products. Additionally, the sensitivity analysis revealed that H+O_2<=>O+OH, O+H_2<=>H+OH, OH+H_2<=>H+HO_2, and H+HO_2<=>2OH are the principal chain branching reactions responsible for the accumulation of H, O, and OH radicals, leading to an enhancement of the overall reaction rate.

Table 4.5 and Table 4.6 show the pathways of H_2 that are generated and consumed. Based on the tables presented, it can be concluded that both the GRI-Mech and reduced mechanisms for H_2 oxidation at different initial temperatures involve the generation of H_2 through the H+HO_2 reaction. Furthermore, both mechanisms include the consumption

reactions of OH+H_2<=>H+H_2O and O+H_2<=>H+OH, which are responsible for the depletion of H_2. The Reduced mechanism also includes the consumption reaction of 2H+M<=>H_2+M, where M represents a third body that assists in the reaction.

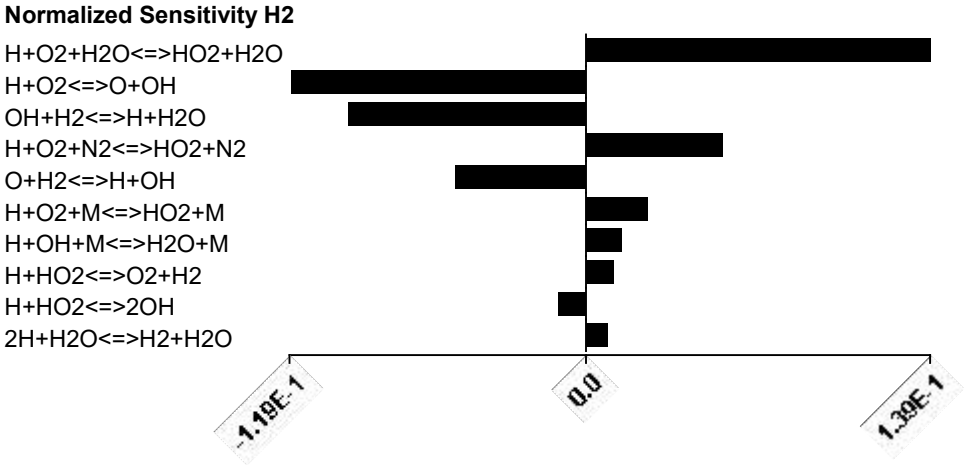


Figure 4.12: Normalized sensitivities of stoichiometric H_2/air flame developed by GRI-Mech mechanism at initial condition, 298 K,1 atm.

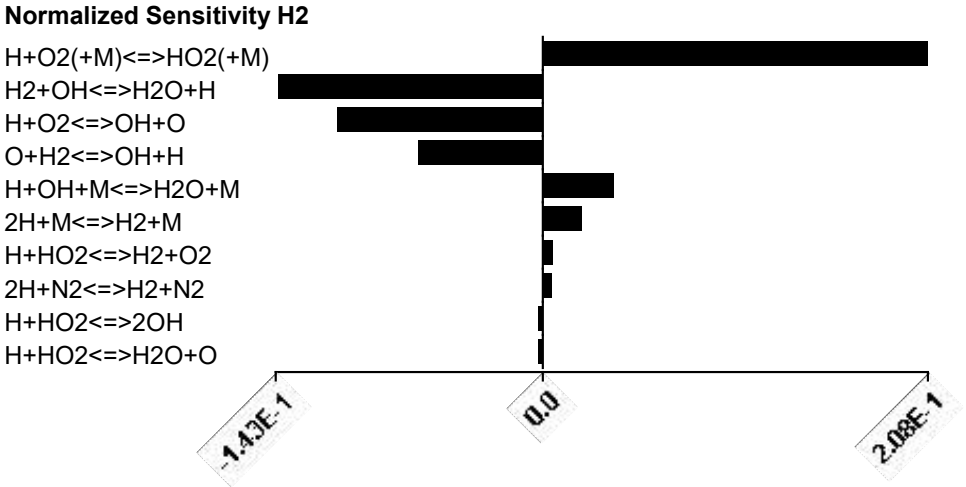


Figure 4.13: Normalized sensitivities of stoichiometric H_2/air flame developed by Reduced mechanism at initial condition, 298 K,1 atm.

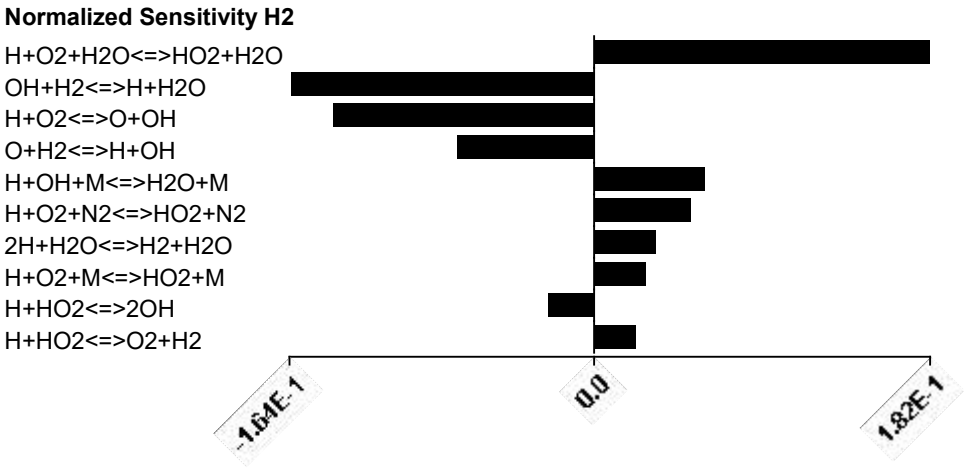


Figure 4.14: Normalized sensitivities of stoichiometric H_2/air flame developed by GRI-Mech mechanism at initial condition, 673 K,1 atm.

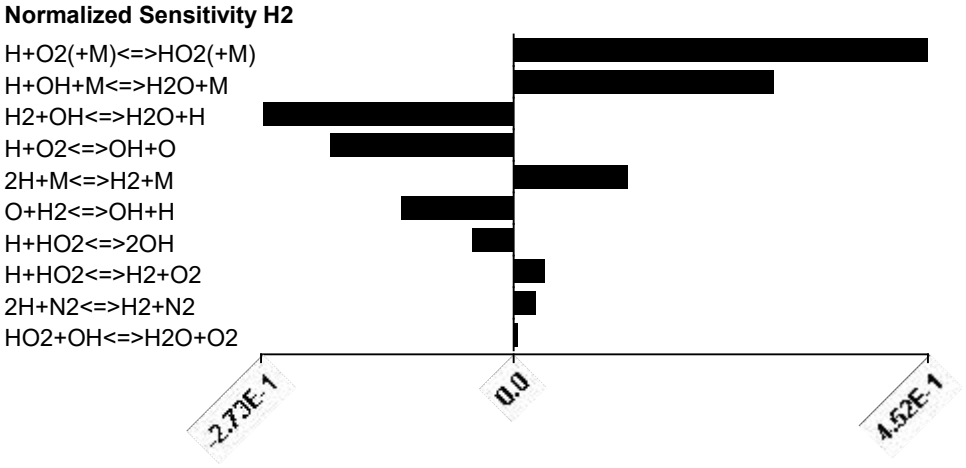


Figure 4.15: Normalized sensitivities of stoichiometric H_2/air flame developed by Reduced mechanism at initial condition, 673 K,1 atm.

Table 4.5: Generation and consumption pathway of the oxidation of H_2/air mixtures at 298 K, 1 atm

Kinetic Mechanism	Generation reactions	Consumption reactions
GRI-Mech mechanism	$H+HO_2=>O_2+H_2$	$OH+H_2<=>H+H_2O$
	$2H+H_2O<=>H_2O+H_2$	$O+H_2<=>H+OH$
Reduced mechanism	$H+HO_2=>O_2+H_2$	$OH+H_2<=>H+H_2O$
	$2H+M<=>H_2+M$	$O+H_2<=>H+OH$

Table 4.6: Generation and consumption pathway of the oxidation of H_2/air mixtures at 673 K, 1 atm

Kinetic Mechanism	Generation reactions	Consumption reactions
GRI-Mech mechanism	$H+HO_2=>O_2+H_2$	$OH+H_2<=>H+H_2O$
	$2H+H_2O<=>H_2O+H_2$	$O+H_2<=>H+OH$
Reduced mechanism	$H+HO_2=>O_2+H_2$	$OH+H_2<=>H+H_2O$
	$2H+M<=>H_2+M$	$O+H_2<=>H+OH$

4.7 Validate Simulation Results of the AFT and S_L of H_2 Oxidation Developed by GRI-Mech Mechanism and Reduced Mechanism

Validation of simulation results is an essential step in any computational study of combustion, particularly when simulating practical applications. In the case of AFT and S_L simulations, validating the results involves comparing them with available data in the literature.

Table 4.7 compares the AFT values obtained from five different studies, including AFTC, Goodger (1977), Tums (2001), Ferguson and Kirkpatrick (2001), and Gordon and McBride Olinger (2004), and two current studies.

The table shows the AFT values for H_2 flame in (K) obtained from each study. AFT values range from 2380 to 2444 K. The table provides a quick reference for comparing the AFT values obtained from various studies. The result is in a reasonable range with the data from previous studies.

Table 4.7: Comparative Analysis of Adiabatic Flame Temperatures (K) in H_2/Air Mixtures: A Comparison Between Previous and Current Studies

Previous Studies	AFTC	2419	**AFT, K**
	Goodger	2444	
	Turns	2382	
	F&G	2383	
	G&M	2400	
Current Studies	GRI-Mech	2380	
	Reduced Mechanism	2380	

Figure 4.16 illustrates the variation of flame speed for H_2/air as a function of the equivalence ratio. These measurements were conducted at atmospheric pressure and 293 K Pareja et al. (2010), Wu & Law (1985), Ilbas et al. (2006), Dahoe (2005). The current simulations are compared with previous research. Notably, the GRI-Mech mechanism results align with Pareja, Egolfopoulos, and Law, while the Reduced Mechanism simulations also fall within an acceptable range when compared to earlier research. The Chemkin simulation results, available in Appendix (F), are presented in text format. These results indicate that the number of grid points has increased from the initial value in the final solution based on the fuel/air ratio. This expanded grid ensures that the temperature and species gradients approach zero. At the cold boundary, the axial velocity represents the relative velocity of the unburned gas to the flame front. This approach allows us to approximate the flame speed of H_2/air combustion at different equivalence ratios. Table 5.7 presents the S_L values based on the model described Table 5.1

Table 4.8: The laminar burning velocity of of H_2 flame at 298K and constant pressure

Reaction Mechanism	S_L at $\phi = 0.6$	S_L at $\phi = 1$	S_L at ϕ 1.3
GRI-Mech Mechanism	73 cm/s	236 cm/s	297 cm/s
Reduced Mechanism	92 cm/s	240 cm/s	296 cm/s

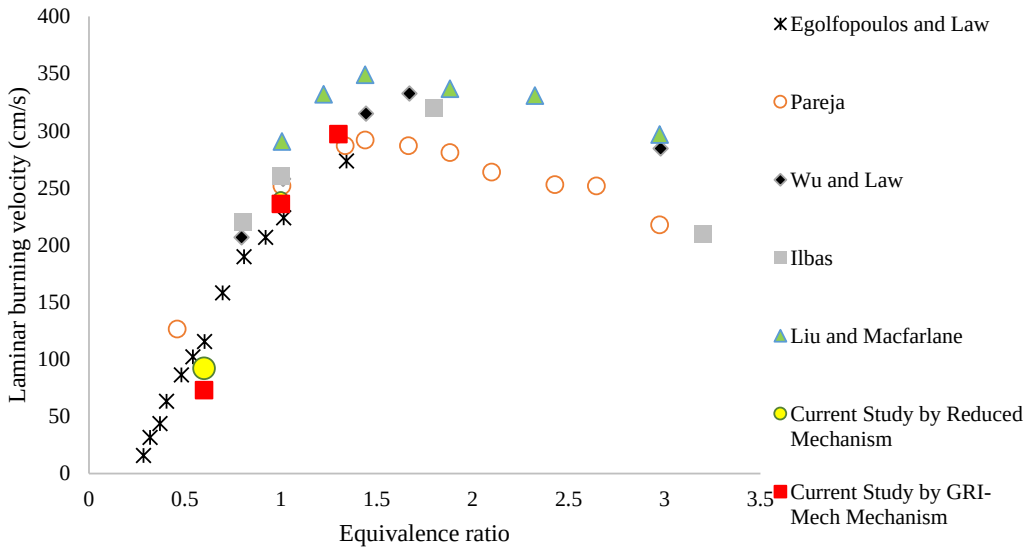


Figure 4.16: The comparison of the laminar burning velocity of H_2/air of current study with previous studies.

4.8 Summary

- To simulate the combustion of a pure H_2/air mixture, both the GRI-Mech reaction mechanisms from the Chemkin library and the Reduced mechanism developed by Konnov have been utilised.
- The S_L of a stoichiometric H_2/air mixture based on the GRI-Mech mechanism at 298 K and 101.33 kPa is 236 cm/s.
- The S_L of a stoichiometric H_2/air mixture based on the Reduced mechanism at 298 K and 101.33 kPa is 240 cm/s.
- The AFT of H_2/air mixture developed by the GRI-Mech mechanism is 2380 K.
- The AFT of H_2/air mixture developed by the Reduced mechanism is 2380 K.
- The flame temperature increases at the same rate for both mechanisms.
- Both the GRI-Mech and Reduced mechanisms provide a detailed description of the production and consumption of species involved in H_2 combustion and can be used to study the impact of different potassium species on these reactions.

- H_2 is mainly consumed through the reactions H_2+OH<=>H_2O+H and H_2+O<=>OH+H.
- The primary contributors to the production of H are the reactions H_2+OH<=>H_2O+H and H_2+O<=>OH+H.
- The primary contributors to the production of OH are the reactions O_2+H<=>OH+O and H_2+O<=>OH+H.
- The combustion of H_2 involves the generation and consumption of several free radicals, including OH, H, and O. These free radicals play crucial roles in the reaction pathways and kinetics of H_2 combustion.
- The simulation results for AFT, S_L, and pathway reactions of H_2/air mixture are found to be in good agreement with previous studies. These results will serve as the foundation for the simulations in the next chapter.
- The next chapter will examine the integration of kinetic mechanisms with K-species reactions. This investigation focuses on the consequences of incorporating K-species reactions into existing kinetic mechanisms.

Chapter 5

Development of Kinetic Reactions Mechanisms (GRI-Mech and Reduced) With the Reactions of Potassium Species

This chapter demonstrates the integration of kinetic mechanisms with K-species reactions. It investigates the consequences of incorporating K-species reactions into kinetic mechanisms, including those found in the hydrogen/ hydrocarbon combustion mechanism as detailed in Appendix (A), as well as the reduced mechanism for H_2 combustion found in Appendix (B). Additionally, this chapter assesses the performance and validity of K-species reactions. The term 'K-species reactions' refers to chemical reactions involving potassium (K) compounds or species. These reactions are of particular interest because some of the K-species serve as key components in fire suppression agents.

Potassium species in this context encompasses a range of chemical species and compounds containing potassium atoms. Understanding the behavior and effectiveness of these potassium species is essential for the development and improvement of fire suppression agents. The K-species reactions model is shown in Section 2.9 The thermodynamics and transport data files of K-species reactions with the species of the hydrocarbon system are documented in Appendix (C) for reference.

The simulations carried out in this chapter focus on modelling stoichiometric H_2/air mixtures. This involves the utilisation of the developed kinetic reaction mechanisms, encompassing GRI-Mech and the Reduced Mechanism, integrated with the reactions of potassium species.

5.1 Develop the Chemical Kinetic Reactions, GRI-Mech with K-Species, and Reduced with K-Species Mechanisms procedure

The development of chemical kinetic reactions, including the GRI-Mech with K-Species and Reduced with K-Species mechanisms, was carried out using the Chemkin-Pro 19R_2 software. The procedure involved a systematic approach to integrate K-Species reactions with existing chemical kinetic mechanisms. The first step was to select the base kinetic mechanisms that serve as a foundation for the study. In this case, the GRI-Mech mechanism and the reduced mechanism for H_2 combustion were chosen as the "Master Mechanism". The identified K-Species reactions (Donor Mechanism) were then

integrated into the selected kinetic mechanisms. This integration entailed adding the chemical reactions involving K-Species into the existing mechanisms. The K-species mechanisms require three essential files, these are, gas phase chemical kinetic reaction, thermodynamic data, and transport data. Collecting data from various sources, including Chemkin and literature reviews, provides accurate thermodynamic and transport data on K and its species.

As in Appendix C, the potassium-containing species included in the reaction file are (K, KH, KO, KO_2, KO_3, K_2O, K_2O_2, KOH, $(KOH)_2$, K_2CO_3, KCO_3 and $KHCO_3$), comprising a total of 85 reactions. Assumptions were made to derive necessary transport data and polynomial coefficients.

For certain potassium-containing species, including K_2O, $KHCO_3$, K_2O_2, K_2CO_3, KO_3, $K_2H_2O_2$, and KCO_3, uniform transport data and polynomial coefficients were assumed. Additionally, to streamline the analysis and modelling process, the polynomial coefficients of KO_2 were used for KO_3, and the polynomial coefficients of K_2CO_3 were applied to $KHCO_3$ and KCO_3. This approach can allow the characterisation of the behaviour and properties of potassium-containing species, even in cases where data from the literature were absent.

Once the mechanisms were developed, testing and validation were performed. This involved simulations to ensure that the integrated mechanisms accurately represented the behaviour of K-Species in the context of hydrogen and hydrocarbon combustion.

5.2 Computational Simulation Method of Development of Kinetic Reactions Mechanisms (GRI-Mech and Reduced) With the Reactions of Potassium Species

Chemical reaction kinetics are simulated using the Chemkin package. The simulations focus on a stoichiometric H_2/air mixture. Four types of reactors have been employed in these simulations:

- A closed equilibrium reactor is utilized to predict AFT.
- A one-dimensional flame-speed reactor (open reactor) is used to calculate the laminar flame speed.
- A perfectly stirred reactor (PSR) is used to predict the flammability limit.
- A closed homogeneous batch reactor is applied to illustrate the behavior of primary species.

Throughout these simulations, it is assumed that all gas species are thermally perfect and uniformly mixed within the reactor, maintaining a constant pressure of 1 atm. The initial temperature is determined based on the prediction parameters. However, for S_L

calculations, the initial gas temperature is set at 673 K instead of the standard 298 K. Figure 4.1 provides further insight into the rationale for using this elevated initial temperature in the development of H_2 flame behaviour through two distinct mechanisms.

5.3 Key Simulation Conditions for Development Mechanism GRI-Mech with K-Species Reactions and Reduced Mechanism of H_2 Combustion with K-Species Reactions

In the context of developing mechanisms for chemical kinetics, it is imperative to outline the key simulation conditions employed during the study of stoichiometric H_2/air mixtures. This section provides a comprehensive summary of these essential simulation conditions, specifically involving two distinct mechanisms: the hydrocarbon/ hydrogen combustion mechanism with reactions of species K and the reduced combustion mechanism of H_2 with reactions of species K.

5.3.1 Case 1: Initial Study of Stoichiometric H_2/air Mixture Using the GRI-Mech Mechanism with K-species Reactions

In the first case, the investigation revolves around the stoichiometric H_2/air mixture. The GRI-Mech Mechanism, augmented by K-species reactions, is employed to model the reaction. The conditions and parameters underpinning this study are of paramount importance in comprehending the behavior of the mixture. This foundational study lays the groundwork for the development and validation of kinetic mechanisms integrated with K-species reactions. Table 5.1 shows the simulation conditions applied in case 1.

Table 5.1: A summary of the simulation conditions used to study the stoichiometric H_2/air mixture based on the GRI-Mech/K-species Mechanism

		Reactor Models Used			
		One dimensional flame speed	Equilibrium	Closed homogeneous(Batch reactor)	Perfectly stirred Reactor
Simulation Conditions		Calculate the flame speed. Normalized sensitivities of the burning velocity	AFT	Species Composition profiles	Flammability limit
	Initial Temperature,K	673	300	1100	1700
	Residence Time,sec	N/A	N/A	N/A	(3×10^{-5})
	Mass Flow Rate (flow rate per area),g/cm^2s	1	N/A	N/A	N/A
	Pressure, atm	1	1	1	1
	Reaction Mechanism Fuel Type	GRI-Mech+K-Species reactions H_2	GRI-Mech+K-Species reactions H_2	GRI-Mech+K-Species reactions H_2	GRI-Mech+K-Species reactions H_2
	Oxidizer Type	air (O_2, N_2)	air (O_2, N_2)	air (O_2, N_2)	air (O_2, N_2)
	Gas Compositions	H_2=0.295 O_2=0.1479 N_2=0.556	H_2=0.295 O_2=0.1479 N_2=0.556	H_2=0.295 O_2=0.1479 N_2=0.556	H_2=1 O_2=0.21 N_2=0.79
Simulation Conditions	Constraints and assumptions	No heat loss and thermal expansion. Constrain the position of the flame. Solve the gas energy equation. Define the reactor dimension. The ambient temperature=298K. The axial velocity obtained from the simulations was assumed to represent the laminar burning velocity.	The reactor is defined at constant pressure and enthalpy. The equilibrium temperature was assumed 2000K	Solver type is transient. Gas energy solvent for accurate heat transfer and energy modelling. Ending time for transient simulations =0.000173s. There is no temperature gradient or heat transfer between the gas and the surface	Solve gas energy equation is chosen as a definition of the model problem. The solver is in a steady state. The reactor volume assumed 64.4cm³
	Wall Boundary	Adiabatic	Adiabatic	Adiabatic	Adiabatic

	Data Required	Gas-phase Kinetic reactions. Thermodynamic data. Transport data	Gas-phase Kinetic reactions. Thermodynamic data.	Gas-phase Kinetic reactions. Thermodynamic data.	Gas-phase Kinetic reactions. Thermodynamic data.

5.3.2 Case 2: Initial Study of Stoichiometric H_2/air Mixture Using the the Reduced Mechanism of H_2 Combustion, Coupled with K-species Reactions

In the second case, the primary focus remains on the stoichiometric H_2/air mixture. However, this investigation uses the reduced mechanism of H_2 combustion in combination with K-species reactions to delve deeper into the behavior of the mixture under stoichiometric conditions. This case represents a crucial step toward future objectives where certain software constraints may require the use of comprehensive kinetic reactions. Assessing the performance and validity of the Reduced mechanism when integrated with K-species reactions is integral to making this determination. Table 5.2 provides an overview of the simulation conditions applied in case 2.

Table 5.2: A summary of the simulation conditions used to study the stoichiometric H_2/air mixture based on the GRI-Mech/K-species Mechanism

		Reactor Models Used			
		One dimensional flame speed	Equilibrium	Closed homogeneous (Batch reactor)	Perfectly stirred reactor
Simulation Conditions		Calculate the Flame speed. Normalised sensitivities of the burning velocity	AFT	Species Composition profiles	Flammability limit
	Initial Temperature,K	673	300	1100	1700
	Residence Time,sec	N/A	N/A	N/A	(3×10^{-5})
	Mass Flow Rate (flow rate per area),g/cm^2s	1	N/A	N/A	N/A
	Pressure, atm	1	1	1	1
	Reaction Mechanism	Reduced Mechanism+K-Species reactions	Reduced Mechanism+K-Species reactions	Reduced Mechanism+K-Species reactions	Reduced Mechanism+K-Species reactions
	Fuel Type	H_2	H_2	H_2	H_2
	Oxidizer Type	air (O_2, N_2)	air (O_2, N_2)	air (O_2, N_2)	air (O_2, N_2)
	Gas Compositions	H_2=0.295 O_2=0.1479 N_2=0.556	H_2=0.295 O_2=0.1479 N_2=0.556	H_2=0.295 O_2=0.1479 N_2=0.556	H_2=1 O_2=0.21 N_2=0.79

	Constraints and Assumptions	No heat loss and thermal expansion. Constrain the position of the flame. Solve the gas energy equation. Defined the reactor dimension. The ambient temperature = 298K. The axial velocity obtained from the simulations was assumed to represent the laminar burning velocity	The reactor is defined at constant pressure and enthalpy. The equilibrium temperature was assumed 2000K	Solver type is transient. Gas energy solvent for accurate heat transfer and energy modelling. End time=0.000173s. There is no temperature gradient or heat transfer between the gas and the surface	Solve gas energy equation is chosen as a definition of the model problem. The solver is in a steady state. The reactor volume assumed 64.4cm³
	Wall Boundary	Adiabatic	Adiabatic	Adiabatic	Adiabatic
	Data Required	Gas-phase Kinetic reactions. Thermodynamic data. Transport data.	Gas-phase Kinetic reactions. Thermodynamic data.	Gas-phase Kinetic reactions. Thermodynamic data.	Gas-phase Kinetic reactions. Thermodynamic data.

Note:

- N/A in the table signifies that specific values or conditions were considered 'not required' for the model or simulation, as they were deemed unnecessary or irrelevant to the analysis.
- Using 'g/cm^{2}s' as a unit of mass flow in one-dimensional reactor simulations simplifies the representation of mass transport, particularly when calculating the flame speed in combustion studies.
- When an ending time is greater than 0.001 sec, the conversion of reactants to products may not be clearly visualised. However, by adjusting the axis bounds for the x-axis (time), this adjustment allows for a more detailed examination of the conversion process in the simulation results, where the y-axis represents mole fractions. It's important to note that with an ending time set to less than 0.00008 sec, there will be no observable change in the reactants, and no product formation is evident. Therefore, the optimal end time for this simulation is 0.0001s, as it provides a clear representation of the reactant-to-product conversion.
- The volume of the reactor in the PSR was systematically varied across a range of values, from 10 cm^3 to 100 cm^3 and beyond. The consistent equilibrium temperature observed throughout these variations suggests that the reactor's volume had no impact on the analysis. In other words, the analysis remains stable

regardless of the specific reactor volume used, affirming the robustness of the chosen idealization of a perfectly stirred reactor for this specific system

5.4 Comparsion Simulations Result of the H_2/air mixture conducted by Case 1 and Case 2

A comparative analysis was performed on the simulation results for the stoichiometric H_2/air mixture. The results indicate a significant level of concurrence between the two cases, suggesting a strong agreement in their findings.

5.4.1 S_L

Figure 5.1, and Figure 5.2 show the temperature profile and the characteristics of axial velocity correlated with the distance above the burner. Figure 5.2 displays a comparison of the S_L of H_2 oxidation modelled using the GRI-Mech/K-species and Reduced/K-species mechanisms, which exhibit a reasonable level of agreement. The solutions obtained in the Chemkin output text format are presented in Appendix (E). These solutions ensure that both temperature and species gradients closely approach zero. At the cold boundary, the axial velocity represents the relative velocity of the unburned gas with respect to the flame front, so that the S_L for H_2/air combustion using 673 K resulting in S_L to be approximately 950 cm/s based on GRI-Mech mechanism and 970 cm/s developed by Reduced mechanism determined through the simulation.

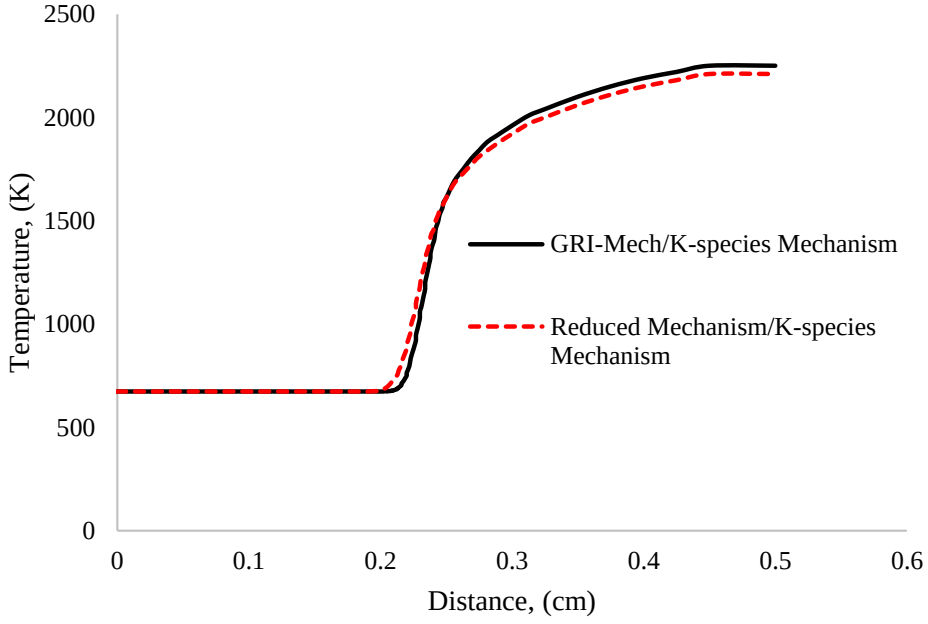


Figure 5.1: The comparison of the gas temperature for H_2/air flame at 673 K and 1 atm between GRI-Mech/K-species and the Reduced/K-species mechanisms.

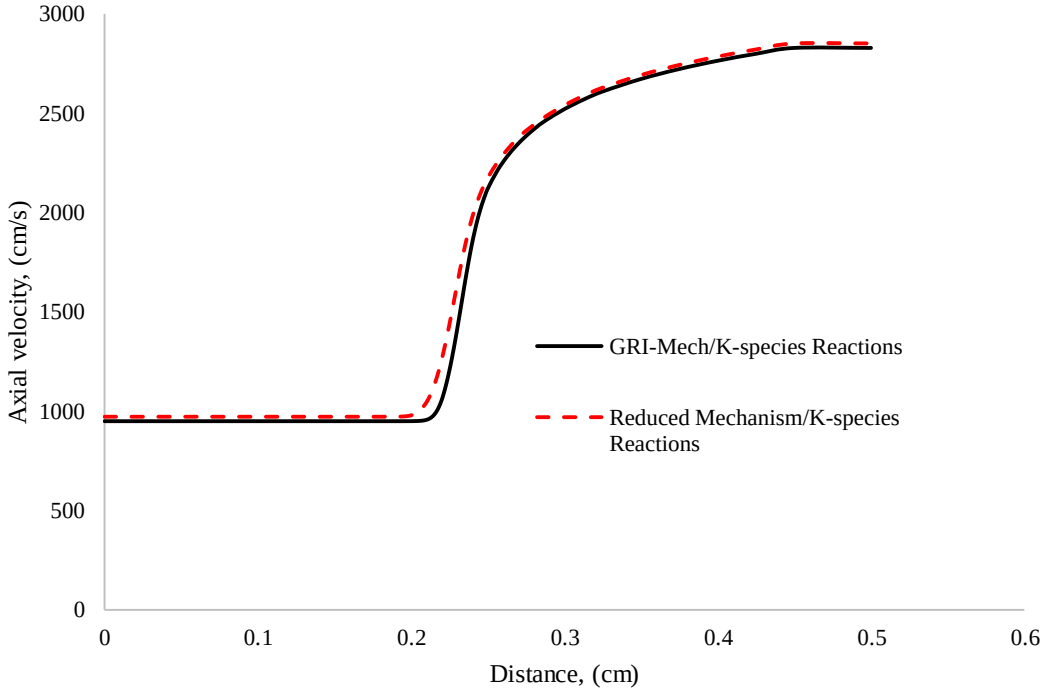


Figure 5.2: The comparison of the axial velocity of the combustion of H_2/air mixture modelled by the GRI-Mech / K-species reaction mechanism and the reduced / K species reactions mechanism.

5.4.2 AFT

Figure 5.3 demonstrates a reasonable agreement between the AFT results for H_2 oxidation modeled using the GRI-Mech/K-species and Reduced/K-species mechanisms. Table 5.3 presents the AFT results of the stoichiometric H_2 / air mixture based on Figure 5.3, and Figure 4.6 in Chapter 4.

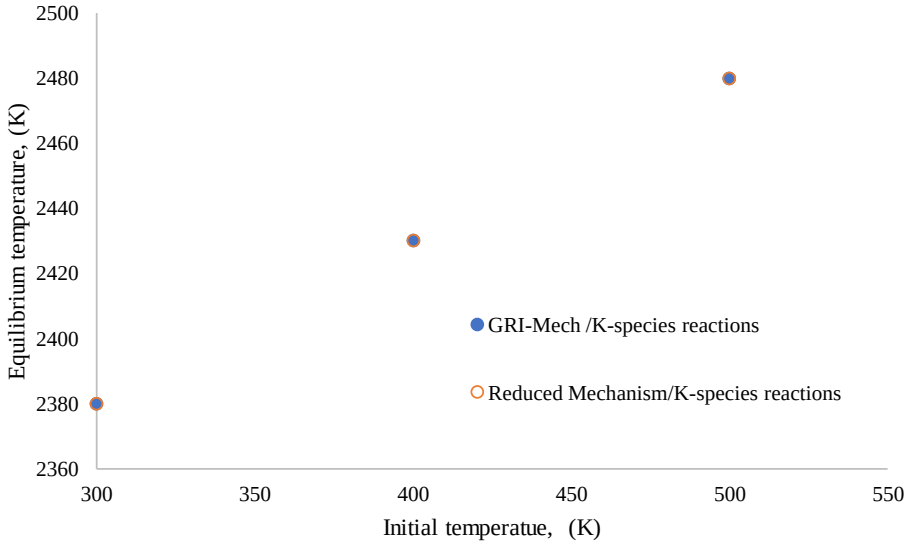


Figure 5.3: Equilibrium temperatures represent the adiabatic flame temperatures for H_2 / air mixture based on GRI-Mech/K-species and Reduced/K-species mechanisms at 300K.

Table 5.3: Comparison of AFT for H_2/air mixture based on different mechanisms

Kinetic Mechanism	**AFT of H_2 / air mixture , K**
GRI-Mech mechanism	2380
Reduced Mechanism	2380
GRI-Mech mechanism + reactions of K-containing species	2380
Reduced mechanism + reactions of K-containing species	2380

5.4.3 Equilibrium Temperature as a Function of Equivalence Ratio

The steady-state temperatures of the combustion mixture H_2/air, simulated using the GRI-Mech/K-species and the Reduced/K-species mechanisms, are presented in figure 5.4. In this case, the temperature exhibits peaks at fuel/air equivalence ratios approximately equal to 1.1 and 1.2, indicating that the highest temperatures are attained under the conditions H_2/air/rich.

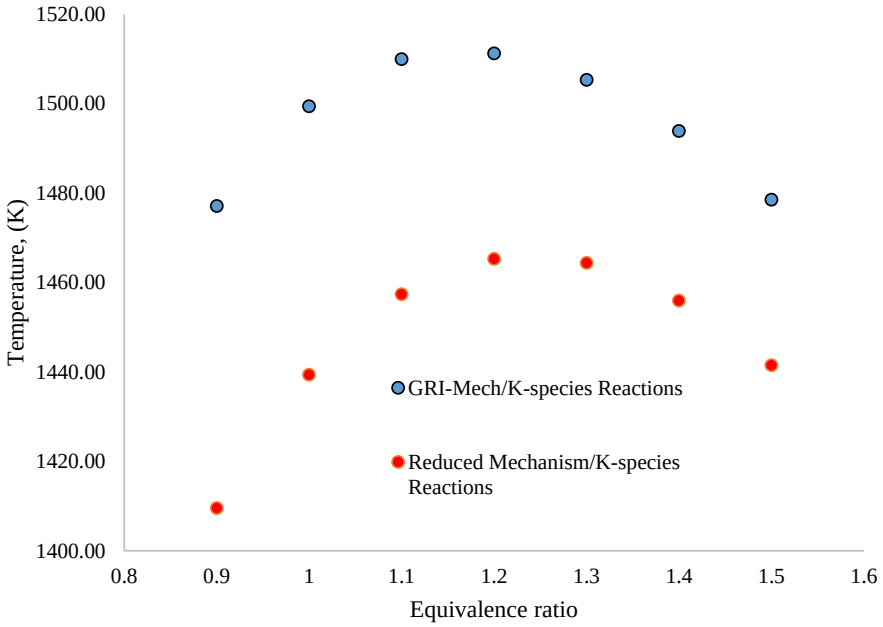


Figure 5.4: Relation between (H_2/air) equivalence ratio and equilibrium temperature developed after the merging mechanisms.

Table 5.4: Equilibrium temperature variation with equivalence ratio of H_2/air mixture based on GRI-Mech mechanism/K-species reactions

Equivalence Ratio	Equilibrium Temperature, (K)
0.9	1477
1	1499
1.1	1510
1.2	1511
1.3	1505
1.4	1494
1.5	1479

Table 5.5: Equilibrium temperature variation with equivalence ratio of H_2/air mixture based on Reduced mechanism/K-species reactions

Equivalence Ratio	Equilibrium Temperature, (K)
0.9	1410
1	1439
1.1	1457
1.2	1465
1.3	1464
1.4	1456
1.5	1442

Based on the batch reactor, Figure 5.5 illustrates the evolution of primary species in the H_2/air mixture over time, as developed by the GRI-Mech+K-species mechanism. In particular, there is a continuous decrease in the mole fraction of H_2 as time progresses. This decline suggests that H_2 serves as a reactant in the ongoing chemical reactions, indicating its consumption during the process. Similarly, the molecular fractions of other species demonstrate an upward trend over time, likely attributed to the formation of reaction products.

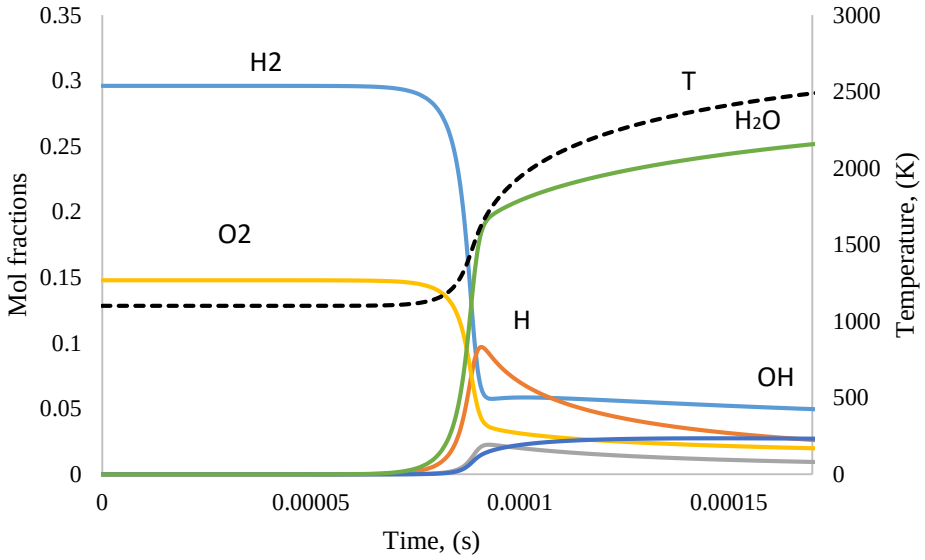


Figure 5.5: Distributions of mole fraction of species in the H_2/O_2 flame based GRI-Mech/K-species reactions as obtained for (ϕ) = 1 and P= 1 atm with initial temperature T = 1100 K).

Using data from the batch reactor, Figure 5.6 provide visual representations of the simulation results, showcasing the dynamic changes in the primary species within the H_2/air mixture over time. These simulations were conducted using the Reduced mechanism/K-species reactions.

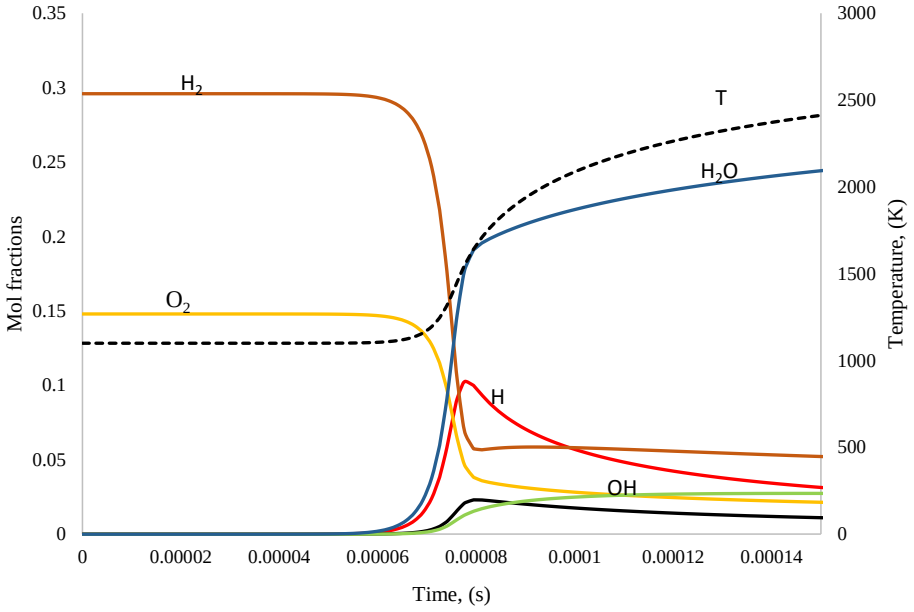


Figure 5.6: Tracking Species Evolution and Temperature Changes in Homogeneous H_2/Air Reactor at Stoichiometric Conditions (ϕ) = 1, P = 1 atm) with an initial temperature of 1100 K using the Reduced/K species mechanism.

5.4.4 Pathway Analysis

Figure 5.7 show the sensitivity analysis for the reaction of oxidation H_2 based on the mechanisms of the GRI-Mech / K species. The main routes for the consumption of H_2 are included; H_2+OH<=>H_2O+H and H_2+O<=>OH+H.

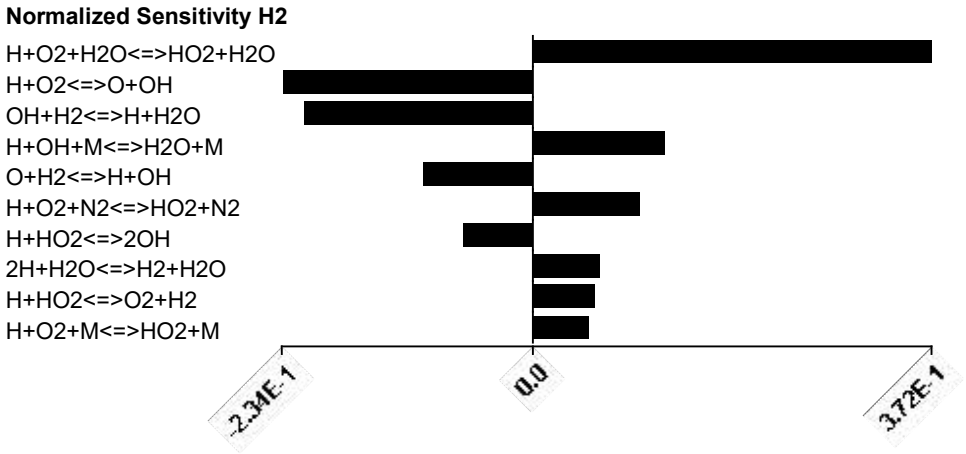


Figure 5.7: Normalized sensitivities of stoichiometric H_2/air flame developed by the GRI-Mech Mechanism / K-species reactions under initial conditions, 673 K,1 atm.

Figure 5.8 shows the sensitivity analysis for the oxidation of H_2 based on the Reduced mechanism/K-species reactions. The analysis highlights the primary pathways for consumption of H_2, which involve the reactions H_2+OH $\rightleftharpoons$ H_2O+H and H_2+O $\rightleftharpoons$ OH+H.

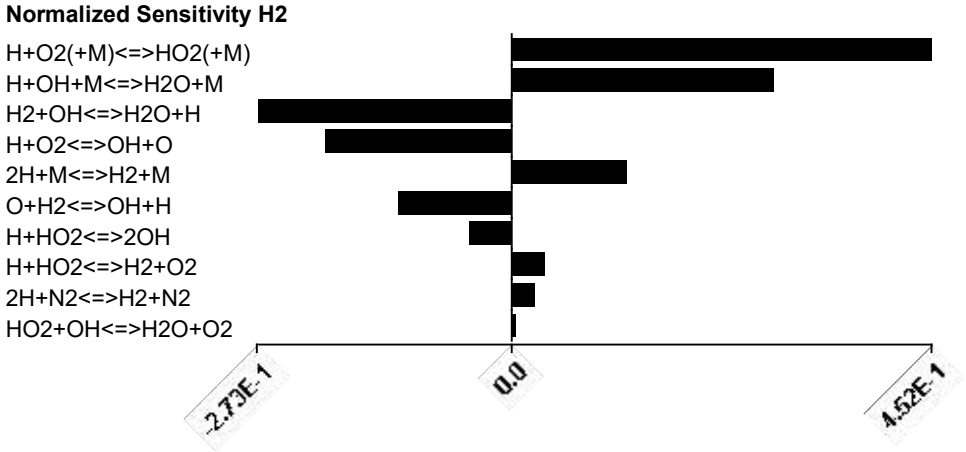


Figure 5.8: Normalized sensitivities of stoichiometric H_2/air flame developed by Reduced Mechanism/K-species reactions at initial condition, 673 K,1 atm.

Table 5.6 shows the production and consumption pathways of H_2 flame. Through sensitivity and pathway analyses of H_2 oxidation reactions developed by different mechanisms, it was discovered that there are two fundamental elementary reactions (H_2+OH<=>H_2O+H and H_2+O<=>OH+H) that serve as the primary pathways for H_2 decomposition. Consequently, the production of H, O, and OH plays a crucial role in the

decomposition of H_2 both before and after the development of the mechanisms. This indicates that reactions involving K-containing species can be integrated into reliable mechanisms that are not currently included in the Chemkin library. Such integration can facilitate the investigation of the impact of K-containing species reactions on various types of flames. Developing Mechanism Generation reactions Consumption reactions

Table 5.6: Generation and consumption pathway of the oxidation of H_2/air mixtures

Developing Mechanism	**Generation reactions**	**Consumption reactions**
GRI-Mech + K-species reactions	H+HO_2=> O_2 +H_2	OH+ H_2<=>H +H_2O
	2H+H_2O<=>H_2O+H_2	O+H_2<=> H +OH
Reduced Mechanism + K-species reactions	H+H_2O=> O_2 +H_2	OH+ H_2<=> H +H_2O
	2H+M<=>H_2+M	O+H_2<=> H +OH

5.5 Comparison of Simulation Results for the H_2/air Mixture: GRI-Mech vs. GRI-Mech/K-species Mechanisms

In this section, the simulation results for the H_2/air mixture in Case 1 from Chapter 4 will be compared with those in Case 1 from Chapter 5. The primary objective here is to validate the results from Chapter 5 through a direct comparison with the results previously validated in Chapter 4. The GRI-Mech/K-species mechanism will be employed to investigate the impact of K-species on a variety of flame types. Additionally, the reduced mechanism with K-species reactions will serve as a valuable tool for future analyses.

5.5.1 AFT

In this section, AFT of the H_2/air mixture is examined, utilizing both the GRI-Mech mechanism before and after its integration with K-species reactions.

The comparison results indicate a significant agreement in the AFT of the H_2/air mixture when employing the GRI-Mech mechanism, both before and after its combination with K-species reactions. This observation suggests that the introduction of the K-species mechanism does not result in substantial alterations to the adiabatic flame temperature characteristics of the mixture. It highlights the resilience of the adiabatic flame temperature, even with the inclusion of the K-species reaction.

Figure 5.9 illustrates the comparison results for the AFT of the H_2/air mixture when utilizing the GRI-Mech mechanism and the GRI-Mech/K-species mechanism.

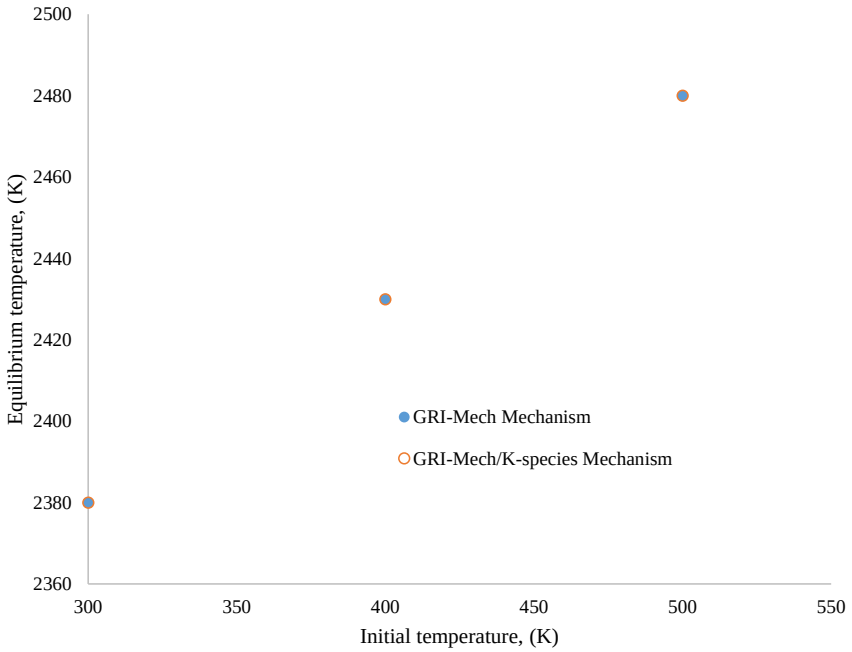


Figure 5.9: AFT of the H_2/air mixture based on the GRI-Mech mechanism and the GRI-Mech/K-species mechanism.

5.5.2 Flame Speed

In this section, the flame speed of H_2 flames developed using both the GRI-Mech mechanism and the GRI-Mech/K-species mechanism will be compared. The analysis aims to evaluate the impact of incorporating the K-species reactions on flame speed characteristics.

Figures 5.10 and 5.11 provide essential visual representations of our analysis. Figure 5.10 presents the temperature profile as a function of the distance above the burner, offering insights into the thermal behaviour of the flames. Meanwhile, Figure 5.11 shows the characteristics of the axial velocity in relation to the distance above the burner.

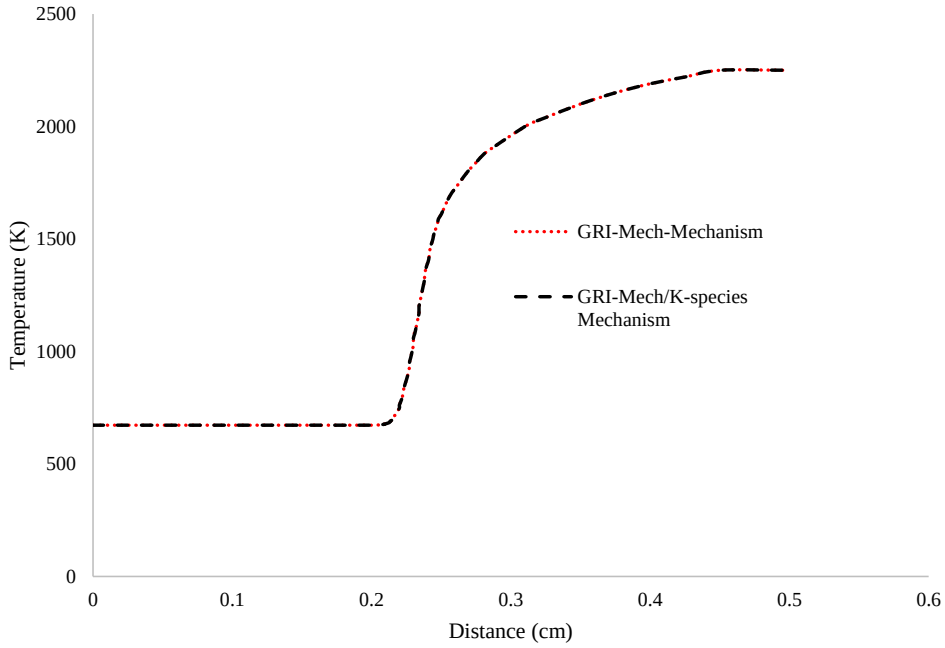


Figure 5.10: The comparison of the gas temperature above burner for the H_2/air flames based GRI-Mech mechanism and GRI-Mech/K-species mechanism at 673 K.

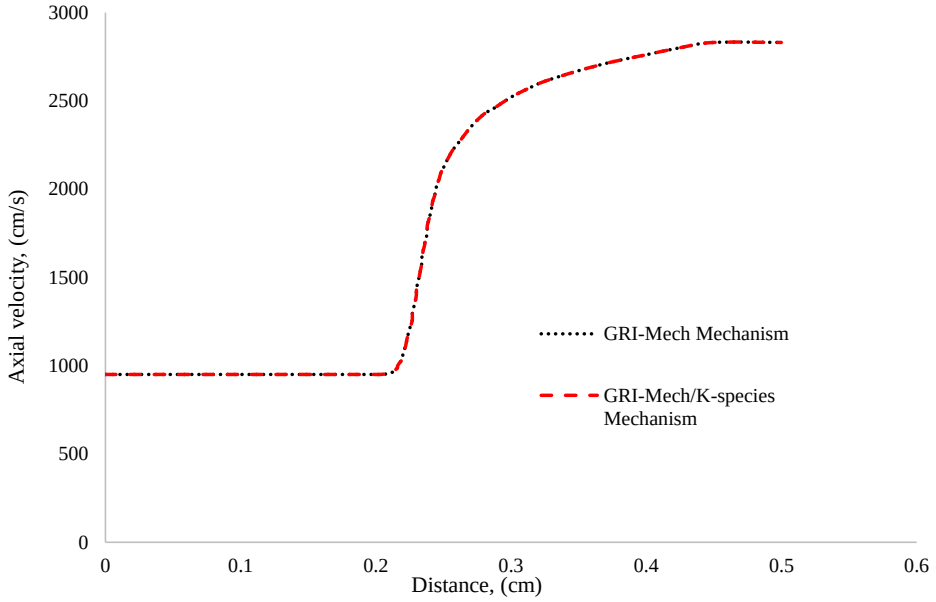


Figure 5.11: The comparison of the axial velocity profile above burner for the H_2/air flames based GRI-Mech mechanism and GRI-Mech/K-species mechanism at 673 K.

Comparison of the laminar burning velocity reveals a high degree of agreement. The flame speed for both the GRI-Mech mechanism and the GRI-Mech/K-species mechanism is calculated at 950 cm/s. This close similarity in flame speed implies that the introduction of K-species reactions into the GRI-Mech mechanism has no observable impact on the laminar burning velocity of H_2 flames. This level of agreement between the two mechanisms establishes confidence in the precision of the combustion models used in the analysis.

5.5.3 Equilibrium Temperature as a function of Equivalence Ratio

The flammability limits within the H_2/air mixture are comparatively analyzed using both the GRI-Mech mechanism and the GRI-Mech/K-species mechanism. The objective is to assess the impact of integrating K-species reactions on these critical boundaries of flammability.

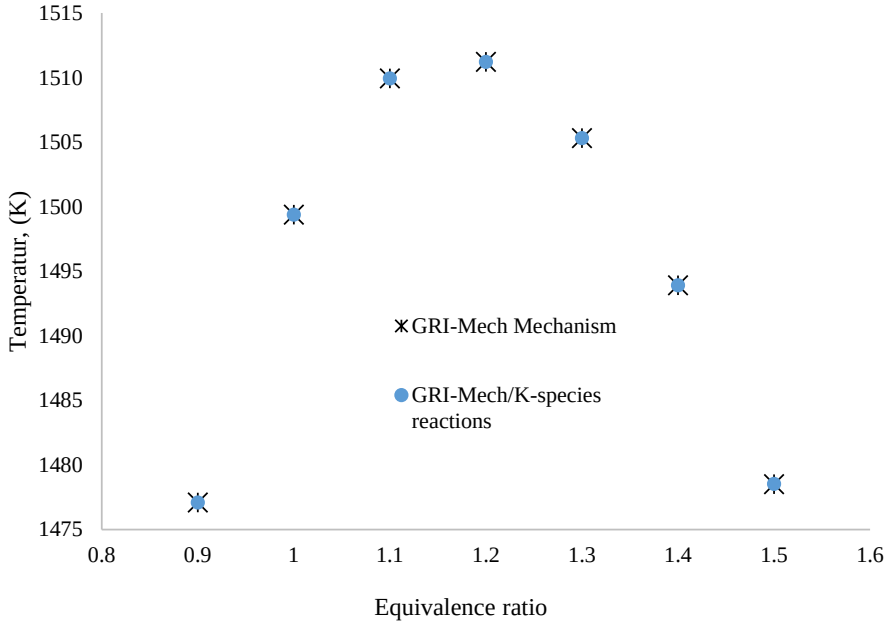


Figure 5.12: The comparison-based equilibrium Temperature as a function of (ϕ) of H_2/air mixture modeled by GRI-Mech mechanism and GRI-Mech/K-species mechanism.

Table 5.12 illustrates how the temperature reaches its peak at fuel/air equivalence ratios of approximately 1.2 in both cases, indicating that the highest temperatures are observed under conditions rich in the mixture of H_2 / air.

Table 5.7: The steady-state temperatures for the combusting H_2/air mixture modelled by GRI-Mech mechanism and GRI- Mech/K-species mechanism.

Equivelance Ratio, ϕ	**Temperature Based GRI-Mech Mechanism, K**	**Temperature Based GRI-Mech/K-species Mechanism, K**
0.9	1477	1477
1	1499	1499
1.1	1509	1509
1.2	1511	1511
1.3	1505	1505
1.4	1494	1494
1.5	1479	1479

5.6 Examining the Potassium-Species Mechanism

Testing has been conducted on K-containing compounds to ensure the proper functioning of the potassium species integrated into gas-phase chemical kinetic mechanisms, such as the GRI-Mech mechanism. This testing validates the readiness of the merged mechanisms for the study of the effects of K-species on flames.

5.6.1 Potassium Oxidation

To simulate the behavior of a potassium (K) oxidation, certain assumptions are made to calculate the mole fractions of K, O_2, and N_2. These assumptions are based on the information presented in Chapter 3. Specifically, the volume of the fire area is considered to be 0.3 m³, which is equivalent to 300 liters. The weight of the fireless unit is 75 grams. The number of moles of air in 300 liters is calculated using the ideal gas law, which is defined as:

$$\text{Moles of air} = \frac{\text{Volume of air (in liters)}}{22.4}$$

The value of 22.4 liters/mol is derived from the ideal gas law and represents the volume occupied by one mol of an ideal gas at standard temperature and pressure (STP).
STP is defined as having a standard pressure (P): 1 atmosphere (atm) and a standard temperature (T): 273.15 K.
When there is 1 mol of an ideal gas at STP ($n = 1$ mol), the ideal gas law as shown in equation 5.2 is rearranged to calculate the volume (V) as follows:

$$PV = nRT \tag{5.2}$$

$$V = \frac{nRT}{P} = \frac{(1\,\text{mol}) \cdot (0.0821\,\text{L atm / K mol}) \cdot (273.15\,\text{K})}{1\,\text{atm}} \approx 22.4\,\text{liters/mol}$$

where:
The ideal gas law, , relates the pressure (P), volume (V), number of moles (n), ideal gas constant (R), and temperature (T) of a gas. With 300 liters of air, the number of moles of air can be calculated as:

$$\text{Moles of air} = \frac{300\,\text{L}}{22.4\,\text{L/mol}} \approx 13.39\,\text{moles of air}$$

There is approximately 13.39 mole of air in 300 liters, recalculate the mole of O_2 and N_2 based on this information:

Mole of O_2 in 300 litres of air:

$$\text{Mole of } O_2 = \text{Mole of air} \times \frac{\text{Percentage of } O_2 \text{ in air}}{100}$$

$$\text{Mole of } O_2 = 13.39\,\text{mol} \times \frac{21}{100} \approx 2.814\,\text{mole of } O_2$$

Mole of N_2 in 300 litres of air:

$$\text{Mole of } N_2 = \text{Mole of air} \times \frac{\text{Percentage of } N_2 \text{ in air}}{100}$$

$$\text{Mole of } N_2 = 13.39\,\text{mole} \times \frac{79}{100} \approx 10.58\,\text{moles of } N_2$$

So, with 300 liters of air containing 21% O_2 and 79% N_2, you have approximately 2.814 mole of O_2 and approximately 10.58 mole of N_2.

To calculate the number of mole of K, based on the mass of fireless unit 75 grams, and the molar mass of K, which is approximately 39.10 g/mol:

$$\text{Number of mole of K} = \frac{\text{Mass of K}}{\text{Molar mass of K}} \tag{5.4}$$

$$\text{Number of mole of K} = \frac{75\,\text{grams}}{39.10\,\text{g/mol}} \approx 1.918\,\text{mole of K}$$

Simulations Condition

The stoichiometric reaction of potassium (K) in air is represented as follows:

$$K + O_2 + N_2 \longrightarrow K_iO_j + N_2$$

Here, K_iO_j may take the form of KO, KO_2, K_2O, or K_2O_2 or other possible products. From the stoichiometric equation, the mole fractions of the reactants as calculated by Chemkin are as shown in Table 5.8

Table 5.8: The reactants mole fractions of K/air mixture

Reactants	**Mole Fraction**
K	0.12526
O_2	0.18378
N_2	0.69096

The mole fractions of the reactants can also be calculated manually using the provided moles for each species. Given that $K = 1.918$ moles, $O_2 = 2.814$ moles, and $N_2 = 10.58$ moles, using the following formulas to calculate the mole fractions:

$$\text{Total number of moles} = 1.918 + 2.814 + 10.58 = 15.312 \text{ mol}$$

$$\text{Mole Fraction of K} = \frac{\text{number of moles of K}}{\text{total number of moles}} = \frac{1.918}{15.312} \approx 0.12526$$

$$\text{Mole Fraction of } O_2 = \frac{\text{number of moles of } O_2}{\text{total number of moles}} = \frac{2.814}{15.312} \approx 0.18377$$

$$\text{Mole Fraction of } N_2 = \frac{\text{number of moles of } N_2}{\text{total number of moles}} = \frac{10.58}{15.312} \approx 0.69096$$

Table 5.9 provides a comprehensive summary of the simulation conditions employed in the study of stoichiometric K/air mixtures using the K-species Mechanism. These conditions encompass different reactor types, initial temperatures, residence times, mass flow rates, pressures, reaction mechanisms, and more. Each set of conditions serves a unique purpose, from predicting equilibrium temperatures to investigating the evolution of reactants within a reactor. The table outlines essential details such as fuel and oxidiser types, gas compositions, constraints, wall boundaries, and the data required for accurate simulations.

Table 5.9: Summary of Simulation Conditions for Investigating the Stoichiometric K/Air Mixture Using the K-Species Mechanism

		Type of Reactors	
		Equilibrium	Plug Flow
Simulation Conditions	Purpose of the Model	Predict the equilibrium temperature	Investigate the evolution of reactants as they traverse a system and examine the behavior of chemical reactions within a reactor characterized by spatial gradients, enable the monitoring of reaction behavior and product formation under the given conditions.
	Initial Temperature,K	300	300
	Residence Time,sec Mass Flow Rate,g/s	N/A N/A	N/A 1
	Pressure, atm	1	1
	Reaction Mechanism	K-Species reactions Mechanism	K-Species reactions Mechanism
	Fuel Type	K	K
	Oxidizer Type	air (O_2, N_2)	air (O_2, N_2)
	Gas Compositions(Mol)	K=1.918 O_2=2.814 N_2=10.58	K=1.918 O_2=2.814 N_2=10.58
	Constraints and Assumptions	The reactor is defined at constant pressure and enthalpy. The equilibrium of species composition is calculated	Solve gas energy equation is chosen as a definition of the model problem. Solve the momentum equations to determine the velocity as a function of distance. Set the starting point or axial positions of the gas inlet as 0 cm. Ending axial positions for the reactor simulation as 5cm. The diameter of the reactor channel is assumed 5.8431 cm, surface temperature is assumed to be the same as the initial temperature.
	Wall Boundary	Adiabatic	Adiabatic
	Data Required	Gas-phase Kinetic reactions. Thermodynamic data.	Gas-phase Kinetic reactions. Thermodynamic data. Transport data.

*In the simulation runs, reactor diameters ranging from 1 cm to 7.2 cm were tested, and variations within this range were observed to not produce significant changes in the simulation results. Notably, with reactor diameters smaller than 5 cm, the conversion of K into KO_2 required a longer time compared to diameters larger than 5cm .

5.6.2 Determine The Equilibrium Temperature of Potassium Oxidation

Figure 5.13 illustrates the equilibrium temperature for the reaction of potassium oxidiser (K) in the air as 1467 K. It represents the temperature at which the chemical reaction between potassium and oxygen reaches a state of thermodynamic equilibrium. In other words, it's the temperature at which the rates of the forward and reverse reactions of the oxidation process are equal, resulting in no net change in the concentrations of the reactants and products.

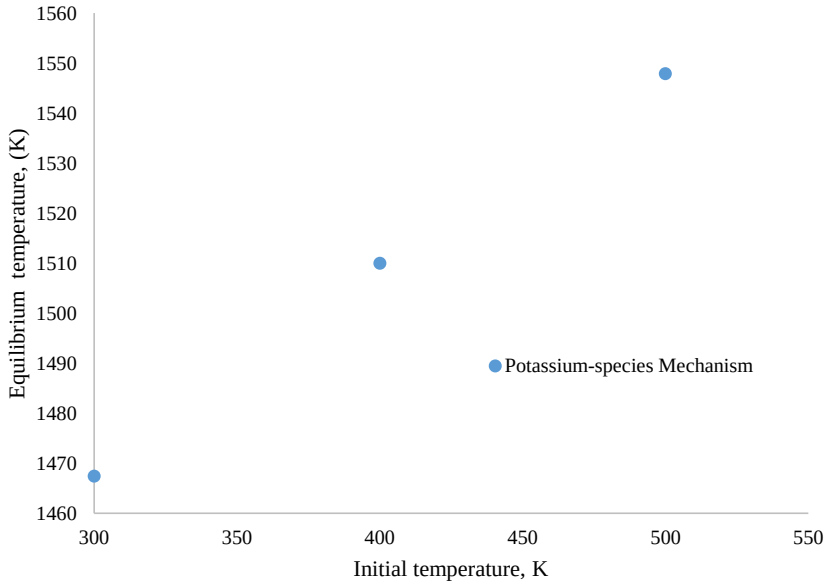


Figure 5.13: Equilibrium temperature for potassium oxidiser in the air at 300 K, 1 atm.

5.6.3 Pathway Analysis for Potassium Oxidation

In sensitivity analysis, negative sensitivity values in a reaction indicate that the reaction is consuming the species associated with the negative sensitivity. This can be interpreted as a decrease in the concentration of that species. On the other hand, positive sensitivity values in a reaction indicate that the reaction is generating the species associated with the positive sensitivity, leading to an increase in the concentration of that species. Figure 5.14 illustrates that in the analysed K/air mixture, K is predominantly consumed through the reaction $K+O_2=KO_2$.



Figure 5.14: Normalized sensitivity analysis for K/air mixture.

At temperatures higher than 1480K, additional K-species will appear, as shown in 5.15. It is evident that KO_2 is generated by two reactions. KO+O = KO_2 and 2KO= KO_2+K



Figure 5.15: Normalized sensitivity analysis for K/air mixture at 1484 K.

5.6.4 Distributions of Mole Fraction of Species in K/air Mixture

The mole fraction of a species in a mixture measures its concentration relative to the total number of moles present. Examining the distributions of mole fractions allows for assessing how different species are distributed throughout the mixture.

Mole Fraction of K vs. Distance

In Figure 5.16, the mole fraction of K is analysed concerning its distribution with distance within the reactor. At the beginning (Distance = 0 cm), the mole fraction of K is 0.1252612, indicating a relatively high potassium concentration at the source. The focus is on a specific region to emphasize potassium consumption. Progressing through the reactor, it becomes evident that potassium gradually depletes, indicating its active involvement in the ongoing chemical reactions. This decrease underscores the transformation of potassium into various reaction products.

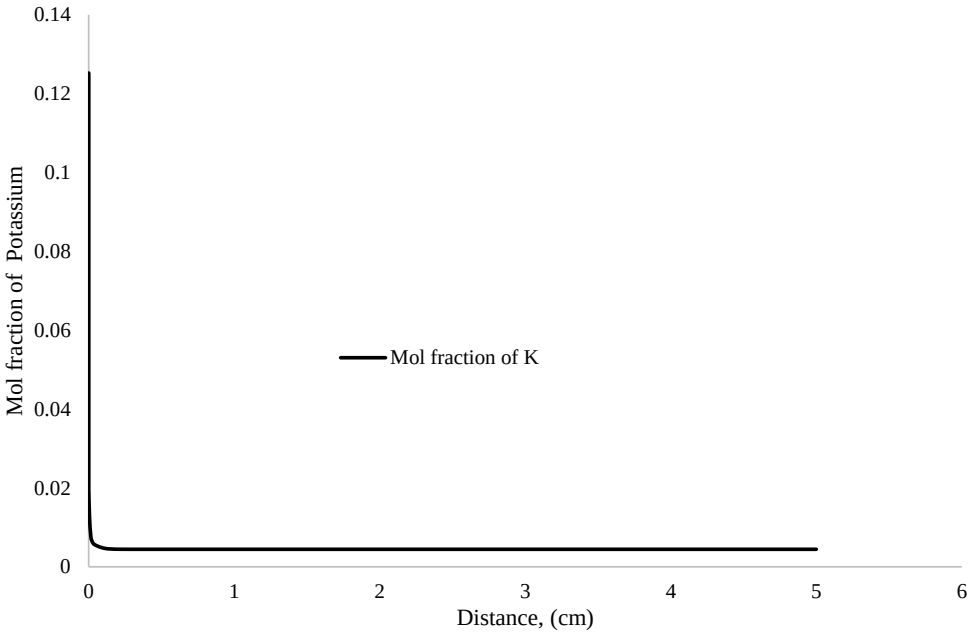


Figure 5.16: Analysis of potassium mole fraction K with respect to distance within the reactor.

Figure 5.17 is a zoomed-in view of a specific region, allowing for a detailed examination of how potassium reduces as it progresses through the reactor. The localized perspective offered by this zoomed-in area provides a clear into the extent of potassium consumption in this particular section of the reactor.

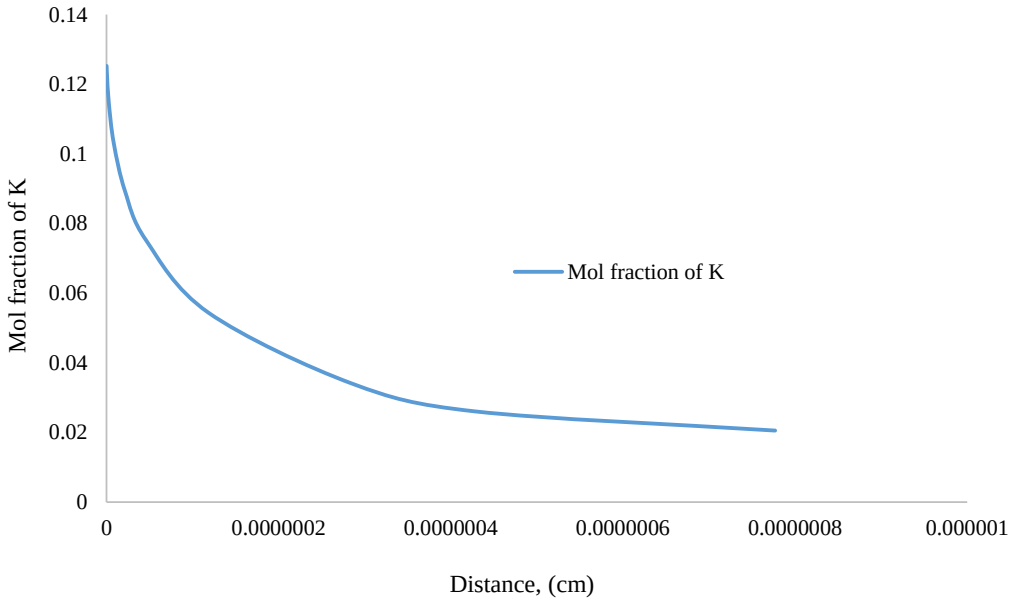


Figure 5.17: Zoomed-in analysis of the mole fraction of K as a function of distance within the reactor.

Mole Fraction of KO_2 vs. Distance

Figure 5.18 illustrates how the mole fraction of KO_2 changes with distance within the reactor. It provides the distribution and concentration of KO_2 and how it evolves as the reaction progresses. The figure demonstrates that the mole fraction stabilizes beyond a certain point, suggesting a dynamic equilibrium between KO_2 generation and consumption.

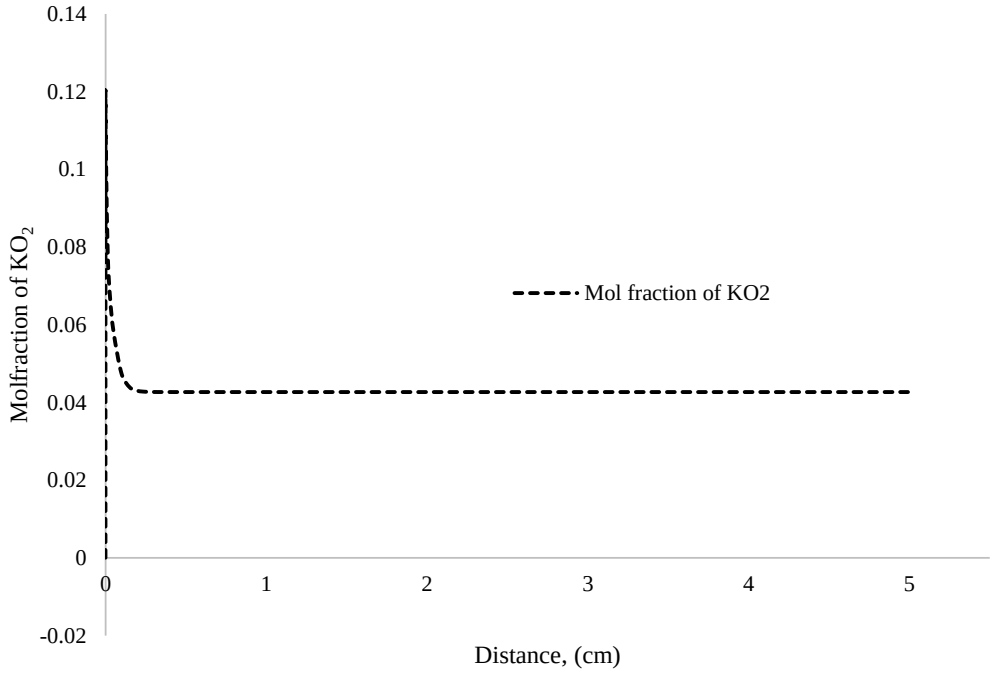


Figure 5.18: Analysis of KO_2 mole fraction with respect to distance within the reactor.

In Figure 5.19, a zoomed-in view of a specific region enables a detailed examination of how KO_2 increases through the reactor. This closer look at the localized area offers a clear view of the extent of KO_2 generation within this particular section of the reactor.

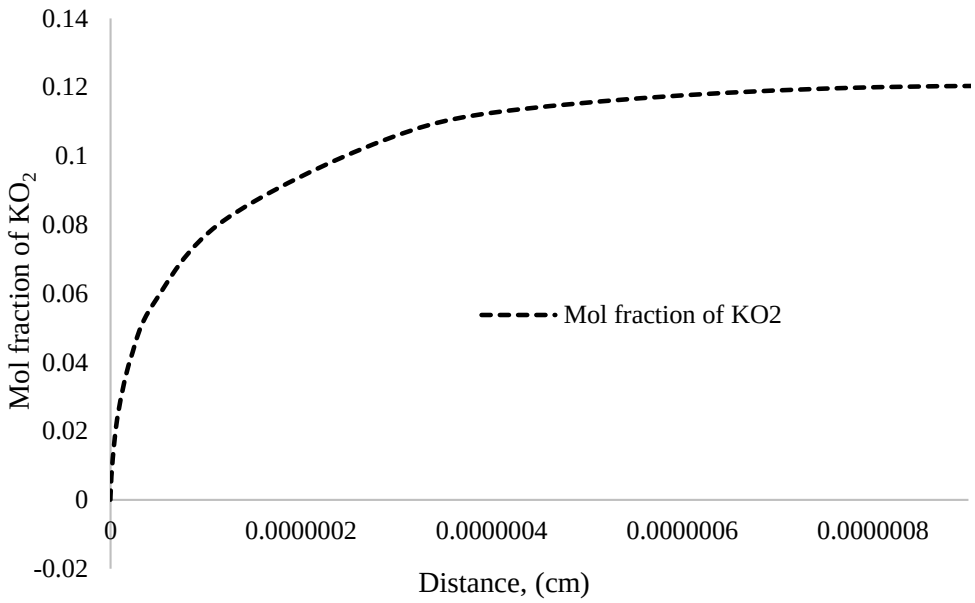


Figure 5.19: Zoomed-in analysis of the mole fraction of KO_2 as a function of distance within the reactor.

At the start (Distance = 0 cm), the mole fraction of KO_2 is 0, indicating that there is no KO_2 present at the source. As the reaction progresses, the mole fraction of KO_2 increases. This suggests that KO_2 is being generated or becoming more concentrated as moving away from the source. Beyond a certain distance, the mole fraction of KO_2 appears to reach a steady state, where it remains relatively constant. This suggests that a dynamic equilibrium is established, where KO_2 generation is balanced by consumption or other reactions. Moreover, In the data, from Distance = 1.88075E-06 cm to Distance = 3.17586E-06 cm, the mole fraction of KO_2 remains almost constant, indicating that the reaction dynamics in this range are relatively stable.

5.7 Summary

- The development of reaction mechanisms, such as GRI-Mech/K-species and Reduced/K-species mechanisms, typically starts at an initial temperature of 337°C.
- Combining kinetic mechanisms with K-species reactions has been tested to study the inhibitory effect of potassium species on flames.
- The adiabatic flame temperature for stoichiometric H_2 flame using the GRI-Mech/K-species and Reduced Mechanism/K-species mechanisms is 2380 K.
- The laminar flame speed for the stoichiometric H_2 flame, developed with the GRI-Mech/K-species reactions at 673 K and 1 atm, is 950 cm/s, which aligns with the laminar burning velocity modelled by the GRI-Mech mechanism at 673 K.
- The flame speed for the stoichiometric H_2 flame, developed with the Reduced Mech/K-species reactions at 673 K and 1 atm, is 968 cm/s. At the same temperature, the flame speed for the stoichiometric H_2 flame developed with the Reduced Mech mechanism is 972 cm/s.
- The primary consumption of H_2 occurs through reactions like H_2+OH<=>H_2O+H and H_2+O<=>OH+H, based on the GRI-Mech/K-species mechanism or Reduced/K-species mechanism.
- The K-species reaction mechanism has been tested, and KO_2 has been identified as the main product based on the numerical simulations.
- Simulations of H_2 combustion kinetics can be conducted using both GRI-Mech 3.0 and Reduced reaction mechanisms. GRI-Mech is preferred for recent simulations, providing more detailed information on hydrocarbon combustion.
- A reduced mechanism that includes potassium species reactions has been developed, combined, and validated for future simulations. These simulations aim to investigate the inhibitory effects of potassium species on flames using commercial computational fluid dynamics (CFD) software, allowing for the simulation of fluid flow, heat transfer, and chemical reactions in fires.
- The gas-phase kinetic model is prepared for studying potassium species' effects on different flames. The GRI-Mech/K-species mechanism will be employed in the subsequent chapters to analyse the kinetic effects of KO_2, $KHCO_3$, and KCO_3 in detail.

Chapter 6

Kinetic Study of the Effect of KO_2, $KHCO_3$, and KCO_3 on Hydrogen Flames

In this chapter, simulations present the speed of the flame and the reduction of the OH mole fraction in H_2 flames with the introduction of KO_2, $KHCO_3$ or KCO_3 molE fractions at various equivalence ratios. The observed changes in flame speed and OH reduction reveal the suppressive effects of these potassium species on H_2 flames, aiding in the identification of the most effective agent. Systematic investigations are conducted on the selected agent to study its impact on flame speed in a wide range of equivalence ratios and to elucidate pathway reactions in H_2/air oxidation under specific conditions.

6.1 Flame speed, (S_L) Modelling Method

To investigate the impact of KO_2, $KHCO_3$, and KCO_3 on a H_2/air mixture, a one-dimensional flame speed calculation model in Chemkin has been employed. This configuration is utilised to determine the burning velocity characteristics of a specific gaseous mixture under predefined pressure and input temperature conditions. It should be noted that this modelling approach does not account for heat losses. Essential input parameters include the gas-phase reaction mechanism, thermodynamic data, and transport properties. The simulation was conducted using the GRI-Mech mechanism, which was integrated with the reactions of K-species. Thermal expansion was not considered in the simulation, so the pressure was constant throughout the calculation, and an unburned gas temperature was set as 673 K. In addition to the parameters mentioned above, a mass flow rate of 1 g/cm²·s was specified for the gaseous mixture incoming. Chapter 4 mentions that the exact mass flow rate is typically determined as part of the flame speed solution. By assuming a fixed mass flow rate during flame speed calculations, the freely propagating flame's position remains constant. The calculation of S_L was conducted at three distinct equivalence ratios, each representing different fuel/air mixtures (0.9, 1, and 1.1). These varying equivalence ratios were chosen to provide valuable insights into the influence of KO_2, $KHCO_3$, and KCO_3 on flame characteristics.

The composition of the reactants was explicitly defined as part of the input data before initiating the model. However, it is important to mention that the expected composition of the products and intermediate fractions was not integrated into the model. For reference,

details of the reactant composition were provided in the input data as in Table 6.1. In the context of this air composition approximation, the balanced chemical equation is represented as follows:

$$2H_2 + O_2 + 3.76N_2 \rightarrow 2H_2O + 3.76N_2$$

Table 6.1: The reactants mole of H_2/air mixture

Reactants	Number of Mole
H_2	2
O_2	1
N_2	3.76

The utilisation of 3.76 moles of N_2, in the reaction equation, is associated with consideration of the composition of the air. When modeling chemical reactions involving air, a typical approach is to approximate dry air as a mixture of 79% N_2 and 21% O_2 by volume. This composition simplifies the representation of air in chemical reactions, allowing for more straightforward modelling and stoichiometry.

6.1.1 Determining Mole Fractions of H_2, O_2 and N_2 in the Presence of K-species at (ϕ), (0.9, 1, 1.1)

The simulations aimed to calculate the mole fractions of H_2, O_2, and N_2 in a chemical reaction involving H_2/air with the addition of K-species in different equivalence ratios. The calculations were based on the chemical reaction:

$$2H_2 + O_2 + 3.76N_2 + z\mathrm{KO}_2 \rightarrow 2H_2O + 3.76N_2 \tag{6.1}$$

Stoichiometric Mixture

To calculate the mole fraction of H_2 in the mixture, the following formula was used:

$$\text{Mole Fraction (X)} = \frac{\text{Moles of the component}}{\text{Total moles in the mixture}} \tag{6.2}$$

For stoichiometric H_2 or O_2 or N_2 , the mole fraction was determined as follows:

$$X = \frac{x}{2 + 1 + 3.76} \tag{6.3}$$

Where: x is the number of moles of H_2 or O_2 or N_2 or KO_2 based on the Equation 6.1.

Lean Mixture

In a lean mixture ($(\phi < 1)$), where there's an excess of air, calculating the mole fraction as follows:

$$X = \frac{x}{2 + 1.1(1 + 3.76)} \tag{6.4}$$

Rich Mixture

In a rich mixture ($(\phi > 1)$), where there's an excess of fuel, you can calculate the mole fraction as follows:

$$X = \frac{x}{2 + 0.9(1 + 3.76)} \tag{6.5}$$

These equations allow calculating the mole fraction (X) of species (e.g., H_2, O_2, or N_2) in the mixture for stoichiometric, lean, and rich mixture conditions based on the (ϕ) and the stoichiometry of the reaction. On the other hand, the mole fraction of unreacted KO_2, $KHCO_3$, or KCO_3 in the mixture was assumed and specified as shown in Table 6.3.

Table 6.2 provides the calculated mole fractions of H_2, O_2, or N_2 at various (ϕ).

This table serves as an illustration of the initial conditions used for the simulation, demonstrating how the mole fractions of the reactants change with variations in the equivalence ratio.

Table 6.2: Mole fractions of H_2, O_2, or N_2 at various (ϕ)

(ϕ)	H_2 Mole Fraction	O_2 Mole Fraction	N_2 Mole Fraction
0.9	2.7439×10^{-1}	1.5244×10^{-1}	5.7316×10^{-1}
1	2.9585×10^{-1}	1.4793×10^{-1}	5.5620×10^{-1}
1.1	3.1609×10^{-1}	1.4367×10^{-1}	5.4021×10^{-1}

6.1.2 Mole Fractions of KO_2, $KHCO_3$, and KCO_3 Tested

Table 6.3 presents the initial moles assumed for calculating the mole fractions of KO_2, $KHCO_3$, and KCO_3 using Equation 6.2 for stoichiometric mixture based on the chemical reaction 6.1. These mole fractions were tested and employed for simulation at various equivalence ratios.

It is essential to note that, for this study, the mol fractions of KO_2, $KHCO_3$, and KCO_3 were maintained at constant values across different equivalence ratios. By ensuring a consistent presence of these potassium species, this approach enables a focused investigation of their influence on flame properties under varying conditions. This guarantees that the variable under examination is the presence of these species rather than their concentrations fluctuating with changes in equivalence ratios.

Table 6.3: The number of moles of KO_2, $KHCO_3$, and KCO_3 assumed for calculating the mole fractions at stoichiometric H_2/air mixture

Number of Mole Assumed	Mole Fraction Calculation
0	0
0.0001	1.47×10^{-5}
0.0002	2.95×10^{-5}
0.0003	4.43×10^{-5}
0.0004	5.91×10^{-5}
0.0005	7.30×10^{-5}
0.0006	8.87×10^{-5}
0.0007	1.03×10^{-4}
0.0008	1.18×10^{-4}
0.0009	1.33×10^{-4}
0.001	1.47×10^{-3}
0.002	2.96×10^{-4}
0.003	4.44×10^{-4}
0.004	5.91×10^{-4}
0.005	7.00×10^{-4}
0.006	8.87×10^{-4}
0.007	1.03×10^{-3}
0.008	1.18×10^{-3}
0.009	1.33×10^{-3}
0.01	1.47×10^{-3}
0.02	2.95×10^{-3}
0.03	4.40×10^{-3}
0.04	5.88×10^{-3}
0.05	7.30×10^{-3}
0.06	8.79×10^{-3}
0.07	1.02×10^{-2}
0.08	1.2×10^{-2}
0.09	1.3×10^{-2}
0.1	1.45×10^{-2}
0.2	2.87×10^{-2}
0.3	4.25×10^{-2}
0.4	5.58×10^{-2}
0.5	6.88×10^{-2}
0.6	8.15×10^{-2}
0.7	9.4×10^{-2}

Tables 6.5, 6.6, and 6.7 show the valid mole fractions for potassium species KO_2, $KHCO_3$ and KCO_3 that are required for the model to run successfully in Chemkin.

6.1.3 Summary of Simulation Conditions

The one-dimensional flame speed reactor was selected as the primary tool to investigate the impact of selected potassium species on H_2 flame behaviour.

The utilisation of this reactor model serves several key purposes. primarily allowing the calculation of flame speed under various equivalence ratios (ϕ). This model also facilitates the study of the influence of the K species on the reduction of OH. Furthermore, the one-dimensional flame speed reactor aids in estimating and discussing the reaction pathways within the H_2/air mixture.

Table 6.4 summarises the simulation conditions used to investigate the behaviour of the H_2/air mixture with added mole fractions of KO_2, $KHCO_3$, or KCO_3.

Table 6.4: Simulation conditions used to study the Effect of KO_2, $KHCO_3$, and KCO_3 Mole fractions on H_2/air mixture

Simulation Conditions	
Model	One-dimensional Flame Speed Reactor
Unburnt Gas Temperature, K	673
Initial Gas Temperature Profile, K	The temperature profile was automatically estimated from equilibrium
Initial Gas Temperature, K	298
Mass Flow Rate, (g/cm²·s)	1
Pressure, atm	1
Reaction Mechanism	GRI-Mech 3.0/K-species Mechanism
Equivalence Ratio, (ϕ)	0.9, 1, 1.1
Fuel Type	H_2
Oxidiser Type	air (O_2, N_2)
Added Species	KO_2 or $KHCO_3$ or KCO_3
Gas Compositions	H_2=2, O_2=1, N_2=3.76
Constraints and Assumptions	Constant pressure, Heat loss and thermal expansion = 0, Gas reaction rate multiplier = 1, The starting axial position of 0 cm, Ending axial position = 0.5cm, the basic tolerance parameters, and advanced controls for the solution are Assigned, Number of uniform grid points =6. No continuations were defined.
Wall Boundary	Adiabatic
Data Required	Gas-phase kinetic, Thermodynamic data, Transport data

6.2 KO_2 Inhibition Effect on the S_L and OH Mole Fraction of H_2 Flame

At different equivalence ratios, the model allows inserting one of the suggested tested K-species with various mole fractions. The change of the flame S_L with equivalence ratio is considered in the simulations.

Figure 6.1 below contains data for the variation of S_L of a H_2/air mixture with the mole fraction of KO_2. The S_L of H_2 in lean, stoichiometric, and rich mixtures was measured in different mole fractions of KO_2.

From Figure 6.1, it can be observed that the laminar flame speed of H_2 decreases as the mole fraction of KO_2 increases. This decrease in S_L is significant at lower KO_2

mole fractions, whereas at higher mole fractions, the flame speed reduction becomes less significant.

Figure 6.2 magnified the range of mole fractions between 0 and 0.001 mole fraction of KO_2 to illustrate the decrease in the flame speed of the H_2 flame, corresponding to the conditions of the [lean/stoichiometric/rich] mixture. This focused examination allows for a detailed analysis of the relationship between the mole fraction of KO_2 and the burning velocity of H_2 flame within the specific concentration range. The decrease in flame speed observed in this range is of particular significance. Indicates a notable impact of KO_2 concentration on the combustion process.

The decrease in S_L is more significant in lean mixtures compared to rich and stoichiometric mixtures.

Table 6.5 shows the simulation results of the flame speed for H_2 flame, indicating the effect of each mole fraction of KO_2 in different equivalence ratios.

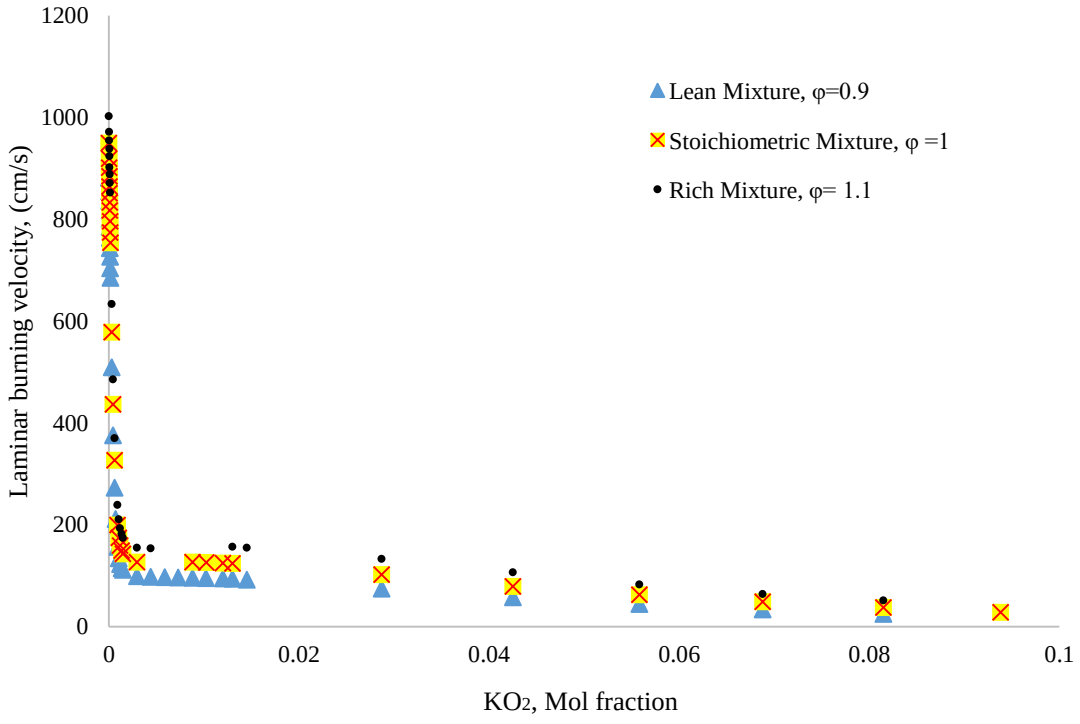


Figure 6.1: The inhibition effect of KO_2 on the laminar burning velocity of H_2/air as a function of the equivalence ratio (initial conditions: 673 K, 1 atm, lean, stoichiometric and rich mixtures,ϕ = 0.9, 1.0, and 1.1).

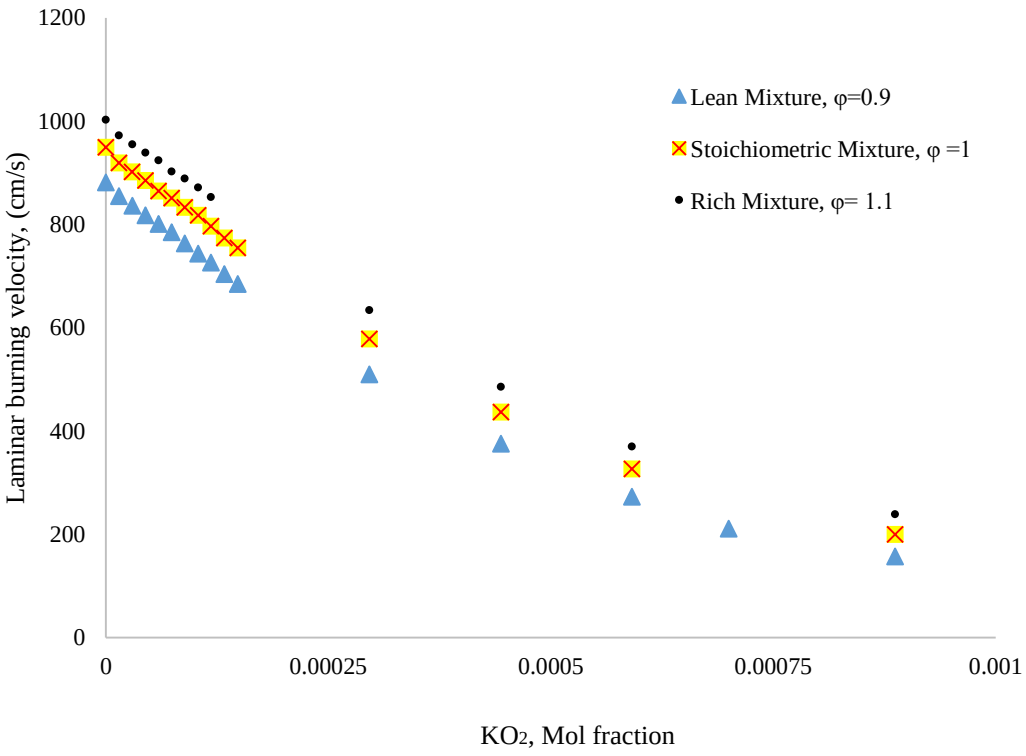


Figure 6.2: Zoomed-out view illustrating the inhibition effect of KO_2 on the laminar burning velocity of H_2/air as a function of equivalence ratio.

Table 6.5: The Inhibition Effect of KO_2 on the Laminar Burning Velocity of H_2 /air Flame

KO_2 Mole fraction	S_L (cm/s) at ϕ =(0.9)	KO_2 Mole fraction	S_L (cm/s) at ϕ = (1)	KO_2 Mole fraction	S_L (cm/s) at ϕ=(1.1)
0.00	881	0.00	950	0.00	1002
1.47×10^{-5}	855	1.47×10^{-5}	919	1.47×10^{-5}	972
2.95×10^{-5}	836	2.95×10^{-5}	902	2.95×10^{-5}	955
4.43×10^{-5}	818	4.43×10^{-5}	885	4.43×10^{-5}	939
5.91×10^{-5}	801	5.91681×10^{-5}	865	5.91×10^{-5}	924
7.30×10^{-5}	785	7.30×10^{-5}	851	7.30×10^{-5}	902
8.87×10^{-5}	763	8.87×10^{-5}	833	8.87×10^{-5}	889
1.03×10^{-4}	744	1.0×10^{-4}	818	1.03×10^{-4}	871
1.18×10^{-4}	726	1.18×10^{-4}	796	1.18×10^{-4}	853
1.33×10^{-4}	704	1.33×10^{-4}	774	2.96×10^{-4}	634
1.48×10^{-4}	685	1.48×10^{-4}	754	4.44×10^{-4}	485
2.96×10^{-4}	510	2.96×10^{-4}	578	5.91×10^{-4}	370
4.44×10^{-4}	376	4.44×10^{-4}	437	8.87×10^{-4}	239
5.91×10^{-4}	273	5.91×10^{-4}	327	1.03×10^{-3}	211
7.00×10^{-4}	211	8.87×10^{-4}	200	1.18×10^{-3}	193
8.87×10^{-4}	157	1.03×10^{-3}	175	1.33×10^{-3}	182
1.03×10^{-3}	134	1.18×10^{-3}	160	1.47×10^{-3}	175
1.18×10^{-3}	123	1.33×10^{-3}	149	2.95×10^{-3}	155
1.33×10^{-3}	115	1.47×10^{-3}	143	4.40×10^{-3}	154
1.47×10^{-3}	111	2.95×10^{-3}	127	1.3×10^{-2}	157
2.95×10^{-3}	99	8.79×10^{-3}	127	1.45×10^{-2}	155
4.40×10^{-3}	98	1.02×10^{-2}	126	2.87×10^{-2}	133
4.40×10^{-3}	98	1.2×10^{-2}	125	4.25×10^{-2}	107
5.88×10^{-3}	97	1.3×10^{-2}	124	5.58×10^{-2}	83
7.30×10^{-3}	97	1.45×10^{-2}	123	6.88×10^{-2}	64
8.79×10^{-3}	96	2.87×10^{-2}	102	8.15×10^{-2}	52
1.02×10^{-2}	95	4.25×10^{-2}	79	9.4×10^{-2}	40
1.2×10^{-2}	95	5.58×10^{-2}	63		
1.3×10^{-2}	94	6.88×10^{-2}	49		
1.45×10^{-2}	92	8.15×10^{-2}	37		
2.87×10^{-2}	74	9.4×10^{-2}	28		
4.25×10^{-2}	58				
5.58×10^{-2}	45				
6.88×10^{-2}	34				
8.15×10^{-2}	25				

The species pathway analysis demonstrated that H, O atoms, and OH radicals play a significant role in the decomposition of H_2. To interrupt the chain reactions by absorbing free radicals, it is necessary to remove the OH radicals from the reaction zone in the flame. Figures 6.3, 6.4, and 6.5 show the hydroxyl radical profiles in H_2/air lean, stoichiometric, and rich flame at various KO_2 mol fractions. As the figures indicate, a KO_2 mole fraction of approximately 0.05% eliminates radical overshoot, and the maximum hydroxyl concentration reaches the flame equilibrium concentration. Adding more concentrations of the agent reduces the equilibrium concentration and, consequently, the equilibrium temperature.

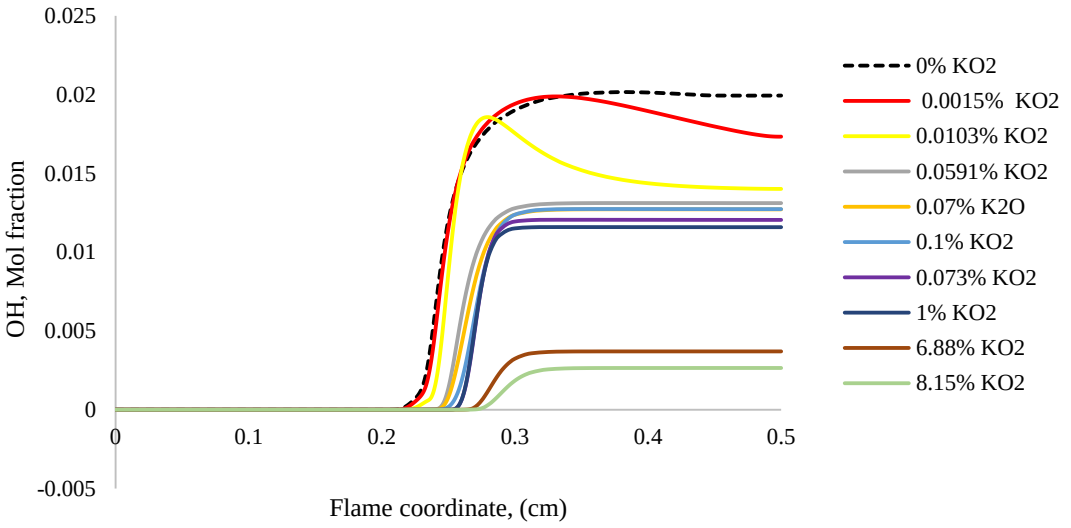


Figure 6.3: Flame concentration profiles of hydroxyl radical at different inhibitor mole fraction of KO_2 loadings (lean H_2/air flame, initial conditions, (673 K,1 atm)).

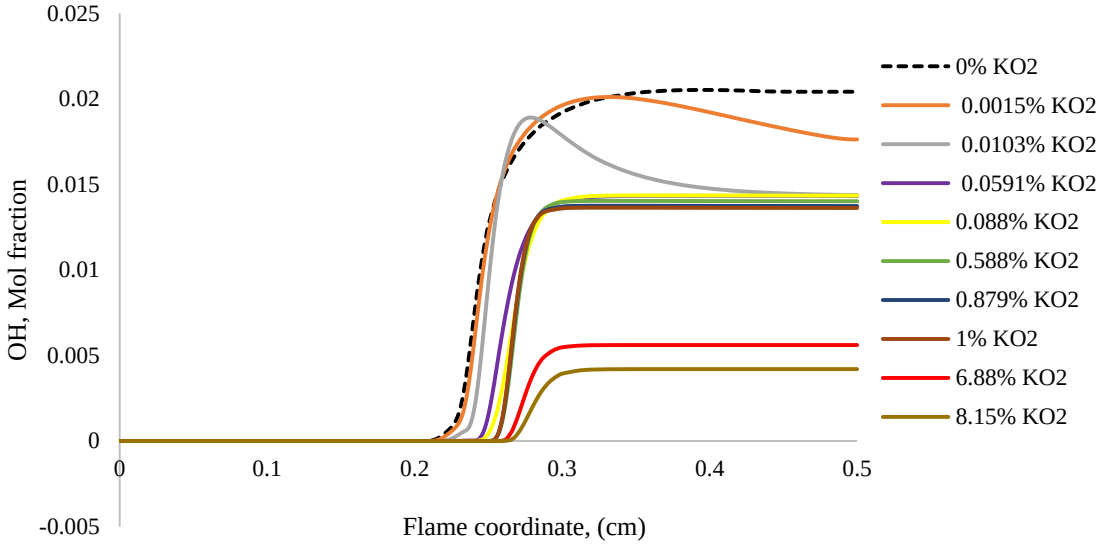


Figure 6.4: Flame concentration profiles of hydroxyl radical at different inhibitor mol fraction of KO_2 loadings (stoichiometric H_2/air flame, initial conditions: (673 K,1 atm)).

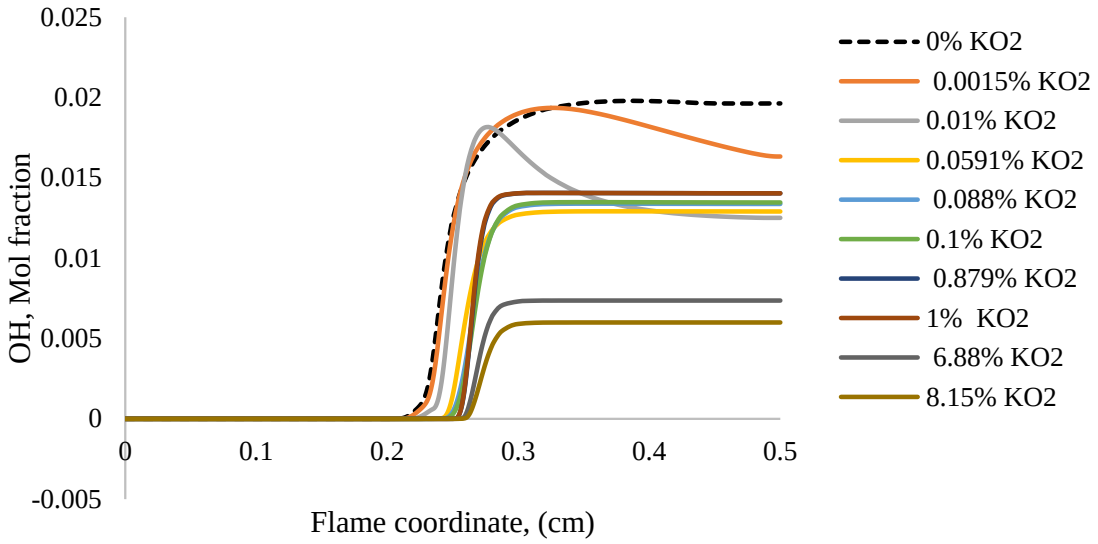


Figure 6.5: Flame concentration profiles of hydroxyl radical at different inhibitor mole fraction of KO_2 loadings (rich H_2/air flame, initial conditions, (673 K, 1 atm)).

6.3 $KHCO_3$ Inhibition Effect on the S_L and OH Mole Fraction

Figure 6.6 shows the flame speed of H_2 flame affected by various mole fractions of $KHCO_3$ at (0.9, 1, 1.1) equivalence ratio. Using an 8% mol fraction of $KHCO_3$ led to reducing the S_L at the lean mixture from 881 to 182 cm/s, and at a rich mixture from 1002 to 217cm/s. The reduction in burning velocity is more pronounced in lean mixtures compared to stoichiometric and rich mixtures, indicating that the addition of $KHCO_3$ has a more significant impact on the combustion of lean mixtures. Overall, Figure 6.6 suggests that the addition of $KHCO_3$ can be an effective way to control the burning velocity of H_2 in different mixtures and Table 6.6 shows the simulation results of flame speed of H_2 affected by $KHCO_3$ mole fractions at various equivalence ratios.

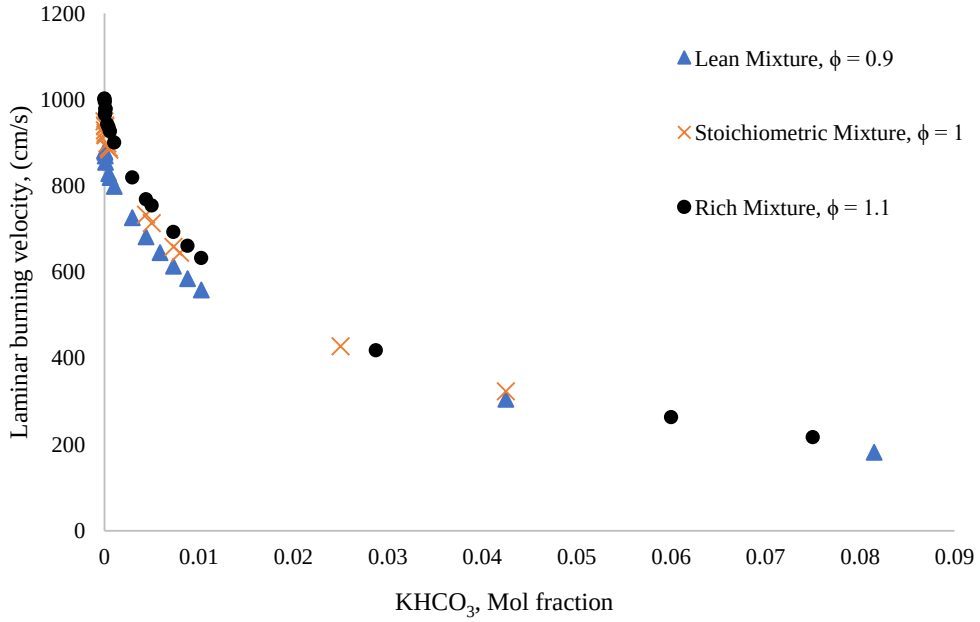


Figure 6.6: The inhibition effect of $KHCO_3$ on the laminar burning velocity of H_2/air as a function of equivalence ratio (initial conditions: 673 K, 1 atm, stoichiometric, lean, and rich mixtures, ϕ = 0.9, 1.0, and 1.1).

Table 6.6: The Inhibition Effect of $KHCO_3$ on the Laminar Burning Velocity of H_2/air Flame

$KHCO_3$ Mole fraction	S_L, (cm/s) at ϕ= (0.9)	$KHCO_3$ Mol fraction	S_L, (cm/s) at ϕ = (1)	$KHCO_3$ Mole fraction	S_L, (cm/s) at ϕ= (1.1)
0.00	881	0.00	950	0.00	1002
1.50×10^{-5}	884	4.43767×10^{-5}	929	1.47927×10^{-5}	1001
4.43767×10^{-5}	878	5.91681×10^{-5}	940	4.44×10^{-5}	995
7.3959×10^{-5}	870	7.3959×10^{-5}	938	5.91×10^{-5}	965
1.00×10^{-4}	855	8.80×10^{-5}	918	8.87×10^{-5}	969
4.44×10^{-4}	828	1.00×10^{-4}	923	1.00×10^{-4}	979
5.91×10^{-4}	819	1.10×10^{-4}	918	1.20×10^{-4}	978
1.03×10^{-3}	799	2.96×10^{-4}	898	3.00×10^{-4}	943
2.95×10^{-3}	726	4.44×10^{-4}	889	4.44×10^{-4}	935
4.40×10^{-3}	682	5.00×10^{-4}	884	5.91×10^{-4}	927
5.88×10^{-3}	645	4.40×10^{-3}	733	1.00×10^{-3}	900
7.30×10^{-3}	614	5.00×10^{-3}	714	2.95×10^{-3}	819
8.79×10^{-3}	585	7.30×10^{-3}	658	4.40×10^{-3}	769
1.02×10^{-2}	559	8.00×10^{-3}	645	5.00×10^{-3}	754
4.25×10^{-2}	305	2.50×10^{-2}	428	7.30×10^{-3}	693
8.15×10^{-2}	182	4.25×10^{-2}	324	8.79×10^{-3}	661
				1.00×10^{-2}	633
				2.87×10^{-2}	418
				6.00×10^{-2}	264
				7.50×10^{-2}	217

Figures 6.7, 6.8, and 6.9 show the hydroxyl radical profiles in H_2/air lean, stoichiometric, and rich flame at different $KHCO_3$ mole fractions. The simulation results show that the radical overshoot disappears at KHO_3 mole fractions higher than 5%.

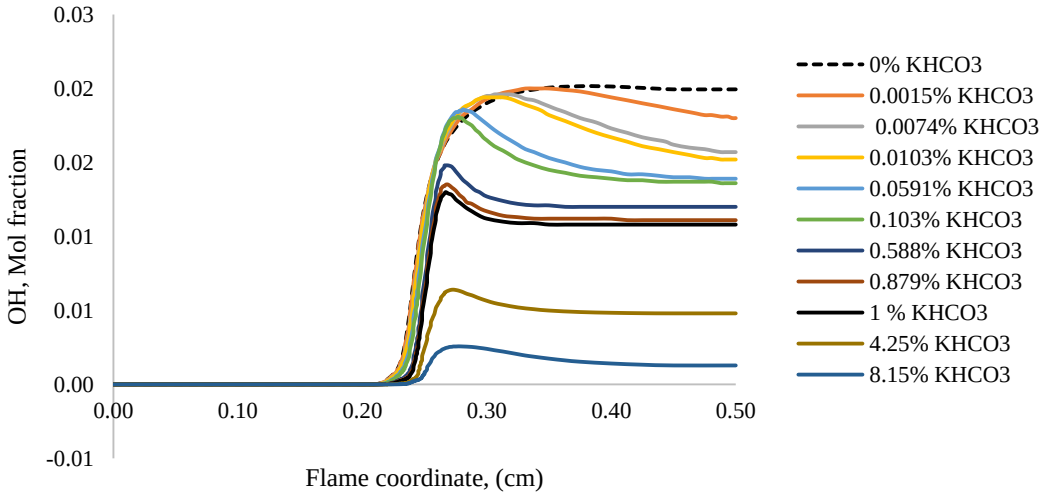


Figure 6.7: Flame concentration profiles of hydroxyl radical at different inhibitor mole fraction of $KHCO_3$ loadings (lean H_2/air flame, initial conditions, (673 K, 1 atm)).

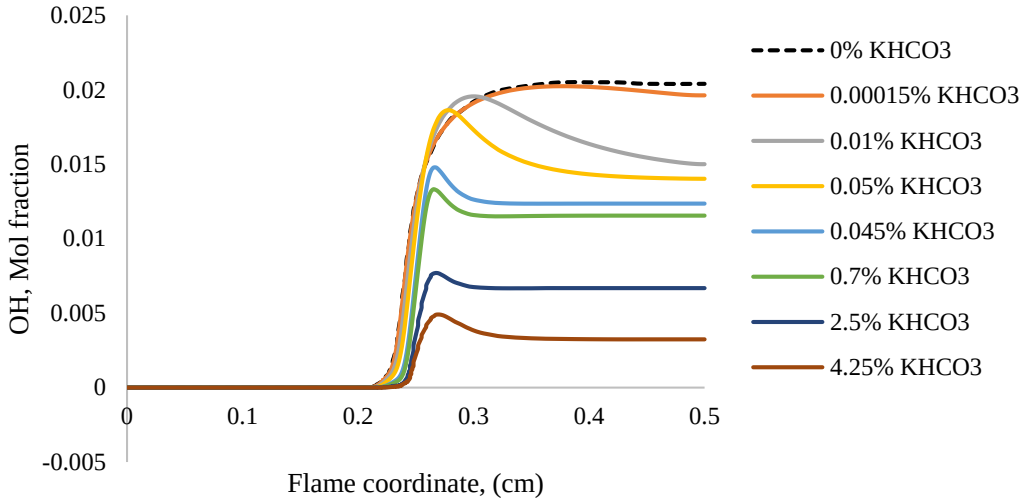


Figure 6.8: Flame concentration profiles of hydroxyl radical at different inhibitor mole fraction of $KHCO_3$ loadings (stoichiometric H_2/air flame, initial conditions, (673 K, 1 atm)).

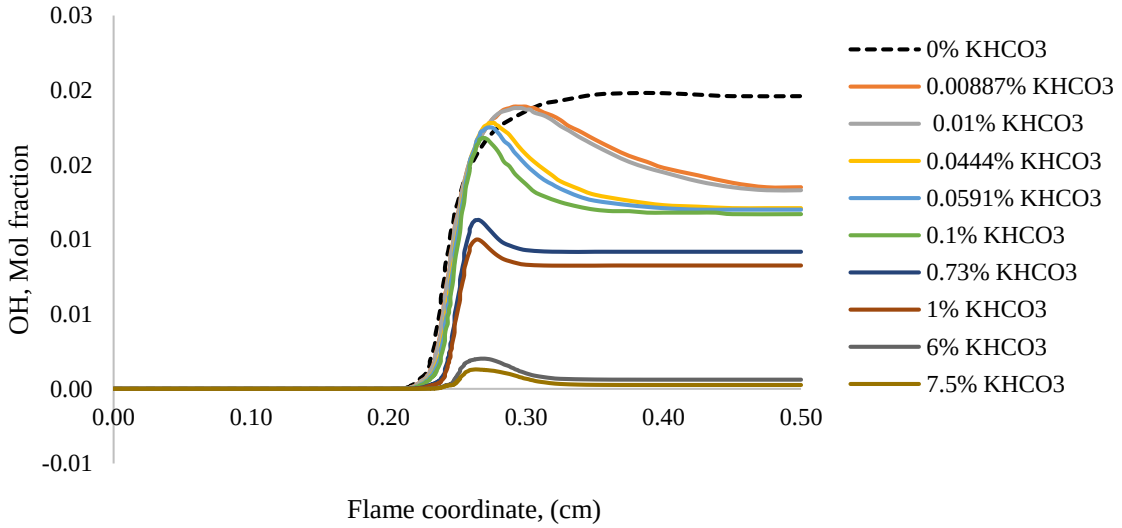


Figure 6.9: Flame concentration profiles of hydroxyl radical at different inhibitor mol fraction of $KHCO_3$ loadings (rich H_2/air flame, initial conditions, (673 K, 1 atm)).

6.4 KCO_3 Inhibition Effect on the S_L and OH Mole Fraction

Using the data provided in Table 6.7, Figure 6.10 illustrates the correlation between the mole fraction of KCO_3 and the laminar burning velocity of H_2 flames across different mixture ratios (lean, stoichiometric, and rich) under specific conditions. The figure illustrates a decrease in the burning velocity of H_2 flames as the mole fraction of KCO_3 increases at all mixture ratios.

Figure 6.10 strongly suggests that the presence of KCO_3 has a notable impact on the burning velocity of H_2 flames, with a more pronounced effect at lower mixture ratios.

The introduction of a 5% mole fraction of KCO_3 in the lean mixture results in a reduced burning velocity from 881 to 192 cm/s, while the effect of a similar mole fraction of $KHCO_3$, which reduces it to 244 cm/s. It can be seen that $KHCO_3$ requires a higher concentration than KCO_3 to suppress the H_2 flame. For comparison, a 5% mole fraction of KO_2 in the lean region reduces the burning velocity to 52 cm/s.

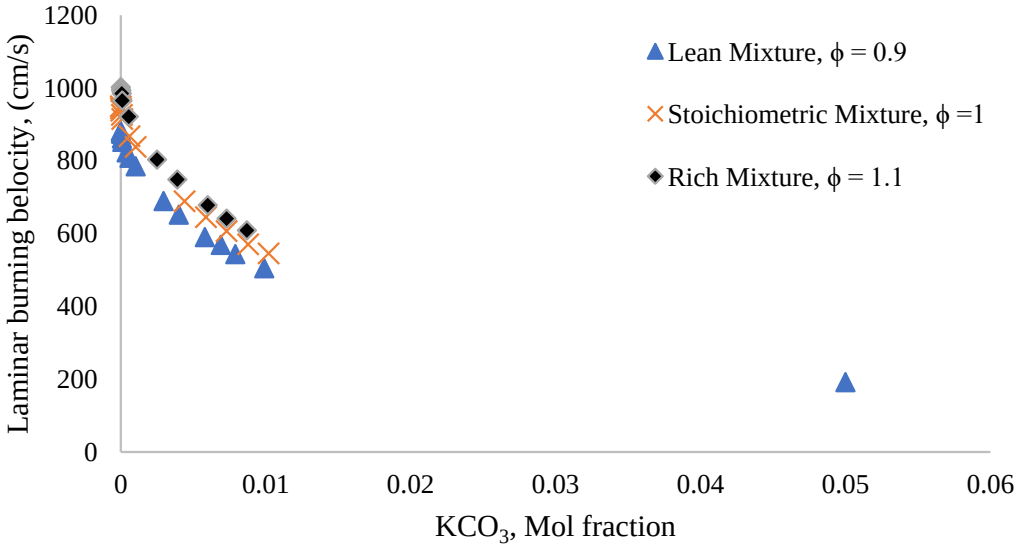


Figure 6.10: The effect of KCO_3 on the laminar burning velocity of H_2/air as a function of equivalence ratio (initial conditions: 673 K, 1 atm, lean, stoichiometric, and rich mixtures, ϕ = 0.9, 1.0, and 1.1).

Table 6.7: The Inhibition Effect of KCO_3 on the Laminar Burning Velocity of H_2/air Flame

KCO_3 Mole fraction	S_L, (cm/s) at ϕ= (0.9)	KCO_3 Mole fraction	S_L, (cm/s) at ϕ = (1)	KCO_3 Mole fraction	S_L, (cm/s) at ϕ= (1.1)
0.00	881	0.00	950	0.00	1002
1.50×10^{-5}	876	1.50×10^{-5}	944	1.50×10^{-5}	996
4.44×10^{-5}	874	7.40×10^{-5}	926	4.44×10^{-5}	992
7.40×10^{-5}	862	9.90×10^{-5}	915	7.00×10^{-5}	985
9.90×10^{-5}	852	6.00×10^{-4}	868	9.90×10^{-5}	966
4.00×10^{-4}	823	1.03×10^{-3}	838	5.50×10^{-4}	921
6.00×10^{-4}	808	4.40×10^{-3}	689	2.50×10^{-3}	803
1.03×10^{-3}	785	5.88×10^{-3}	645	3.90×10^{-3}	749
2.95×10^{-3}	689	7.30×10^{-3}	607	6.00×10^{-3}	678
4.00×10^{-3}	652	8.79×10^{-3}	570	7.30×10^{-3}	641
5.80×10^{-3}	590	1.02×10^{-2}	545	8.70×10^{-3}	609
6.90×10^{-3}	569				
7.90×10^{-3}	544				
9.90×10^{-3}	505				
5.00×10^{-2}	192				

Figures 6.11, 6.12, and 6.13 show the hydroxyl radical profiles in H_2/air lean, stoichiometric, and rich flame at different KCO_3 mole fractions. At the KCO_3 mole fraction higher than 5%, radical overshoot disappears. The equilibrium concentration and the equilibrium temperature decrease with the future addition of KCO_3.

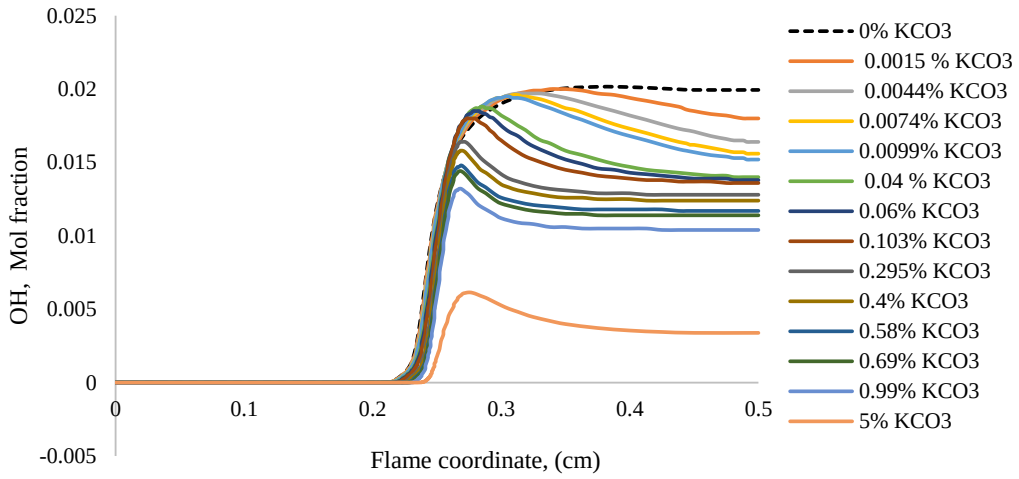


Figure 6.11: Flame concentration profiles of hydroxyl radical at different inhibitor mole fraction of KCO_3 loadings (lean H_2/air flame, initial conditions, (673 K, 1 atm)).

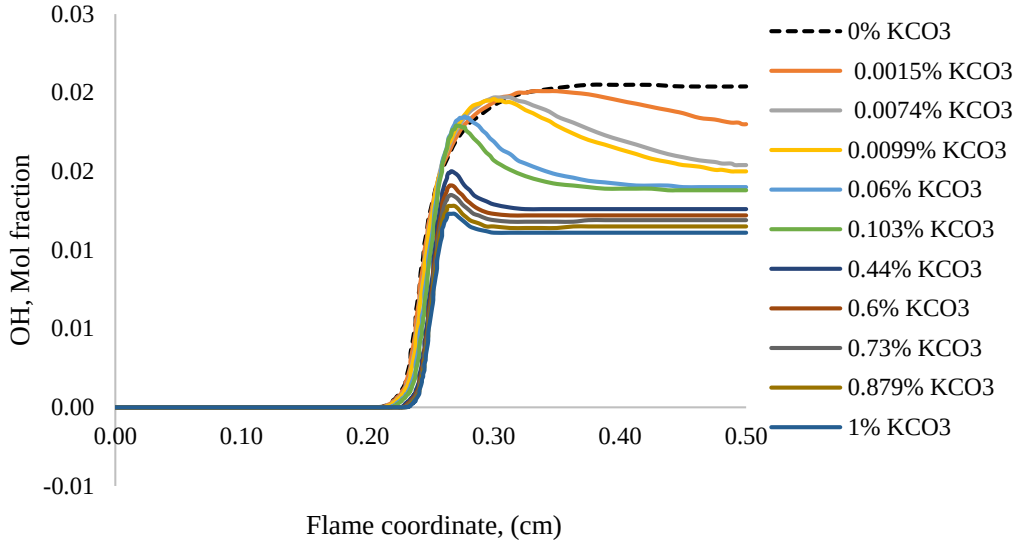


Figure 6.12: Flame concentration profiles of hydroxyl radical at different inhibitor mole fraction of KCO_3 loadings (stoichiometric H_2/air flame, initial conditions, (673 K, 1 atm)).

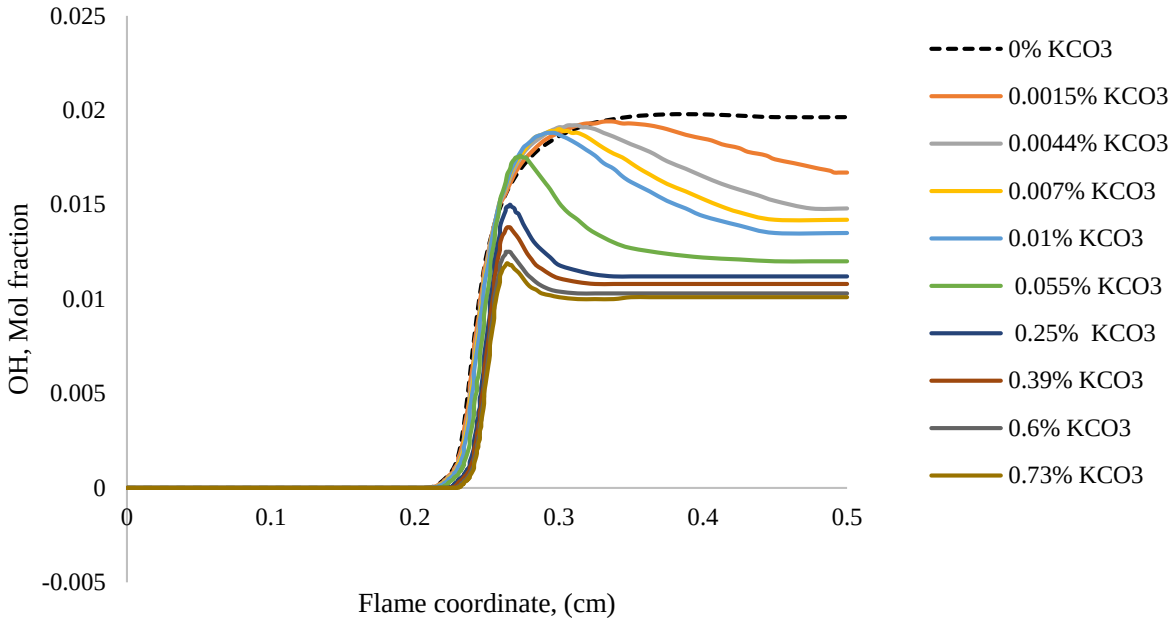


Figure 6.13: Flame concentration profiles of hydroxyl radical at different inhibitor mole fraction of KCO_3 loadings (rich H_2-air flame, initial conditions, (673 K, 1 atm)).

6.5 Comparison the Simulation Results

The results obtained from the numerical modelling of homogeneous reaction kinetics for mixtures involving H_2/air with KO_2, $KHCO_3$, and KCO_3 indicate that all three substances effectively inhibit H_2 flames in different ways. Among them, KO_2 demonstrates higher efficacy in suppressing H_2 flames compared to $KHCO_3$ and KCO_3. Furthermore, the predicted values for the laminar burning velocity suggest that KCO_3 has a faster impact on the reduction of the burning velocity compared to $KHCO_3$.

6.6 Analysing the Comparison Results

6.6.1 The Impact of KO_2 on the Flame speed of H_2/air Mixture at Different Equivalence Ratio

The data file is used to predict the flame speed of H_2/air mixture, which is influenced by various mole fractions of KO_2 (0.001%, 0.29%, and 4%). This data was obtained by simulating the one-dimensional flame speed model (see Table 6.4), considering the range of equivalence ratio (0.8 to 1.2) using continuations.

Figure 6.14 shows the relationship between the equivalence ratio and flame speed in the presence of varying concentrations of KO_2. It can be seen that the presence of KO_2 has a substantial impact on the speed of the flame.

Specifically, an increase in the mole fraction of KO_2 leads to a noticeable reduction in flame speed. This is most evident at equivalence ratios less than 1, indicating lean

conditions. At this point, the flame speed experiences a sharp decline with higher concentrations of KO_2.

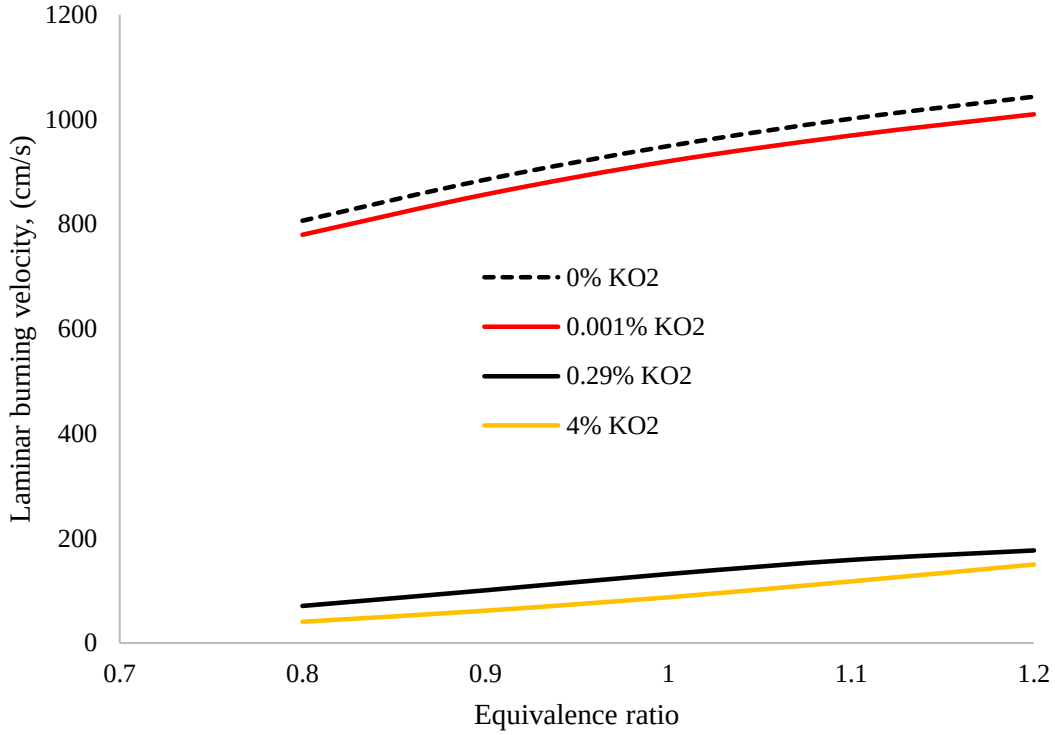


Figure 6.14: The impact of KO_2 mole fraction on the flame speed of H_2 flame using equivalence ratio (0.8 to 1.2).

6.6.2 Determining the Pathway Analysis of Stoichiometric H_2/air Mixture with Adding KO_2

To investigate the interactions between KO_2 and the most crucial free radicals of the H_2 flame, varying mole fractions of KO_2, specifically 0.0001, 0.00147, and 0.08 have been employed. These fractions are used to investigate how KO_2 influences the behavior and reactions of fundamental species, including OH, O, and H, in the context of the stoichiometric H_2 flame.

0.01% Mole Fraction of KO_2

Figure 6.15 illustrates the analysis of the reactions of the stoichiometric H_2 flame with the addition 0.0001 mole fraction of KO_2. The analysis is illustrated at a location, 0.2607188 cm from the ignition source, and at a temperature of 2014.99 K.

In this analysis, it can be observed that HKO consumes H atoms in the reaction HKO + H $\rightleftharpoons$ K + H_2O. This consumption of H atoms may reduce their availability for other reactions, potentially slowing the overall combustion process.

Additionally, the reaction involving the formation of HKO by consuming H and KO is significant. HKO is a reactive species that can participate in subsequent reactions,

potentially increasing its concentration in the flame.

Furthermore, the reactions O + $H_2 \rightleftharpoons$ H + OH and OH + $H_2 \rightleftharpoons$ H + H_2O result in the consumption of H_2 in H and OH. These reactions are crucial for the production of OH and H radicals, which play essential roles in combustion.

The reaction H + $HO_2 \rightleftharpoons$ 2OH represents the formation of OH radicals through the consumption of H and HO_2. Additionally, H atoms are consumed by reacting with HO_2 to generate H_2 + O_2. While this reaction doesn't directly affect combustion, it can influence the concentrations of reactants and intermediates.

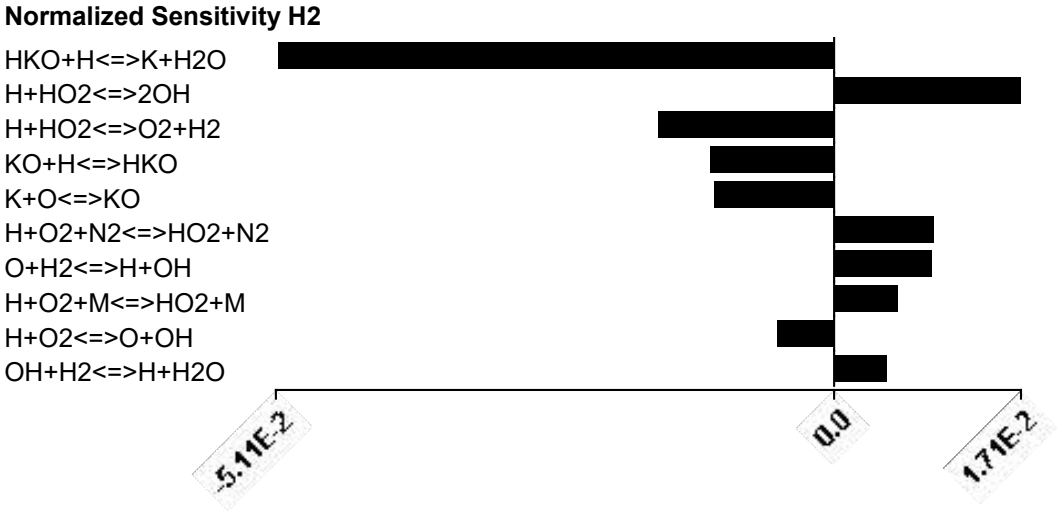


Figure 6.15: Sensitivity analysis of H_2/air mixture developed by GRI-Mech/K-species Mechanism at initial condition, 673K,1atm, and 0.01% mole fraction of KO_2.

0.147% Mole Fraction of KO_2

Figure 6.16 shows the analysis of the path to adding the 0.00147 KO_2 to the stoichiometric flame H_2, the sensitivity analysis is located at distance 0.265625 cm and temperature 2268.6 K. It's clear from Figure 6.16 that H_2 is consumed through the reactions OH + $H_2 \rightleftharpoons$ H + H_2O and O + $H_2 \rightleftharpoons$ H + OH.

At a KO_2 mole fraction of 0.147%, the reaction KO + O $\rightleftharpoons$ KO_2 illustrates the conversion of KO to KO_2 through its interaction with O.

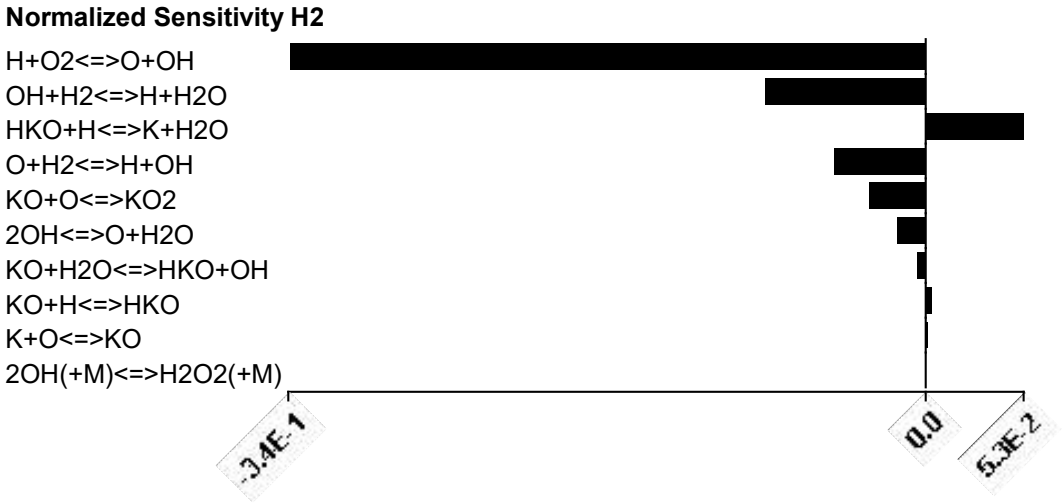


Figure 6.16: Sensitivity analysis of H_2/air mixture developed by GRI-Mech/K-species Mechanism at initial condition, 673K,1atm, and 0.147% mole fraction of KO_2.

8% Mole Fraction of KO_2

Figure 6.17 presents the pathway analysis of a stoichiometric H_2/air mixture with 8% mole fraction of KO_2 at a 0.260156 cm from the ignition source, and a temperature of 1586 K. In this analysis, the focus is on the normalised sensitivity of H_2 concerning various reactions involving OH, H_2, O, and the potassium species, KO, KO_2, and HKO. The consumption of H_2 is represented by the reaction OH + H_2 $\rightleftharpoons$ H + H_2O and O + H_2 $\rightleftharpoons$ H + OH, However, KO_2 clearly reacting with H_2, OH, and H through the following reactions:

$KO_2 + H_2 \rightleftharpoons HKO + OH$ $KO_2 + OH \rightleftharpoons HKO + O_2$ and $KO_2 + H \rightleftharpoons HKO + O$

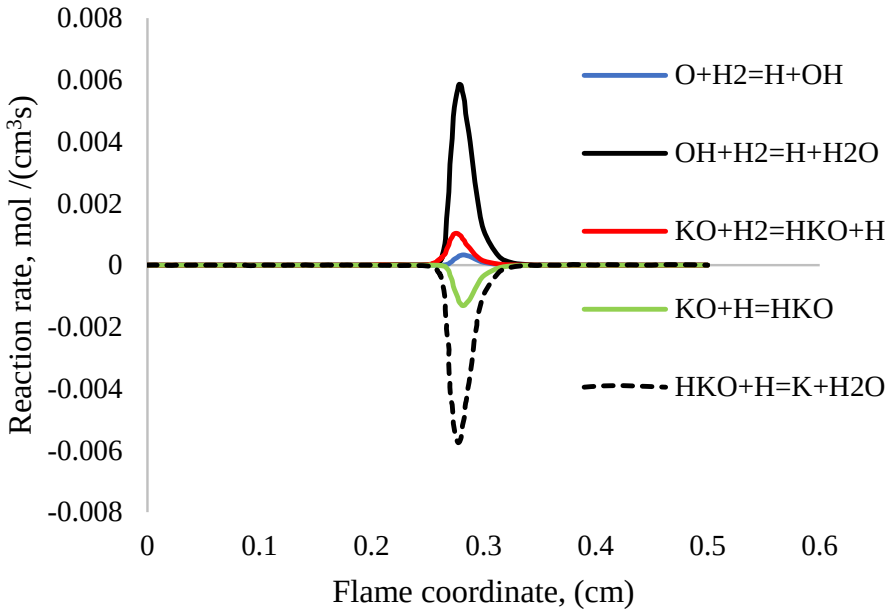
where KO + O contributes to the generation of KO_2 in the flame reacting.



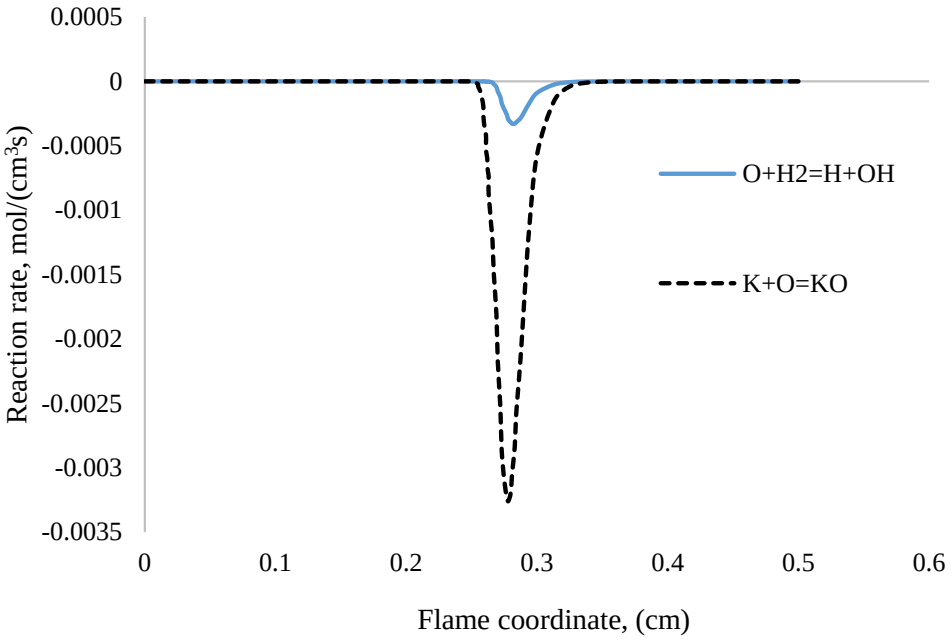
Figure 6.17: Sensitivity analysis of H_2/air mixture developed by GRI-Mech Mechanism at initial condition, 673 K,1 atm, and 8% mole fraction of KO_2.

6.6.3 Reaction Rate Profiles as a Function of Flame Position in a Stoichiometric H_2/air Mixture with 8% KO_2

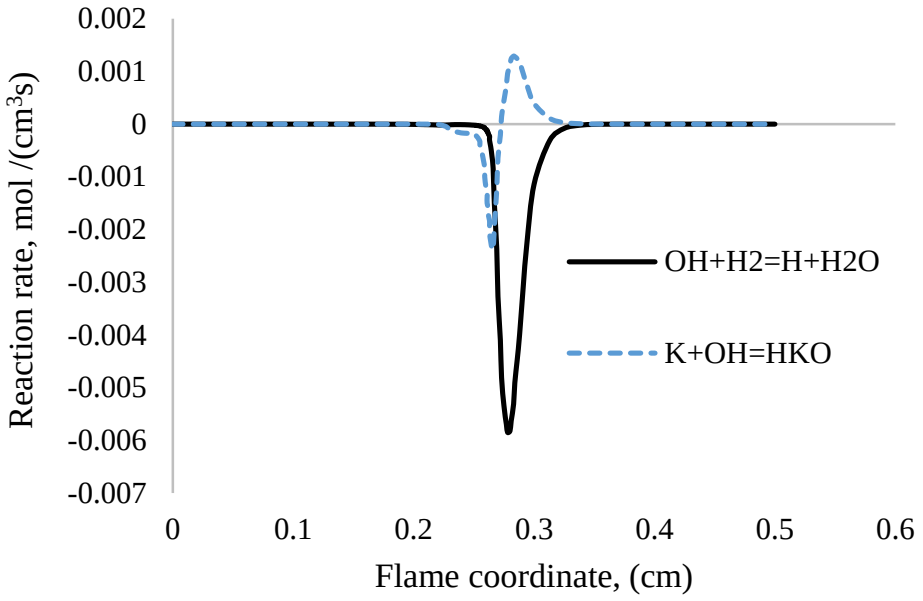
Figures 6.18a, 6.18b, and 6.18c demonstrate the reaction rate profiles of the main reactions for consumption of H, O, and OH radicals, and Figure 6.18d illustrates the main reactions for the formation and consumption of K-atom in the main reaction zone of the flame. H and O atoms are consumed by K-species and the reactions are HKO+H=K+H_2O, KO+H= HKO, and K+O=KO. However, OH radical is mostly consumed by the reaction OH+H_2=H+H_2O, and HKO is generated by consuming OH where K+OH= HKO.



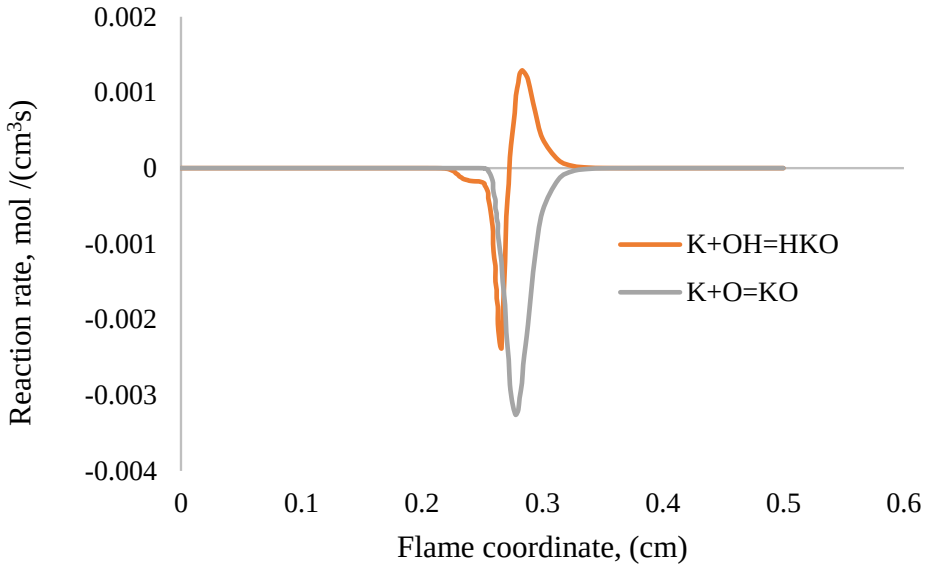
(a)


0.0005
0
-0.0005
-0.001
-0.0015
-0.002
-0.0025
-0.003
-0.0035
Reaction rate, mol/(cm3s)
0
0.1
0.2
0.3
0.4
0.5
0.6
Flame coordinate, (cm)
O+H2=H+OH
K+O=KO

(b)


0.002
0.001
0
-0.001
-0.002
-0.003
-0.004
-0.005
-0.006
-0.007
Reaction rate, mol /(cm3s)
0
0.1
0.2
0.3
0.4
0.5
0.6
Flame coordinate, (cm)
OH+H2=H+H2O
K+OH=HKO

(c)



(d)

Figure 6.18: Reaction rate profiles as a function of position in the flame, for the main reactions of (a) H atom (b) O atom consumption (c) OH radical (d) formation and consumption of potassium atom (stoichiometric H_2/air flame, 673 K, 1 atm, KO_2 mole fraction of 0.08).

6.6.4 Adiabatic Flame Temperature of Stoichiometric H_2/air Mixture with Mole Fractions of KO_2

As illustrated in Figure 6.19, the graph demonstrates the effect of different mole fractions of KO_2 (0.01%, and 10%) on the adiabatic flame temperature of stoichiometric H_2/air mixture at an initial temperature of 300K and constant pressure. The data indicates that a high concentration of KO_2 can dramatically reduce the adiabatic flame temperature of H_2 flame.

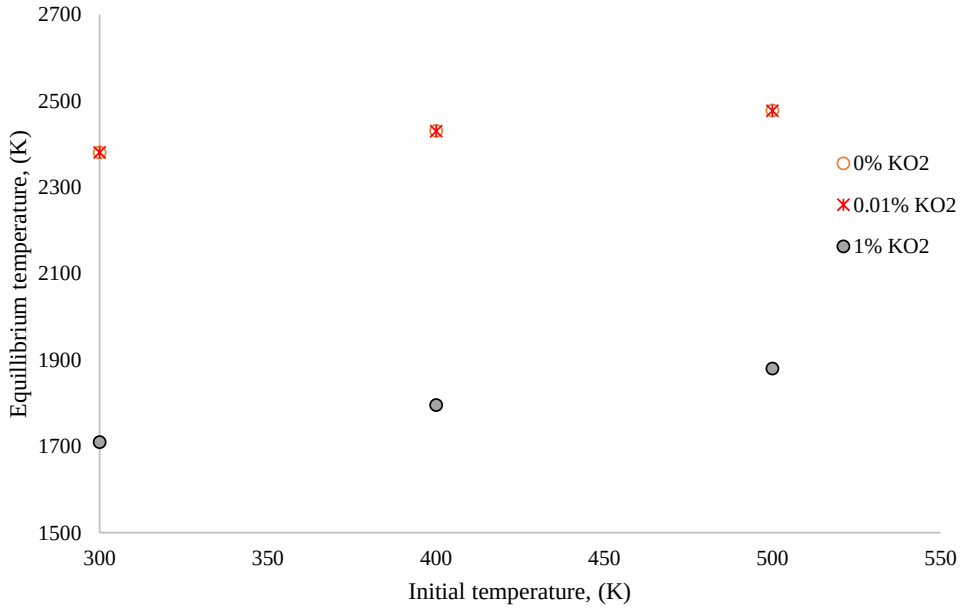


Figure 6.19: AFT H_2/air mixture adding different mole fractions of KO_2.

6.7 Discussion

In this investigation, the focus extends beyond the examination of the impact of KO_2 on critical combustion parameters such as flame speed and reduction of OH radicals. Instead, the emphasis is placed on estimating the flame speed under a range of equivalence ratios and explaining the intricate reactions within the flame pathway.

6.7.1 H_2 Flame Behaviour Under Different Equivalence Ratio and Mole Fractions of KO_2

Investigating the influence of various mole fractions of KO_2 (0.001%, 0.29%, and 4%) on the flame speed of H_2 / air mixture has led to valuable conclusions. When a low concentration of about 0.001% KO_2 is introduced, the flame speed of the H_2 flame is slightly lower than the flame speed of pure H_2 flame at the same equivalence ratio. Upon close examination, it becomes evident that the presence of KO_2 plays a significant role in shaping the flame speed characteristics. An increase in the mole fraction of KO_2 results in a substantial reduction in flame speed, and this effect is most pronounced under lean conditions $(\phi < 1)$.

6.7.2 Reaction Rate as a Function of Position in the Flame

Consumption of H and O atoms by K-Species: K-species, particularly represented by HKO and KO, play a significant role in the consumption of H and O atoms within the flame. This consumption leads to the formation of K atoms, indicating a direct influence of K species on flame chemistry.

OH Radical Reduction: OH radicals are mostly consumed by the reaction

$OH + H_2 \rightarrow H + H_2O$

This reaction is influenced by the K-species.

Formation and Consumption of K-atoms: The reaction K+OH=HKO indicates the consumption of potassium (K) as it reacts with OH to form potassium hydroxide (HKO). The initial negative slope of the curve would represent the decrease in potassium (K) concentration as it's consumed to form HKO. The subsequent positive slope would indicate the generation of HKO from the consumed K and OH. K atoms are consumed when they react with oxygen (O) to form potassium oxide (KO). This is represented by the reaction: $K + O \rightarrow KO$ As a result, K atoms are no longer present as free atoms but are incorporated into the potassium monoxide molecule.

6.7.3 Pathway Analysis

At a low concentration of KO_2 (0.0001 mole fraction), the pathway analysis revealed that HKO consumes H atoms in the reaction $HKO + H = K + H_2O$. This consumption of H atoms can potentially limit their availability for other reactions, which could result in a deceleration of the overall combustion process. Furthermore, significant HKO formation through consumption of H and KO has the potential to increase its concentration in the flame.

In addition, there were reactions involving the conversion of H_2 into H and OH. It appears that, at this specific level of KO_2 concentration, the presence of KO_2 has minimal impact on the pathway reactions of the H_2 flame.

With a higher concentration of KO_2 (0.00147 mole fraction), the analysis of the pathway showed that H_2 is still consumed through reactions $OH + H_2 \rightleftharpoons H + H_2O$ and $O + H_2 \rightleftharpoons H + OH$. Additionally, KO_2 is involved in the reaction $KO + O \rightleftharpoons KO_2$.

At a significantly higher concentration of KO_2, significant consumption of H_2 was observed in reactions involving KO_2. KO_2 clearly reacts with H_2, OH, and H, indicating that KO_2 has a pronounced effect on the H_2 flame by interrupting the chain reaction.

6.8 Summary

- KO_2 stands out as the most effective suppression agent on H_2 flame. It reduces the flame speed at a faster rate compared to $KHCO_3$ and KCO_3 when utilising the same mole fraction.
- KO_2 requires a lower concentration to effectively reduce the OH mole fraction within the flame zone.
- $KHCO_3$ and KCO_3 require concentrations exceeding the 5% mole fraction to disappear the overshoot of the OH radical.
- The presence of KO_2 reduces the flame speed in the range (0.8 to 1.2).

- KO_2 plays a pivotal role in the combustion process by actively consuming H, O atoms and H_2 itself, leading to the formation of HKO.
- At a high concentration of KO_2, a significant reduction in the adiabatic flame temperature of H_2 flames can be observed.
- The next chapter will focus on studying the effects of KO_2, $KHCO_3$, and KCO_3 on CH_4 flames.

Chapter 7

Effect of KO_2, $KHCO_3$, and KCO_3 on Methane Flames

This chapter presents numerical modelling to simulate the flame speed of a CH_4 flame with the addition of KO_2 or $KHCO_3$ or KCO_3 in different equivalence ratios. It also estimates the reduction of the mole fraction of OH. The changes in the flame speed of the CH_4/air mixture concerning the equivalence ratio are demonstrated. Additionally, the chapter studies the pathway analysis of CH_4 flames affected by KCO_3 mole fractions.
In this chapter, the effect of $KHCO_3$ on the CH_4 flame is compared with the findings of the previous study.

7.1 Flame Speed of CH_4/air Mixture Modelling Method

Numerical modelling of flame speed is carried out using a one-dimensional flame speed calculation model within Chemkin. This model employs the boundary value method to calculate the speed of the adiabatic flame. The purpose is to determine the burning velocity characteristics of a specific gaseous mixture under specified pressure and inlet temperature conditions. Notably, the modeling neglects heat losses. The input parameters include the gas-phase reaction mechanism, thermodynamic data, and transport properties. The simulation uses the GRI-Mech 3.0/K-species reaction mechanism, which encompasses the fundamental steps for CH_4 oxidation.

The initial gas pressure is set at 1 atm and the unburned gas temperature is 673 K, without considering heat loss or thermal expansion, resulting in constant pressure throughout the calculation. In addition, an initial temperature profile is automatically estimated. The initial gas temperature was set at 298 K. The starting point was given as 0 cm, which means that the starting position was just above the burner. The ending axial position was set at 0.5 cm, which covers the reaction zone of the CH_4 flame. An initial number of points in the grid was required to be given to initially solve the problem. The initial number of the grid points was given and adjusted between 6-11, depending on if the solution could be found. In addition to these parameters, the mass flow rate of the inlet gaseous mixture is supplied. It is essential to note that the final solution's sensitivity to the mass flow rate is minimal as it will be determined as part of the flame speed solution. Assuming a mass flow rate for flame speed calculations keeps the freely propagating flame at fixed coordinates. The composition of the reactants is specified as input before running

the model, whereas the expected composition of the products and intermediate fractions is not included in the model.

The number of grid points has increased from the initial value of 6 to the final solution. The solution ensures that the temperature and species gradients are close to zero. The axial velocity at the cold boundary is the relative velocity of the unburned gas to the flame front. flame speed for the pure CH_4/air mixture based on GRI-Mech +K-species reactions is approximately 166 cm/s, as obtained from the simulation at 673 K and 1 atm.

Figure 7.1 shows the relationship between the axial velocity and the initial temperature of CH_4/air combustion developed by different mechanisms (GRI-Mech mechanism and GRI-Mech with the reaction of K-species). A relatively low initial temperature, such as room temperature, does not cause a reaction in the modelling developed by the GRI-Mech/ K-species reaction mechanism. Modelling this mechanism with K-species mole fraction starts from 500 K. This figure shows the reason behind selecting an unburned temperature higher than 298 K.

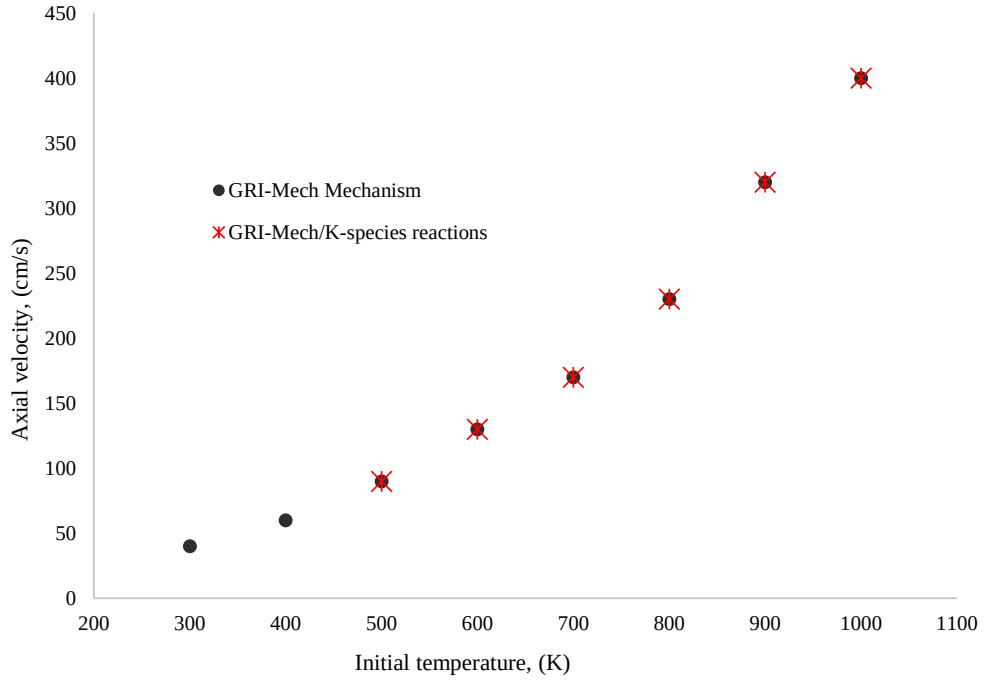


Figure 7.1: The relation between initial temperature and axial velocity of different kinetic reaction mechanisms of CH_4/air mixture.

7.1.1 Summary of Simulation Conditions

The one-dimensional flame speed reactor was selected to investigate the impact of selected potassium species on CH_4 flame behaviour.

The utilisation of this reactor model serves several key purposes. First and foremost, it allows for the calculation of flame speed under various equivalence ratios (ϕ). This enables the study of how the presence of specific potassium species influences the flame speed of CH_4 flame. Furthermore, the one-dimensional flame speed reactor aids in

estimating and discussing the reaction pathways within the CH_4/air mixture. Table 7.1 summarises the simulation conditions used to investigate the behaviour of the CH_4/air mixture with added mole fractions of KO_2, or KCO_3, or $KHCO_3$.

Table 7.1: Simulation Conditions for Studying the Effect of KCO_3 and $KHCO_3$ Mole Fractions on CH_4/air Mixture

Simulation Conditions	
Model	One-Dimensional Flame Speed Reactor
Unburnt Gas Temperature, K	673
Initial Gas Temperature Profile, K	The temperature profile was automatically estimated from equilibrium.
Initial Gas Temperature, K	298
Mass Flow Rate, (g/cm²·s)	1
Pressure, atm	1
Reaction Mechanism	GRI-Mech/K-species Mechanism
Fuel Type	CH_4
Oxidiser Type	air (O_2, N_2)
Equivalence Ratio (ϕ)	0.9, 1, 1.1
Constraints and Assumptions	Constant pressure, Heat loss and thermal expansion = 0, Gas reaction rate multiplier = 1, The starting axial position of 0 cm, Ending axial position = 0.5cm, the basic tolerance parameters, and advanced controls for the solution are Assigned, Number of uniform grid points = 6
Wall Boundary	Adiabatic
Data Required	Gas-phase kinetic, Thermodynamic data, Transport data

Note:

- The polynomial coefficients for KCO_3 and $KHCO_3$ have been assumed to be the same as those for K_2CO_3.
- The transport data for KCO_3 and $KHCO_3$ are assumed to be equivalent to the transport data for KO_2.
- The assumptions of transport data are not expected to significantly affect the results. This is because Chemkin utilises a mixture-averaged transport properties method to solve the transport properties in the model.

7.1.2 Mole Fraction of Reactant

Various mole fractions of KO_2, $KHCO_3$ and KCO_3, as shown in Tables 7.3, 7.4 and 7.5, were considered, ranging from 0 to 20% in the mixture. In the simulation, the reaction of CH_4 with air is carried out under stoichiometric conditions.

$$CH_4 + 2\,(O_2 + 3.76\,N_2) \longrightarrow CO_2 + 2\,H_2O + 7.52\,N_2$$

Table 7.2 illustrates the calculated mole fractions of CH_4, O_2, and N_2 at various equivalence ratios (ϕ). These mole fractions were used in the simulation to investigate the impact of the $KHCO_3$ and KCO_3 mole fractions on the CH_4 flame.

Table 7.2: Calculated mole fractions of CH_4, O_2, and N_2 at various (ϕ), applied with $KHCO_3$ and KCO_3 mole fractions in the simulation

(ϕ)	CH_4 Mole Fraction	O_2 Mole Fraction	N_2 Mole Fraction
0.9	8.6319×10^{-2}	1.9182×10^{-1}	7.2185×10^{-1}
1	9.5×10^{-2}	1.90×10^{-1}	7.15×10^{-1}
1.1	1.035×10^{-1}	1.8819×10^{-1}	7.0820×10^{-1}

7.2 The Inhibition Effect of KO_2 on S_L and OH Mole Fraction

From figure 7.2, it becomes evident that the laminar burning velocity of CH_4 flames experiences a notable increase with an increasing mole fraction of KO_2. This finding suggests that KO_2 is not an effective fire suppression agent for CH_4 flames. The table 7.3 presents flame speed values of CH_4 at different concentrations of KO_2, ranging from 0 to 0.2 mole fractions. Across all equivalence ratios, the trend indicates a significant enhancement in flame speed with higher KO_2 concentration. Specifically, in lean, stoichiometric, and rich mixtures, the laminar burning velocity of CH_4 consistently increases as the mole fraction of KO_2 increases. For instance, in the lean mixture, the laminar burning velocity of CH_4 increases from 159 to 210 cm/s as the mole fraction of KO_2 increases from 0 to 0.02.

In real-world scenarios, this suggests that the use of KO_2 as a fire suppression agent for CH_4 fires may not be effective.

Given that higher flame speeds can lead to more rapid flame propagation and increased fire intensity, the observed increase in flame speed with KO_2 concentration could potentially exacerbate fire situations rather than suppress them. This raises concerns about the suitability of KO_2 as a fire suppression agent in environments where CH_4 is the primary fuel source.

Furthermore, the findings underscore the importance of carefully evaluating the efficacy of fire suppression agents in different fire scenarios. While KO_2 may be effective in certain contexts, such as fires involving different fuel sources, its application in CH_4 fires requires careful consideration and further investigation to ensure safe and effective fire management practices.

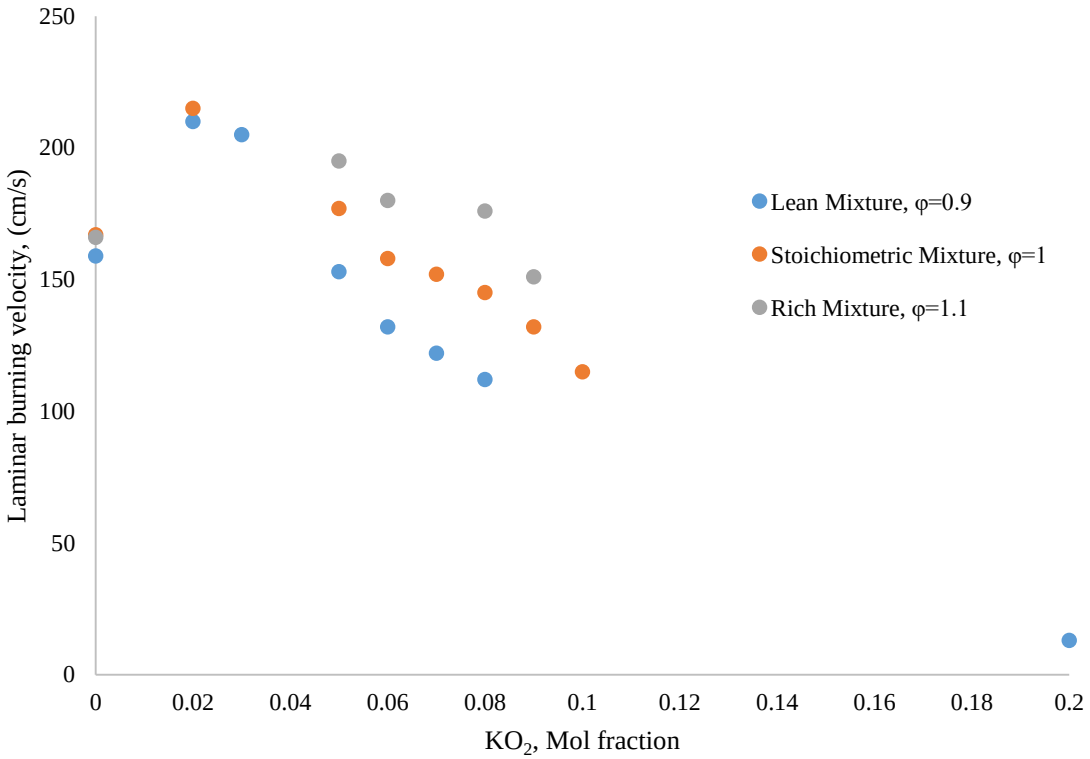


Figure 7.2: The effect of KO_2 on S_L of CH_4/air as a function of equivalence ratio (initial conditions: 673 K, 1 atm, lean, stoichiometric, and rich mixtures, ϕ = 0.9, 1.0, and 1.1).

Table 7.3: The Inhibition Effect of KO_2 Mole Fraction on the Laminar Burning Velocity of CH_4/air Flame

KO_2 Mole fraction	S_L, (cm/s) of CH_4 at ϕ= (0.9)	KO_2 Mole fraction	S_L, (cm/s)of CH_4 at ϕ = (1)	KO_2 Mole fraction	S_L, (cm/s) of CH_4 at ϕ= (1.1)
0.00	159	0.00	167	0.00	166
2×10^{-2}	210	2×10^{-2}	215	5×10^{-2}	195
3×10^{-2}	205	5×10^{-2}	177	6×10^{-2}	180
5×10^{-2}	153	6×10^{-2}	158	8×10^{-2}	176
6×10^{-2}	132	7×10^{-2}	152	9×10^{-2}	151
7×10^{-2}	122	8×10^{-2}	145		
8×10^{-2}	112	9×10^{-2}	132		
2×10^{-1}	13	1×10^{-1}	115		

Figures 7.3, 7.4, and 7.5 depict the relationship between distance and mole fraction of OH at varying concentrations of KO_2. The data indicates a trend where the mole fraction of OH increases with higher concentrations of KO_2. However, at a 20% concentration of KO_2 results in a notable decrease in the mole fraction of OH and effectively eliminates the OH overshoot phenomenon. Additionally, concentrations higher than 5% lead to the disappearance of the OH overshoot, although the OH concentration continues to increase.

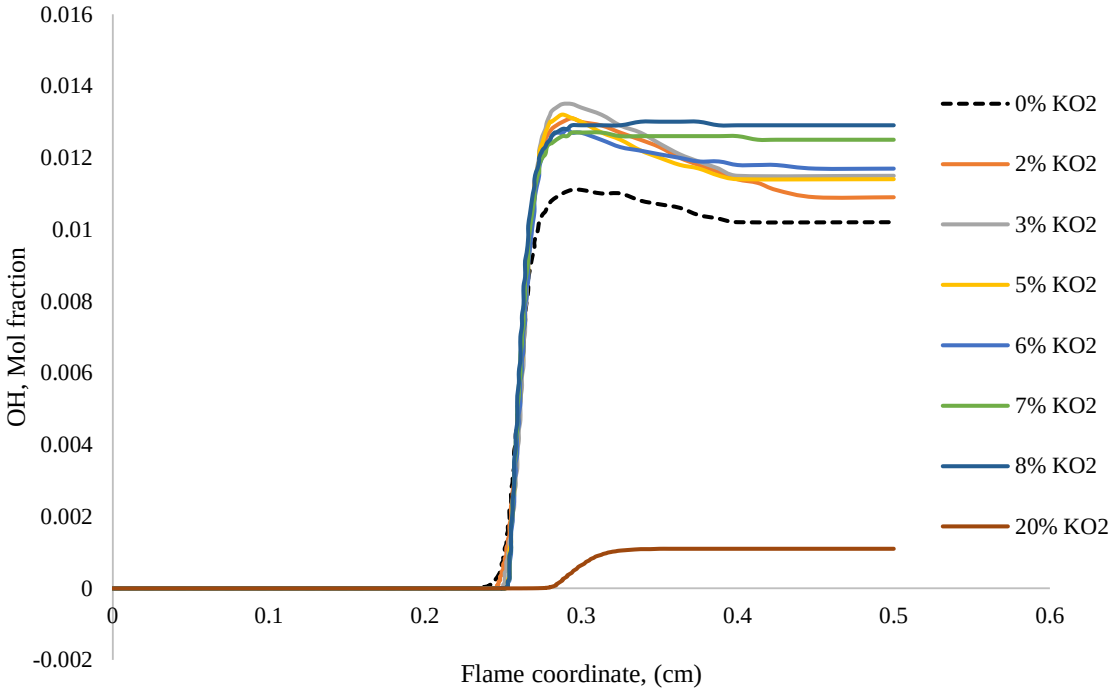


Figure 7.3: Flame concentration profiles of hydroxyl radical at different inhibitor mole fraction of KO_2 loadings (lean CH_4/air flame, initial conditions, (673 K,1 atm)).

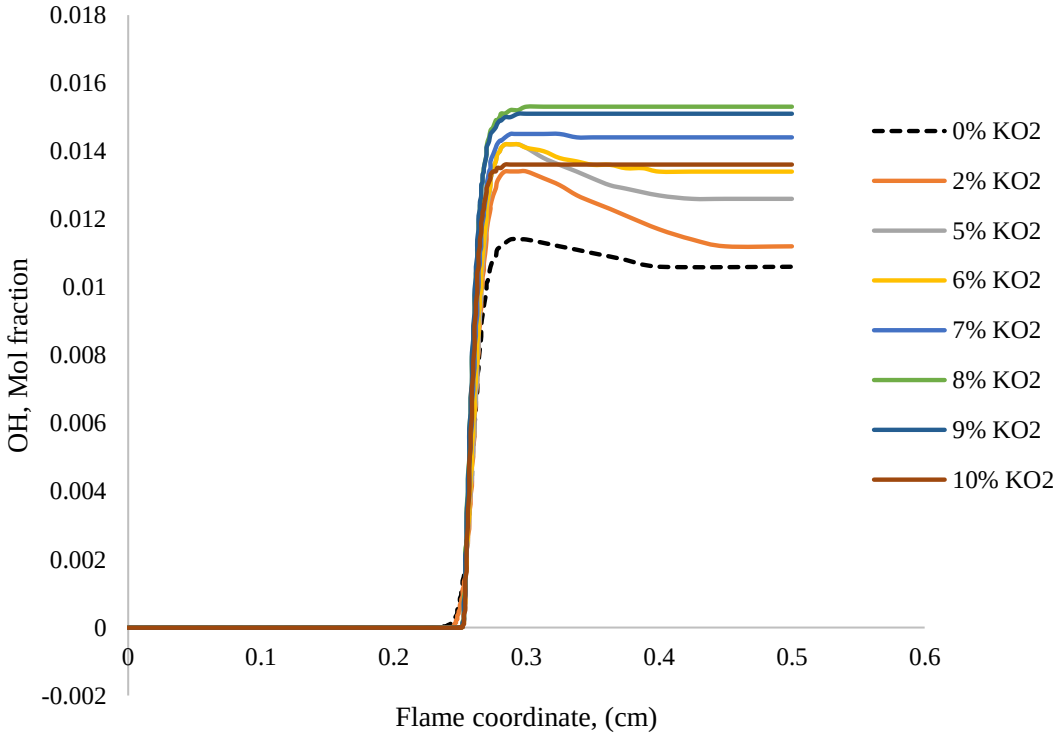


Figure 7.4: Flame concentration profiles of hydroxyl radical at different inhibitor mole fraction of KO_2 loadings (stoichiometric CH_4/air flame, initial conditions, (673 K,1 atm)).

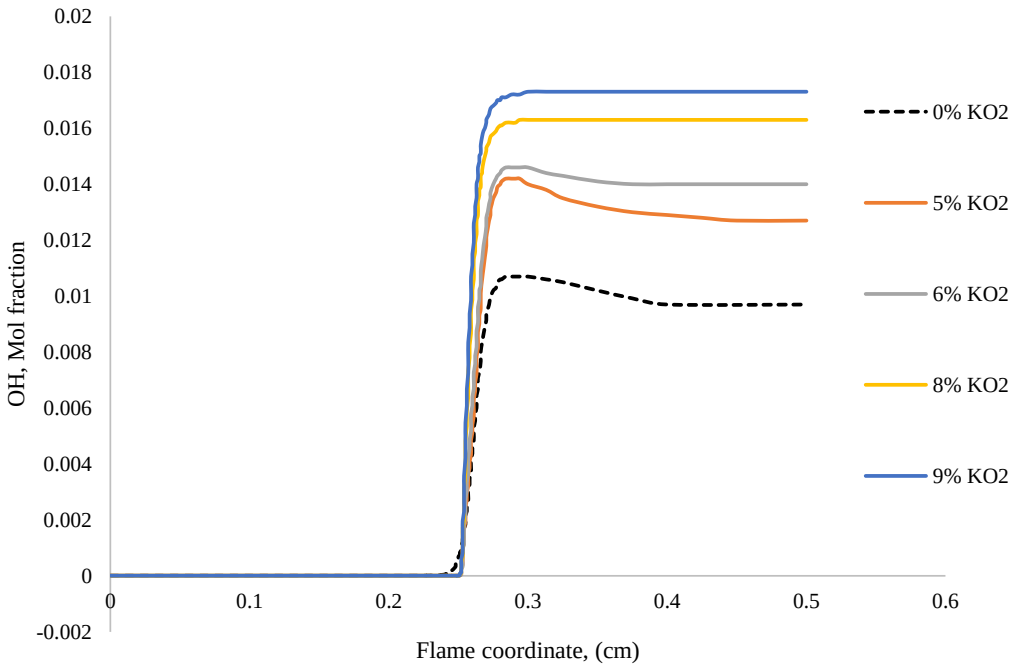


Figure 7.5: Flame concentration profiles of hydroxyl radical at different inhibitor mole fraction of KO_2 loadings (rich CH_4/air flame, initial conditions, (673 K,1 atm)).

7.3 The Inhibition Effect of $KHCO_3$ on S_L and OH Mole Fraction

From Figure 7.6, it can be seen that as the mole fraction of $KHCO_3$ increases, S_L of CH_4 decreases for all three mixtures. This indicates that adding $KHCO_3$ to the mixture slows down the combustion of CH_4. Figure 7.6 presents the flame speed values of CH_4 at different concentrations of $KHCO_3$, ranging from a fraction of 0 to 0.0938 mole. In lean, stoichiometric, and rich mixtures, the flame speed values remain relatively constant until a $KHCO_3$ mole fraction of around 0.01, after which they begin to decrease more rapidly. In the lean mixture, the S_L of CH_4 ranges from 159 to 158 cm/s as the mole fraction of $KHCO_3$ increases from 0 to 0.00103. In the stoichiometric mixture, the S_L of CH_4 ranges from 167 to 166 cm/s as the mole fraction of $KHCO_3$ increases from 0 to 0.00103. In the rich mixture, S_L of CH_4 ranges from 166 to 164 cm/s as the mole fraction of $KHCO_3$ increases from 0 to 0.001. In general, the addition of $KHCO_3$ to the mixture CH_4/air results in a decrease in the flame speed of CH_4, and this effect is more pronounced in the rich mixture compared to the lean and stoichiometric mixtures. Table 7.4 shows the effect of $KHCO_3$ on the flame speed of CH_4 in lean, stoichiometric, and rich mixture.

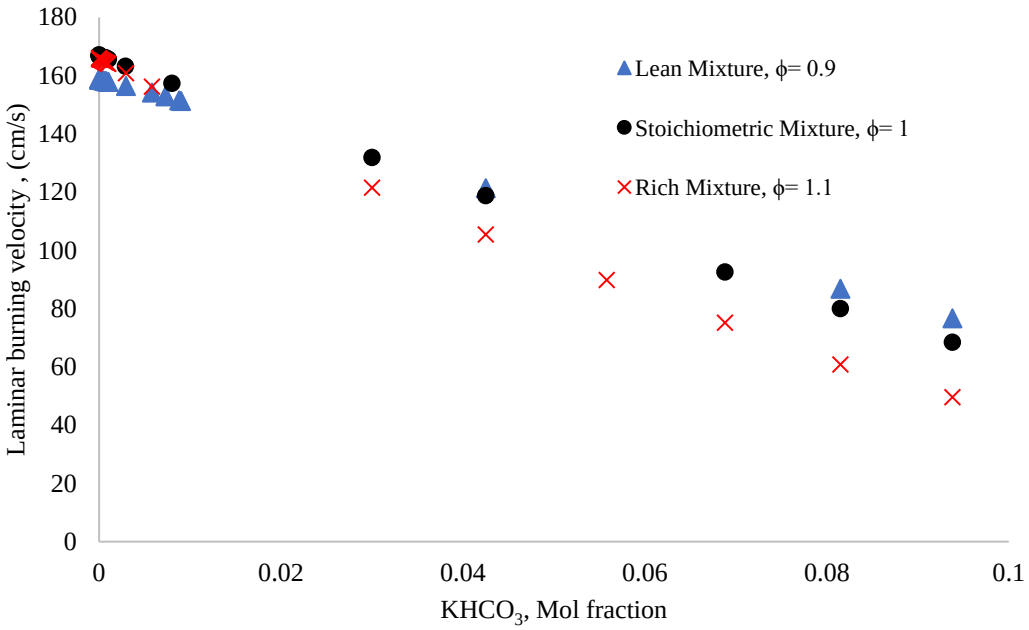


Figure 7.6: The effect of $KHCO_3$ on S_L of CH_4/air as a function of equivalence ratio (initial conditions: 673 K, 1 atm, lean, stoichiometric, and rich mixtures, $\phi = 0.9$, 1.0, and 1.1).

Table 7.4: The Inhibition Effect of $KHCO_3$ Mole Fraction on the Laminar Burning Velocity of CH_4/air Flame

$KHCO_3$ Mole fraction	S_L, (cm/s) of CH_4 at ϕ= (0.9)	$KHCO_3$ Mole fraction	S_L, (cm/s)of CH_4 at ϕ = (1)	$KHCO_3$ Mole fraction	S_L, (cm/s) of CH_4 at ϕ= (1.1)
0.00	159	0.00	167	0.00	166
1.50×10^{-5}	159	1.50×10^{-5}	167	1.50×10^{-5}	166
2.95×10^{-5}	159	2.95×10^{-5}	167	2.95×10^{-5}	166
4.44×10^{-5}	159	4.44×10^{-5}	167	4.44×10^{-5}	166
5.90×10^{-5}	159	5.90×10^{-5}	167	5.90×10^{-5}	166
7.40×10^{-5}	159	7.40×10^{-5}	167	7.40×10^{-5}	166
8.87×10^{-5}	159	8.87×10^{-5}	167	8.87×10^{-5}	166
1.03×10^{-4}	159	1.03×10^{-4}	167	1.03×10^{-4}	165
2.96×10^{-4}	158	2.96×10^{-4}	166	2.90×10^{-4}	165
4.44×10^{-4}	158	4.44×10^{-4}	166	4.44×10^{-4}	165
5.91×10^{-4}	158	6.00×10^{-4}	166	5.91×10^{-4}	165
7.40×10^{-4}	158	7.40×10^{-4}	166	6.99×10^{-4}	165
8.00×10^{-4}	158	8.00×10^{-4}	166	8.87×10^{-4}	164
1.03×10^{-3}	158	1.03×10^{-3}	166	1.00×10^{-3}	164
2.95×10^{-3}	156	2.90×10^{-3}	163	2.95×10^{-3}	161
5.80×10^{-3}	154	8.00×10^{-3}	157	5.80×10^{-3}	156
7.30×10^{-3}	153	3.00×10^{-2}	132	3.00×10^{-2}	121
8.79×10^{-3}	151	4.25×10^{-2}	119	4.25×10^{-2}	105
9.00×10^{-3}	151	6.88×10^{-2}	93	5.58×10^{-2}	90
4.25×10^{-2}	121	8.15×10^{-2}	80	6.88×10^{-2}	75
8.15×10^{-2}	87	9.38×10^{-2}	68	8.15×10^{-2}	61
9.38×10^{-2}	77			9.38×10^{-2}	50

Figures 7.7, 7.8, and 7.9 show the relationship between distance and mole fraction of OH at different concentrations of $KHCO_3$. The distance is in centimetres (cm) and the mole fraction of OH is represented in decimal form. The concentrations of $KHCO_3$ used in the evaluation are 00015%, 0.0103%, 0.0591%, 0.103%, 4.25% and 8.15%. The data suggests that as the concentration of $KHCO_3$ increases, the mole fraction of OH decreases. Additionally, the mole fraction of OH increases as the distance from the source of the mixture decreases. However, in the lean mixture, for example, at 0.256 cm with a concentration of 8.15% $KHCO_3$, the mole fraction of OH suddenly drops from 0.011 to 0.00382.

The reduction of OH in the rich mixture is higher than in the lean and stoichiometric mixtures.

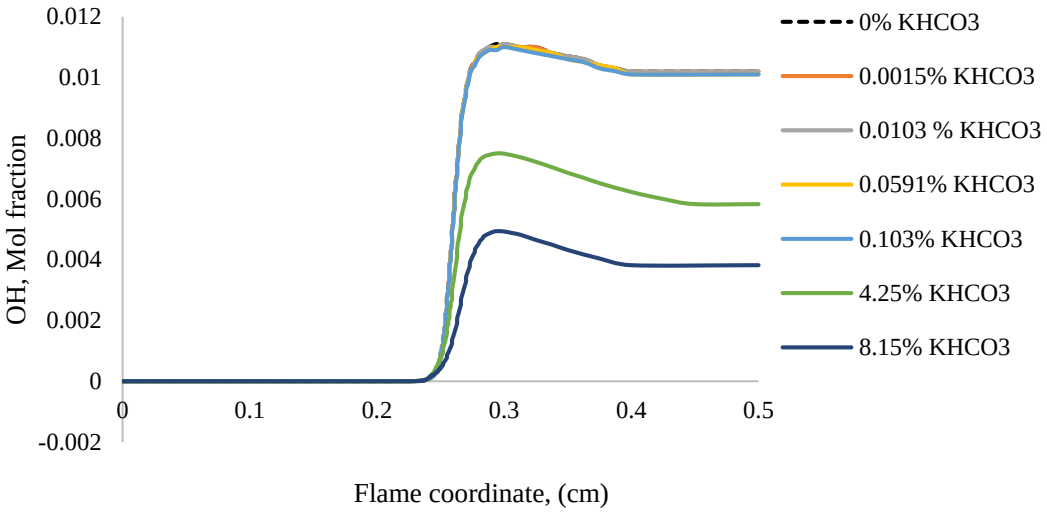


Figure 7.7: Flame concentration profiles of hydroxyl radical at different inhibitor mole fraction of $KHCO_3$ loadings (lean CH_4/air flame, initial conditions, (673 K,1 atm)).

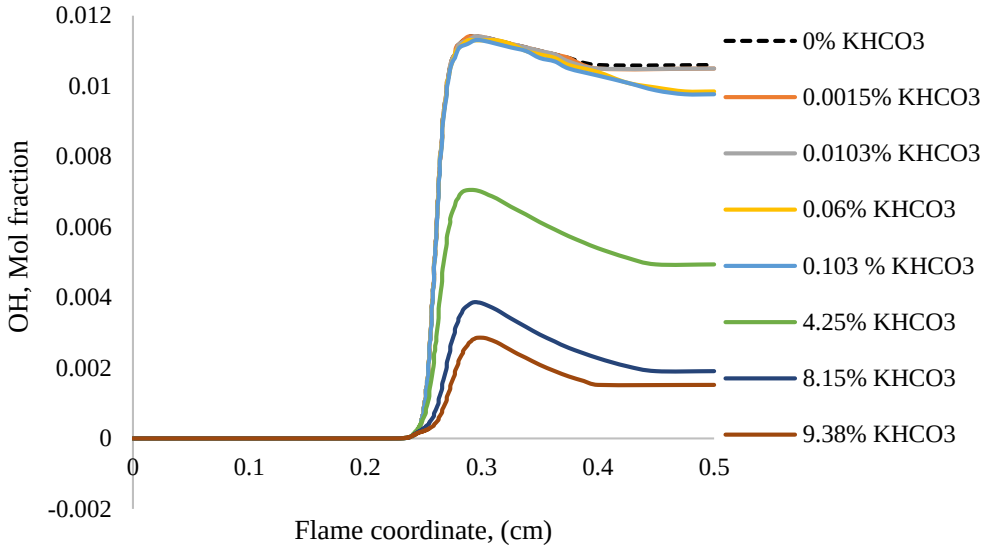


Figure 7.8: Flame concentration profiles of hydroxyl radical at different inhibitor mole fraction of $KHCO_3$ loadings (stochiometric CH_4/air flame, initial conditions, (673 K,1 atm)).

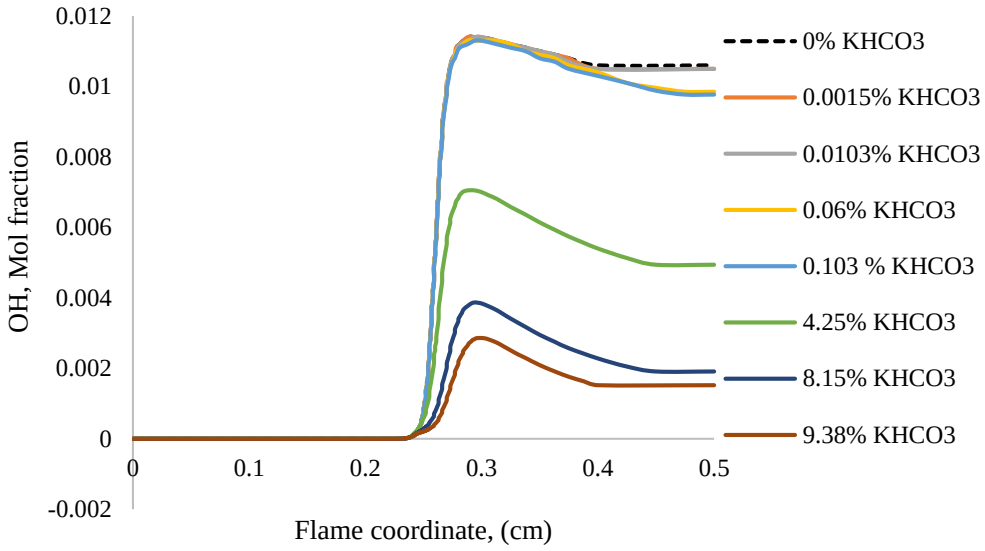


Figure 7.9: Flame concentration profiles of hydroxyl radical at different inhibitor mole fraction of $KHCO_3$ loadings (rich CH_4/air flame, initial conditions, (673 K,1 atm)).

7.4 The Inhibition Effect of KCO_3 on S_L and OH Mole Fraction

Figure 7.10 presents an analysis of the impact of varying KCO_3 mole fractions on the flame speed (S_L) of CH_4 across different equivalence ratios.

The figure systematically provides data on the flame speed of CH_4 flame for lean, stoichiometric, and rich mixtures, with varying KCO_3 mole fractions. As the KCO_3 mole fraction increases from 0 to 0.1. Notably, there is a clear trend of decreasing S_L for CH_4 across all equivalence ratios with the increase in the KCO_3 mole fraction. However, it should be noted that the influence of KCO_3 on S_L of CH_4 is not linear in all scenarios. Some irregularities emerge within the data set. At lower KCO_3 mole fractions, the S_L values for all air-fuel ratios remain relatively high, but they exhibit a rapid decline as KCO_3 mole fractions increase. This trend is observable in stoichiometric, rich, and lean mixtures alike. While S_L of CH_4 in rich and stoichiometric mixtures experiences a noticeable decrease with higher KCO_3 mole fractions, there is a slight increase in S_L at lean mixtures. This indicates that the influence of KCO_3 on combustion behaviour can lead to non-linear effects under certain conditions, as shown in Table 7.5.

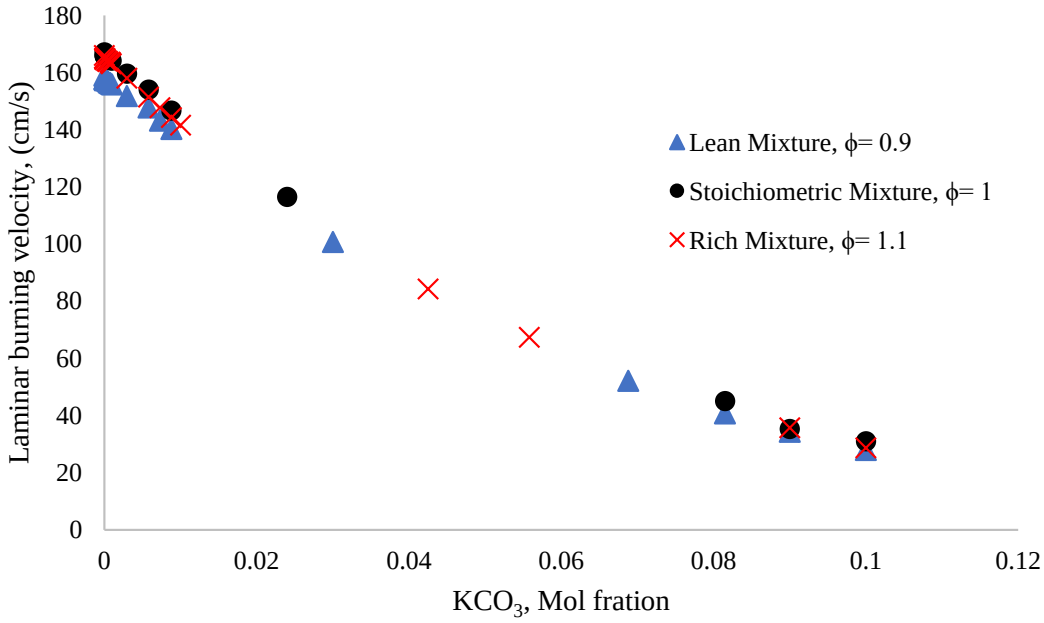


Figure 7.10: The effect of KCO_3 on the laminar burning velocity of CH_4/air as a function of equivalence ratio (initial conditions: 673 K, 1 atm, lean, stoichiometric, and rich mixtures, ϕ = 0.9, 1.0, and 1.1).

Table 7.5: The Inhibition Effect of KCO_3 Mole Fraction on the Laminar Burning Velocity of CH_4/air Flame

KCO_3 Mole fraction	S_L, (cm/s) of CH_4 at ϕ= (0.9)	KCO_3 Mole fraction	S_L, (cm/s) of CH_4 at ϕ = (1)	KCO_3 Mole fraction	S_L, (cm/s) of CH_4 at ϕ= (1.1)
0.00	159	0.00	167	0.00	166
1.50×10^{-5}	158	1.50×10^{-5}	166	1.50×10^{-5}	165
2.95×10^{-5}	158	2.95×10^{-5}	166	2.95×10^{-5}	165
4.44×10^{-5}	158	5.9×10^{-5}	166	5.90×10^{-5}	165
5.90×10^{-5}	157	7.00×10^{-5}	166	7.00×10^{-5}	165
7.00×10^{-5}	158	1.00×10^{-4}	166	8.87×10^{-5}	165
8.87×10^{-5}	158	2.00×10^{-4}	166	2.96×10^{-4}	164
1.00×10^{-4}	158	5.90×10^{-4}	165	4.44×10^{-4}	164
2.00×10^{-4}	158	7.40×10^{-4}	165	7.40×10^{-4}	164
4.00×10^{-4}	157	9.30×10^{-4}	164	8.00×10^{-4}	163
5.90×10^{-4}	156	2.95×10^{-3}	160	9.00×10^{-4}	163
7.40×10^{-4}	156	5.5×10^{-3}	154	2.95×10-3	158
8.20×10^{-4}	156	8.79×10^{-3}	147	5.80×10^{-3}	151
9.90×10^{-4}	156	2.40×10^{-2}	117	7.30×10^{-3}	148
2.95×10^{-3}	152	8.15×10^{-2}	45	8.79×10^{-3}	144
5.00×10^{-3}	148	9.38×10^{-2}	35	1.00×10^{-2}	142
7.30×10^{-3}	143	1.00×10^{-1}	31	4.25×10^{-2}	84
8.79×10^{-3}	140			5.58×10^{-2}	67
3.00×10^{-2}	101			9.00×10^{-2}	36
6.88×10^{-2}	52			1.00×10^{-1}	29
8.15×10^{-2}	41				
9.00×10^{-2}	34				
1.00×10^{-1}	28				

Figures 7.11, 7.12, and 7.13 below offer an analysis of the mole fraction of OH radicals at various distances from the model, in different equivalence ratios. These figures provide critical information on the role of KCO_3 concentration in influencing the formation of OH radicals in the combustion process. In this model, variations in the concentration of KCO_3 were systematically investigated to understand its impact on the generation of OH radicals. Figures present data for a wide range of KCO_3 concentrations, ranging from 0.0015% to 10%.

From the figures below, it can be seen that the effect is not uniform across all concentrations of KCO_3. At lower KCO_3 concentrations, specifically ranging from 0.0015% to 0.08%, the mole fraction of OH radicals remains relatively unaffected. This phenomenon could be attributed to a threshold effect, indicating that KCO_3 starts exerting a significant influence on the formation of OH radicals only beyond a certain concentration.

Furthermore, the influence of KCO_3 on the mole fraction of OH radicals is not uniform across all distances from the model. As the distance increases, the effect becomes more

pronounced. For example, at a distance of 0.5 cm, the decrease in the mole fraction of OH radicals due to KCO_3 is notably higher compared to the effect observed at 0.3 cm.

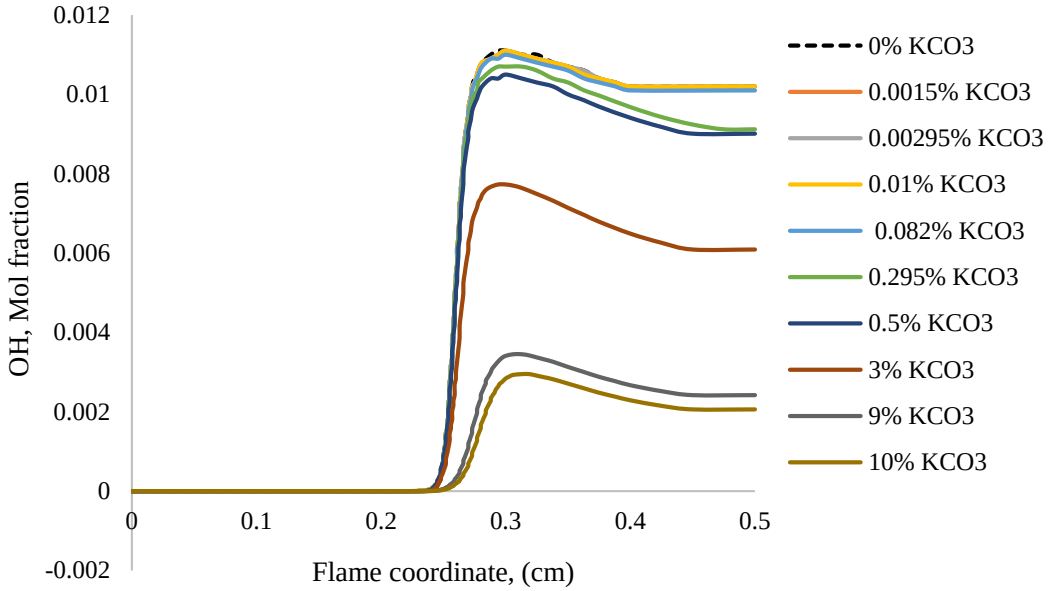


Figure 7.11: Flame concentration profiles of hydroxyl radical at different inhibitor mole fraction of KCO_3 loadings (lean CH_4/air flame, initial conditions, (673 K,1 atm)).

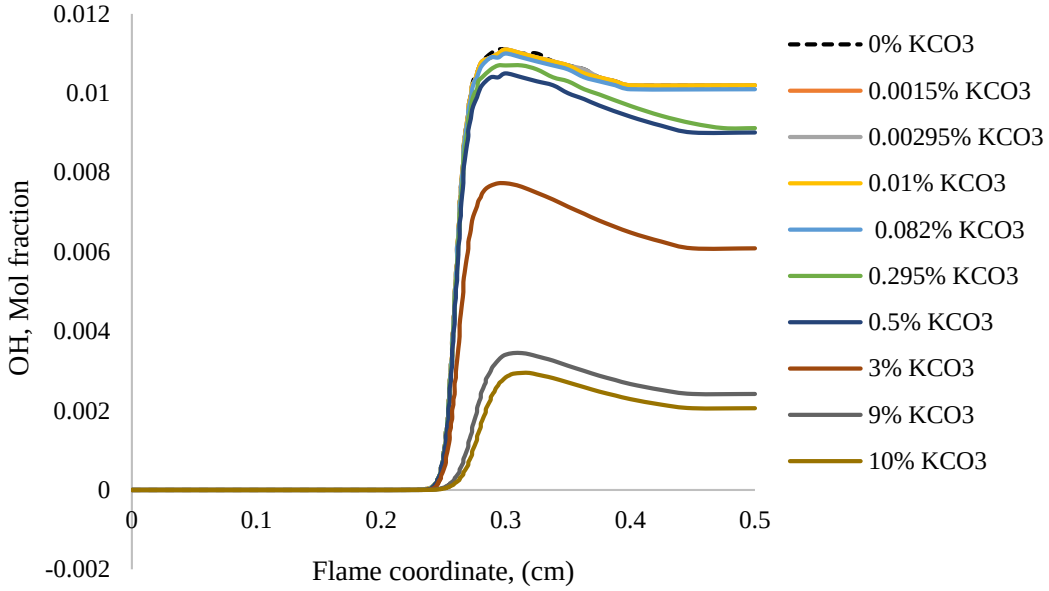


Figure 7.12: Flame concentration profiles of hydroxyl radical at different inhibitor mole fraction of KCO_3 loadings (stochiometric CH_4/air flame, initial conditions, (673 K,1 atm)).

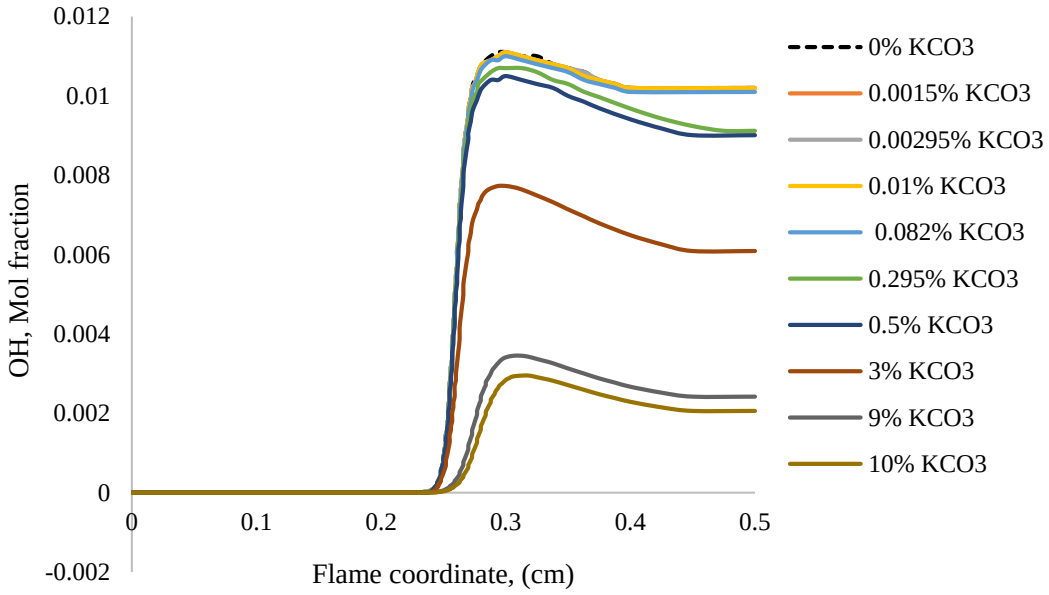


Figure 7.13: Flame concentration profiles of hydroxyl radical at different inhibitor mole fraction of KCO_3 loadings (rich CH_4/air flame, initial conditions, (673 K,1 atm)).

The study's findings focus on the behaviour of $KHCO_3$ and KCO_3 in their role as OH radical reducers within the flame of CH_4. The OH reduction performance of $KHCO_3$ is on par with that of KCO_3, suggesting that both compounds exhibit similar capabilities in influencing the combustion dynamics of CH_4 flames.

However, when the concentration of $KHCO_3$ or KCO_3 exceeds the threshold 5% or at concentrations above this critical point, the OH consumption during the reaction becomes disproportionately high.

The reduction of S_L and the alteration of the OH mole fraction within the CH_4 flame are notably sensitive to the concentration of $KHCO_3$ or KCO_3. This underscores the complex interaction between these potassium-containing compounds and the combustion process, where subtle changes in concentration can lead to significant changes in flame characteristics.

7.5 Comparison Simulation Results

Numerical modeling of homogeneous reaction kinetics was employed to investigate the impact of $KHCO_3$ and KCO_3 on the combustion of CH_4. The focus was on understanding how the presence of these potassium-based compounds affects the flame speed of CH_4 in various mixture ratios, ranging from lean to stoichiometric to rich mixtures.

The results of the simulations show a consistent trend: as the mole fraction of KCO_3 or $KHCO_3$ increases, the S_L of CH_4 decreases.

When comparing the impact of $KHCO_3$ and KCO_3, it is evident that the latter exerts a slightly more pronounced effect on the reduction of the speed of the flame in the CH_4 flames. This implies that KCO_3 has a slightly higher inhibitory effect on combustion in CH_4 flames compared to $KHCO_3$.

7.6 Numerical Simulations Based KCO_3

7.6.1 Predict the Behaviour of CH_4 Flame Under Different Equivalence Ratios and Mole Fractions of KCO_3

The addition of KCO_3 as a suppression agent can introduce challenges with the stability of a flame CH_4. Certain reactions or interactions can lead to numerical instabilities when chemical species such as KCO_3 are incorporated into combustion simulations, especially detailed chemical kinetic models. These instabilities can hinder the convergence of the simulation, causing the simulation to fail or providing inaccurate results.

Figure 7.14 illustrates the impact of two different mole fractions of KCO_3 on the flame speed of CH_4. The database is provided in Appendix (I).

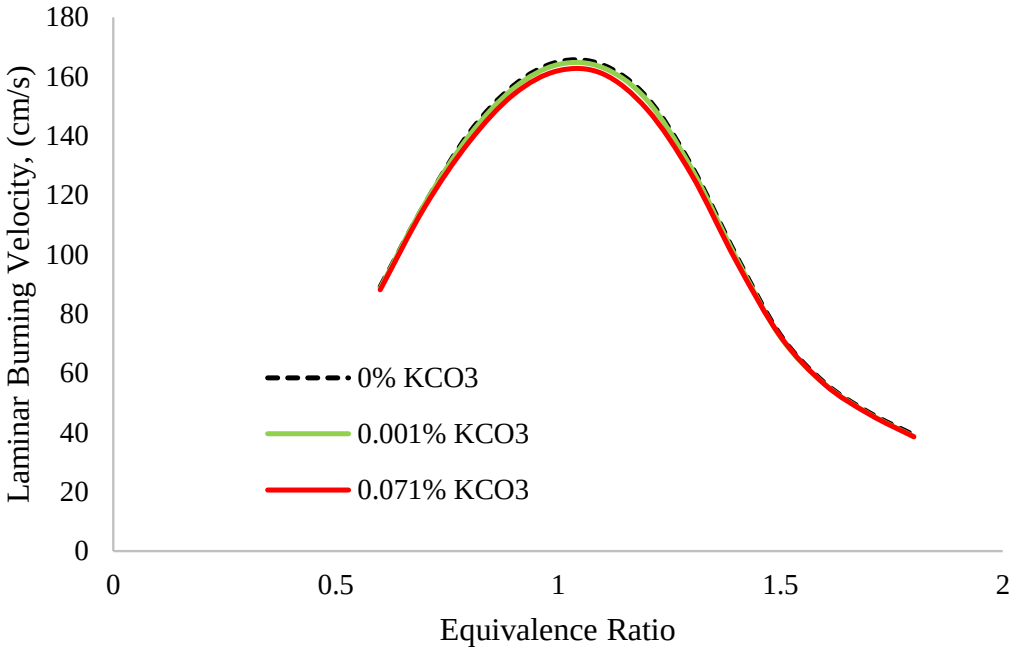


Figure 7.14: Flame speed of CH_4 in various KCO_3 mole fraction.

The graph illustrates that the presence of KCO_3 does not exert a substantial influence on the flame speed of CH_4. Throughout the range of concentrations and equivalence ratios examined, the flame speed of pure CH_4 remains consistently stable. This consistency implies that CH_4 retains its flammable properties within the specified conditions, even in the presence of KCO_3.

These findings suggest that, at the concentrations tested, KCO_3 does not significantly alter the flammability characteristics of CH_4. The flame speed of CH_4 remains well within the flammable range, indicating that KCO_3, under these specific conditions, does not have a pronounced inhibitory effect on CH_4 combustion.

7.6.2 The Influence of KCO_3 and $KHCO_3$ on the Adiabatic Flame Temperature of Stoichiometric CH_4/air Mixture

As illustrated in Figures 7.15 and 7.16, the graphs depict the influence of varying concentrations of KCO_3 and $KHCO_3$ on the equilibrium temperature of the flame under different initial temperature conditions. As observed, the introduction of KCO_3 and $KHCO_3$ results in notable changes in the adiabatic flame temperature across the examined temperature range (from 300 K to 500 K) and constant pressure. The graphs clearly illustrate the sensitivity of the flame temperature to different levels of KCO_3 and $KHCO_3$, with higher concentrations leading to a reduction in equilibrium temperatures.

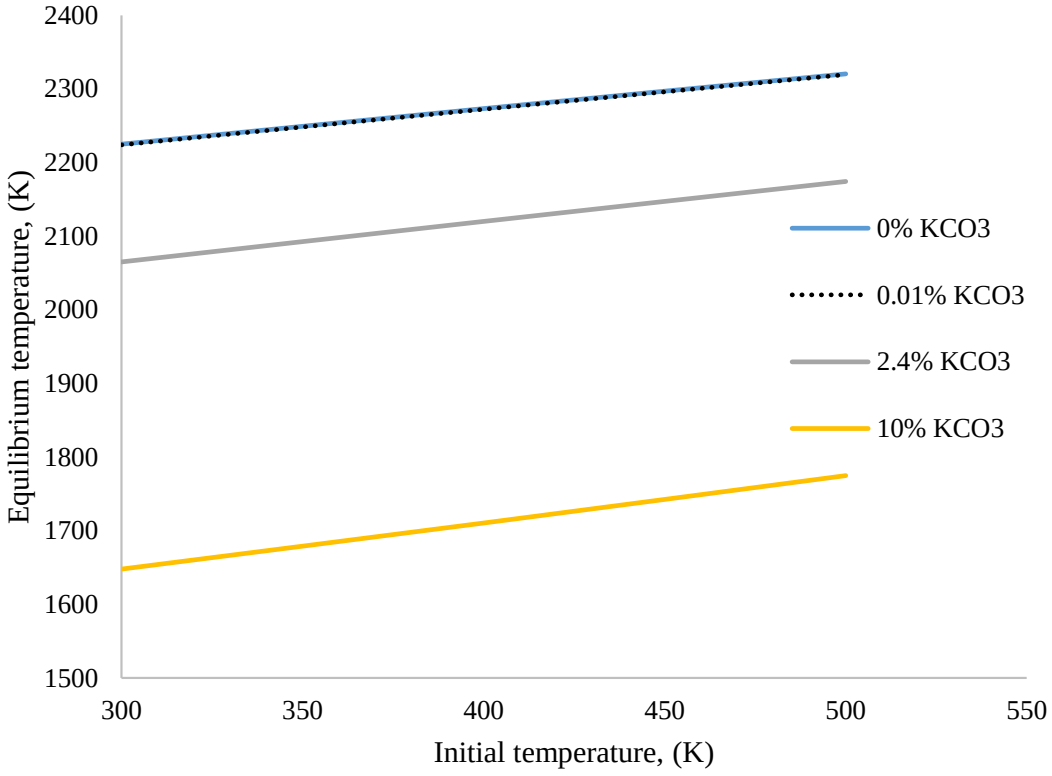


Figure 7.15: The effect of KCO_3 on the AFT of stoichiometric CH_4 flame based on GRI-Mech/K-species mechanism.

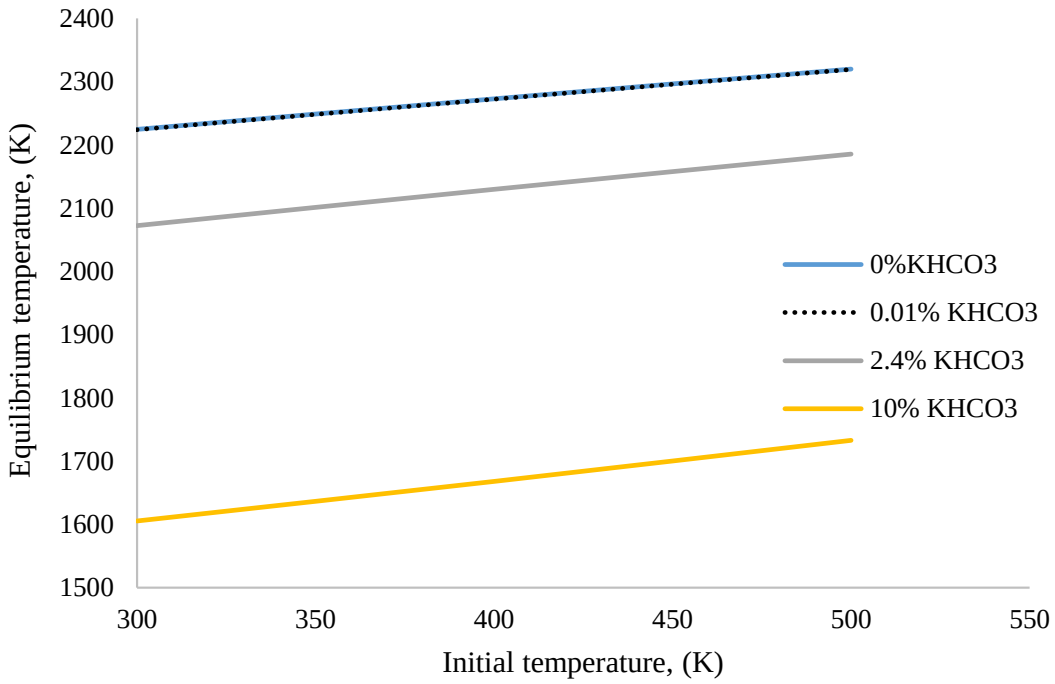


Figure 7.16: The effect of $KHCO_3$ on the AFT of stoichiometric CH_4 flame based on GRI-Mech/K-species mechanism.

7.6.3 Pathway Analysis of Stoichiometric CH_4/air Mixture with Adding KCO_3

Figure 7.17 illustrates the reactions of the primary pathway reactions involved in a CH_4 flame. In this combustion process, CH_4 is a crucial fuel source that undergoes a series of chemical reactions leading to the production of various reaction intermediates and final products Wang et al. (2018).

The figure visually represents the key reactions that occur during the combustion of CH_4 and shows the behaviour of this flame. It can be seen that CH_4 is consumed during reactions that involve atomic OH, H, and O.

These reactions are depicted below:

$H + CH_4 <=> CH_3 + H_2$

In this reaction, the H atom reacts with CH_4, leading to the formation of a methyl radical (CH_3) and H_2. This represents a fundamental step in the combustion of CH_4.

$OH + CH_4 <=> CH_3 + H_2O$

OH participates in a reaction with CH_4, resulting in the generation of CH_3 and H_2O. This reaction contributes to the conversion of CH_4 within the flame.

$O + CH_4 <=> OH + CH_3$

O atom reacts with CH_4 to produce OH and CH_3. This reaction is significant for the conversion of CH_4 in the flame.

One notable aspect of this figure is that it serves as a valuable tool to investigate the impact of KCO_3 on the behaviour of the CH_4 flame.

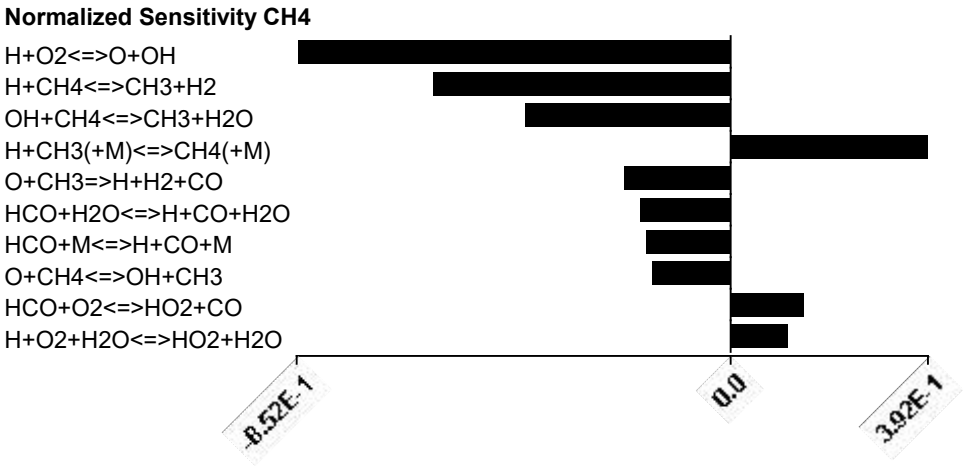


Figure 7.17: Normalized Sensitivity analysis of stoichiometric CH_4/air mixture developed by GRI-Mech/K-species Mechanism at initial condition, 673 K,1 atm, and 0% mole fraction of KCO_3.

0.001% Mole Fraction of KCO_3

Figure 7.18 shows a set of chemical reactions that are relevant to the combustion of CH_4 in the presence of an extremely small amount of KCO_3 added to the mixture (0.00001 KCO_3, which corresponds to 0.001% mole fraction of KCO_3). These reactions are essential in understanding how the addition of KCO_3 influences the combustion process. It is clear that KCO_3 does not exert a substantial impact on the pathway of the CH_4 flame. The primary reactions involved in the combustion of CH_4 appear to remain largely unaffected by the presence of KCO_3.

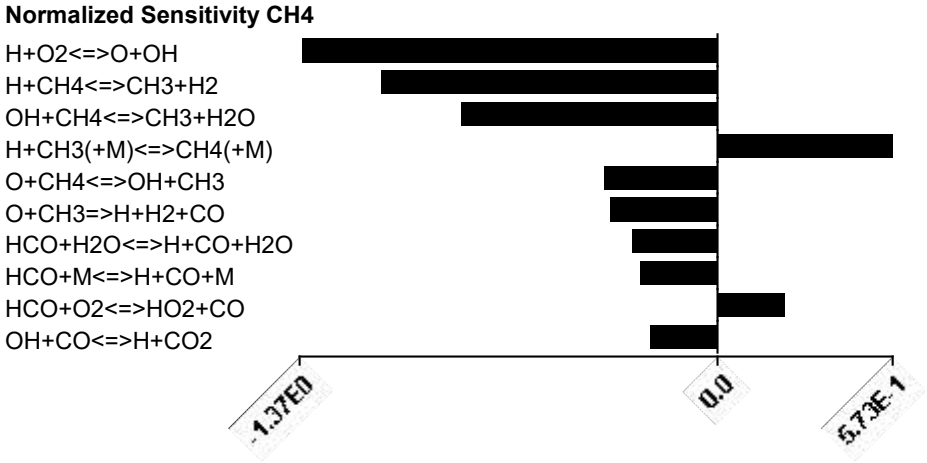


Figure 7.18: Normalized Sensitivity analysis of stoichiometric developed by GRI-Mech/K-species Mechanism at initial condition, 673 K,1 atm, and 0.001% mole fraction of KCO_3.

8.15% Mole Fraction of KCO_3

The provided set of reactions and their associated normalized sensitivity values correspond to the combustion of CH_4 with the introduction of 8.15% mole fraction of KCO_3 is shown in Figure 7.19.

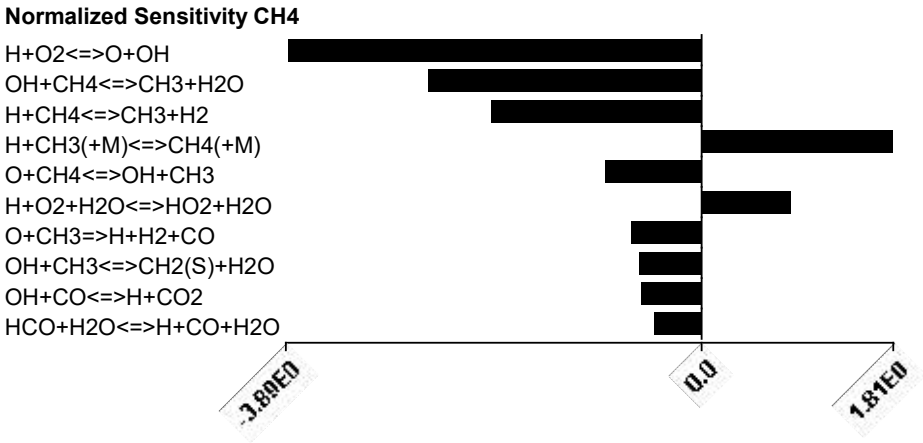


Figure 7.19: Normalized Sensitivity analysis of stoichiometric CH_4/air mixture developed by GRI-Mech/K-species Mechanism at initial condition, 673K,1atm, and 8.15% mole fraction of KCO_3.

It is evident that, under these specific conditions, KCO_3 does not induce substantial alterations in the combustion pathway of CH_4. This underscores the sensitivity of KCO_3's impact on its concentration.

10% Mole Fraction of KCO_3

Figure 7.20 presents the reactions and their corresponding normalized sensitivity values, which represent the essential chemical reactions involved in the combustion of CH_4 with the introduction of a 10% mole fraction of KCO_3. At a higher concentration of KCO_3 (10% mole fraction), a clear impact on the combustion pathway of CH_4 becomes evident. It can be seen that specific reactions that involve the consumption and generation of chemical species are significantly influenced by KCO_3, indicating its substantial role in altering combustion dynamics. Consequently, under these specific conditions, a 10% mol fraction of KCO_3 substantially reshapes the CH_4 combustion pathway, exerting notable effects on reaction kinetics and overall combustion processes. Furthermore, at elevated temperatures, Figure 7.21 illustrates the production of KCO_3 through the reaction $OH+KHCO_3=KCO_3+H_2O$.

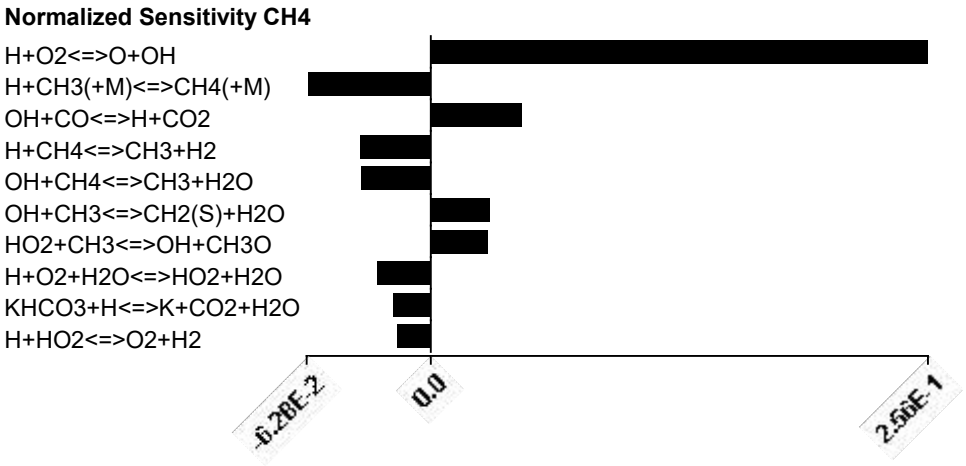


Figure 7.20: Normalized Sensitivity analysis of stoichiometric CH_4/air mixture developed by GRI-Mech/K-species Mechanism at initial condition, 673 K,1 atm, and 10% mole fraction of KCO_3.

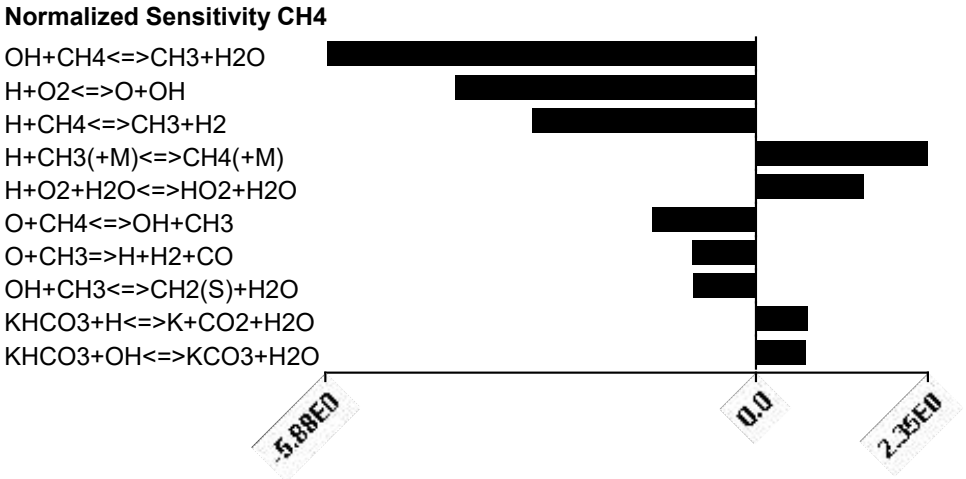
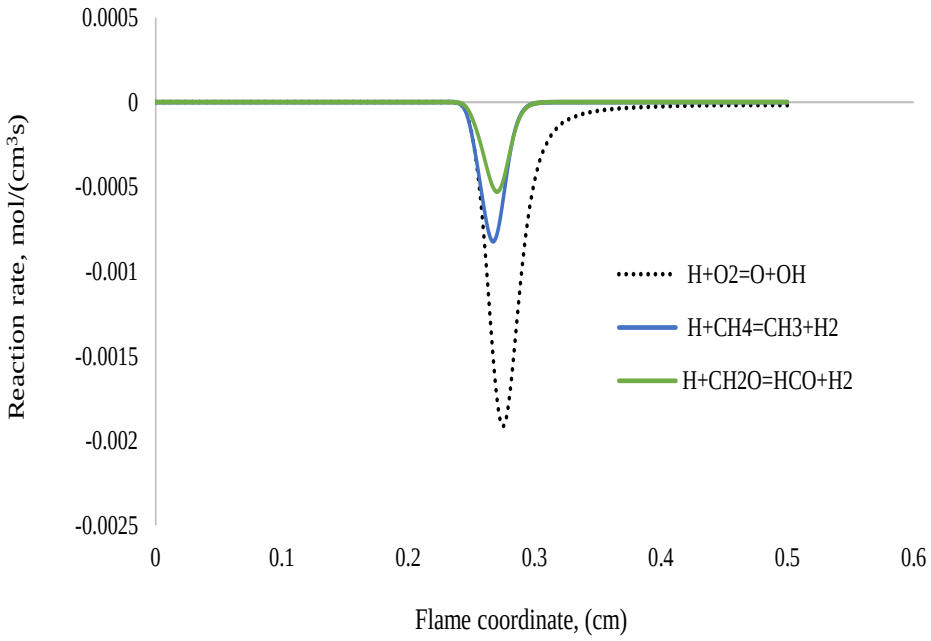


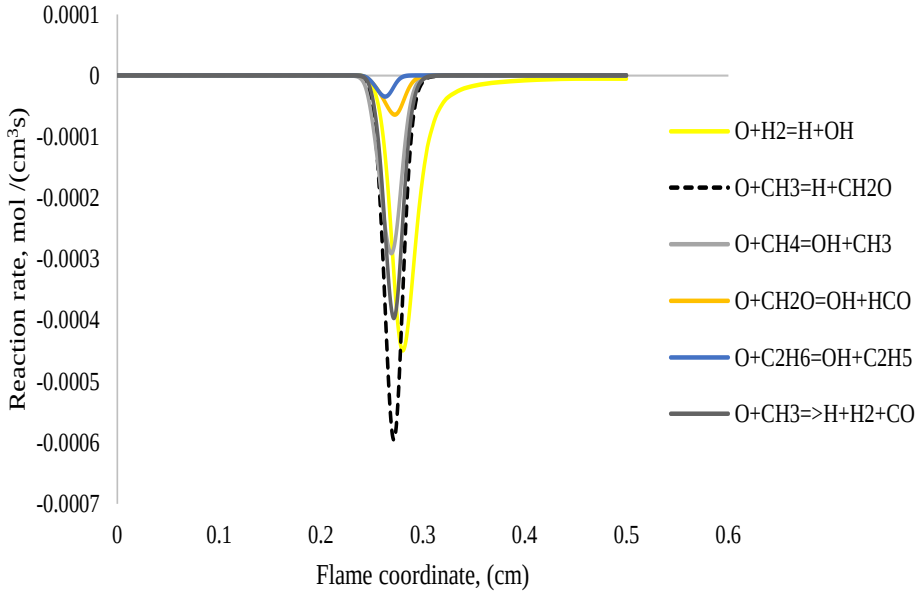
Figure 7.21: Normalized Sensitivity analysis of stoichiometric CH_4/air mixture developed by GRI-Mech/K-species Mechanism at initial condition, 673 K,1 atm, and 10% mole fraction of KCO_3 at specific flame distance (1823 K, and 0.5 cm).

7.6.4 Reaction Rate Profiles as a Function of Flame Position in a Stoichiometric CH_4/KCO_3 Mixture

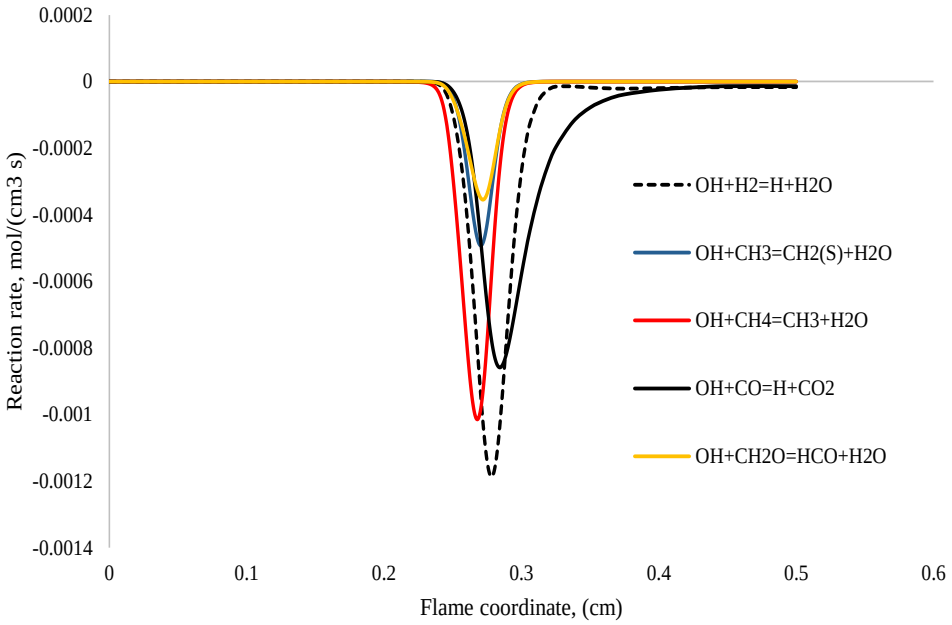
The chosen agent for analyzing the pathway reactions of CH_4 combustion, with a particular focus on investigating the interactions between K-species and the most crucial free radicals within the CH_4 flame (OH, CH_3, and H), is KCO_3. In these simulations, a 0.1 mole fraction of KCO_3 has been introduced. Figures 7.22a, 7.22b, 7.22c, and 7.22d present the reaction rate profiles of the primary reactions responsible for the consumption of H, O, OH, and CH_3 radicals, respectively. Furthermore, Figure 7.22e provides insight into the main reactions governing the formation and consumption of K atoms within the main reaction zone of the flame.


0.0005
0
-0.0005
-0.001
-0.0015
-0.002
-0.0025
Reaction rate, mol/(cm³s)
0
0.1
0.2
0.3
0.4
0.5
0.6
Flame coordinate, (cm)
H+O2=O+OH
H+CH4=CH3+H2
H+CH2O=HCO+H2

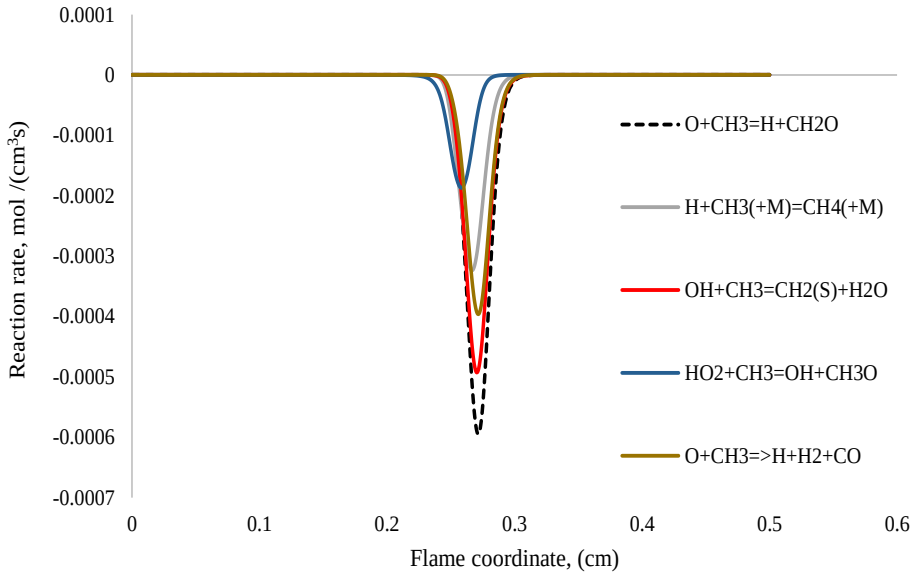
(a)


0.0001
0
-0.0001
-0.0002
-0.0003
-0.0004
-0.0005
-0.0006
-0.0007
Reaction rate, mol /(cm³s)
0
0.1
0.2
0.3
0.4
0.5
0.6
Flame coordinate, (cm)
O+H2=H+OH
O+CH3=H+CH2O
O+CH4=OH+CH3
O+CH2O=OH+HCO
O+C2H6=OH+C2H5
O+CH3=>H+H2+CO

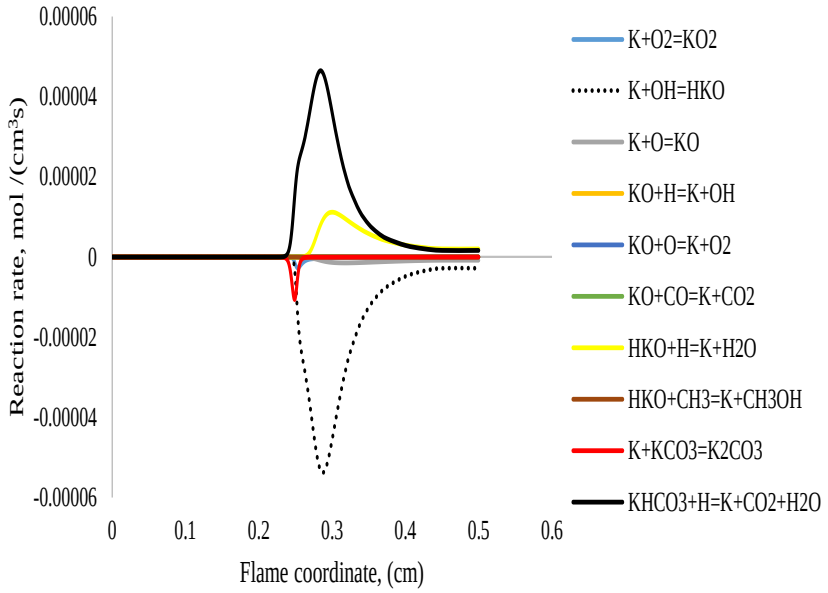
(b)


0.0002
0
-0.0002
-0.0004
-0.0006
-0.0008
-0.001
-0.0012
-0.0014
Reaction rate, mol/(cm3 s)
0
0.1
0.2
0.3
0.4
0.5
0.6
Flame coordinate, (cm)
OH+H2=H+H2O
OH+CH3=CH2(S)+H2O
OH+CH4=CH3+H2O
OH+CO=H+CO2
OH+CH2O=HCO+H2O

(c)



(d)



(e)

Figure 7.22: Reaction rate profiles as a function of position in the flame, for the main reactions of (a) H atom (b) O atom consumption (c) OH radical (c) CH_3 radical (e) formation and consumption of potassium atom (stoichiometric CH_4/air flame, 673 K, 1 atm, KCO_3 mole fraction of 0.1).

One notable observation is that O atoms are consumed primarily through the reaction $O + \mathrm{CH_3} = H + \mathrm{CH_2O}$. Conversely, OH radicals are consumed by CH_4, H_2, and CO, leading to the production of various products. H radicals, on the other hand, are mostly absorbed through the reaction:

$H + O_2 = O + OH$

Lastly, CH_3 radicals are consumed via various reactions:
$O + CH_3 = H + CH_2O$
$OH + CH_3 = H + CH_2 + H_2O$
$O + CH_3 = H + H_2 + CO$
$H + CH_3 + M = CH_4 + M$
$HO_2 + CH_3 = OH + CH_3O$

The analysis reveals that the reactions involving the K species, despite their presence within the combustion model, do not appear to significantly affect the behaviour of the H, O, OH, and CH_3 radicals, as suggested by the graphs depicting the relationship between reaction rates and flame coordinates. This phenomenon might be attributed to the kinetic parameters or relative concentrations of the K-species reactions in comparison to the other dominant reactions in the combustion process.

Contribution of OH Radical to Consumed K: Figure 7.22e illustrates the contribution of OH radicals to the consumption of K through a reaction: K + OH = HKO. The presence of this reaction pathway indicates that OH radicals actively participate in the removal or consumption of K species within the combustion environment.

Contribution of H Atom to Producing K: Figure 7.22e shows the contribution of H atoms to the production of K. This is achieved through a reaction involving HKO, through the reaction HKO + H = K + H_2O. This reaction pathway illustrates how H atoms, which are abundantly present within combustion environments, can lead to the production of K.

7.7 Numerical Simulations Based on $KHCO_3$

7.7.1 Comparison Study of the Potassium Species ($KHCO_3$) in CH_4/air Mixture with a Previous Study

This section elucidates the kinetic impact of integrating K-species reactions into the GRI-mech mechanism. Based on previous investigations, the influence of $KHCO_3$ mol fractions on stoichiometric CH_4 flame has been examined. Specifically, Babushok et al. (2017) have developed a gas-phase kinetic model of $KHCO_3$ inhibition on CH_4/air flames. The computational analysis in their work was performed using the Chemkin tool. Notably, the flame speed was calculated at the initial conditions: 298 K and 1 atm. and the resultant outcomes were subsequently compared against the experimental data documented in the literature, where they used experimental data from Rosser Jr et al. (1963) and Hoffmann (1971) to investigate the impact of $KHCO_3$ on the burning velocity of a stoichiometric CH_4/air flame. It is important to note that $KHCO_3$ is introduced into flames in the form of solid particles, with varying diameters within two specified ranges: 2.2 μm (as reported by Rosser Jr et al. (1963)) and 32–40 μm (as detailed in Hoffmann, 1971). The graph illustrates the normalized burning velocity of premixed stoichiometric CH_4/air flames. It

compares the measured values with those predicted numerically, showcasing a reasonable agreement, as the $KHCO_3$ volume fraction (introduced as solid particles) varies.

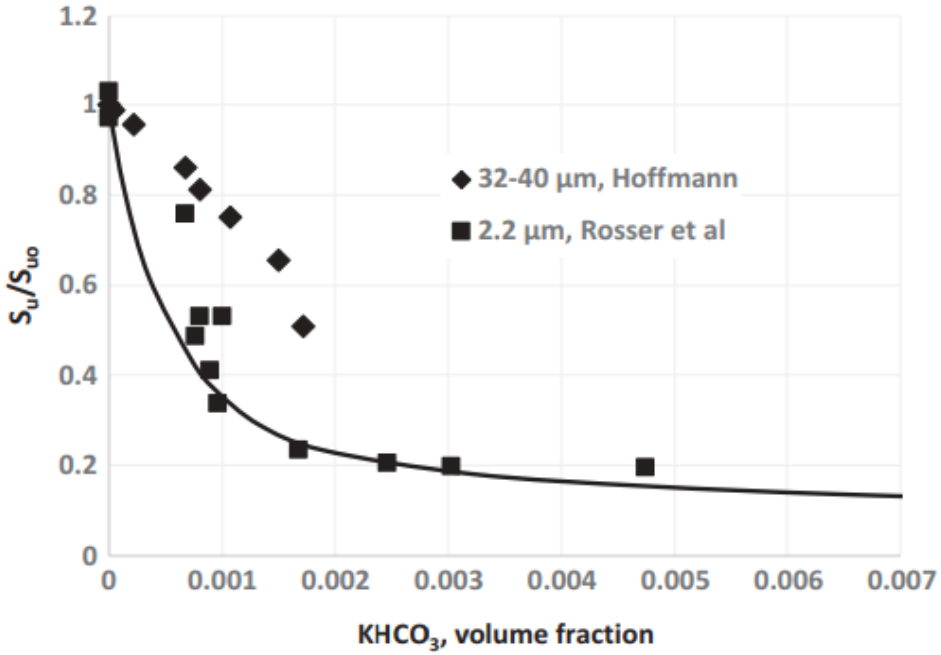


Figure 7.23: Dependence of burning velocity S_u normalized by the uninhibited burning velocity S_{uo} on $KHCO_3$ volume fraction for stoichiometric methane-air flame (line: calculations; symbols: experimental data; initial conditions: 298 K, 1 atm) Babushok et al. (2017).

The present investigation has produced Figure 7.24, which shows the predicted burning velocity of the premixed stoichiometric CH_4/air flame, plotted against the $KHCO_3$ concentration at initial conditions of 673 K and 1 atm. The predicted burning velocity, which incorporates the added $KHCO_3$ mole fraction, exhibits a significant level of concordance with the findings reported by Babushok et al. (2017), particularly regarding the reduced burning velocity resulting from the presence of $KHCO_3$.

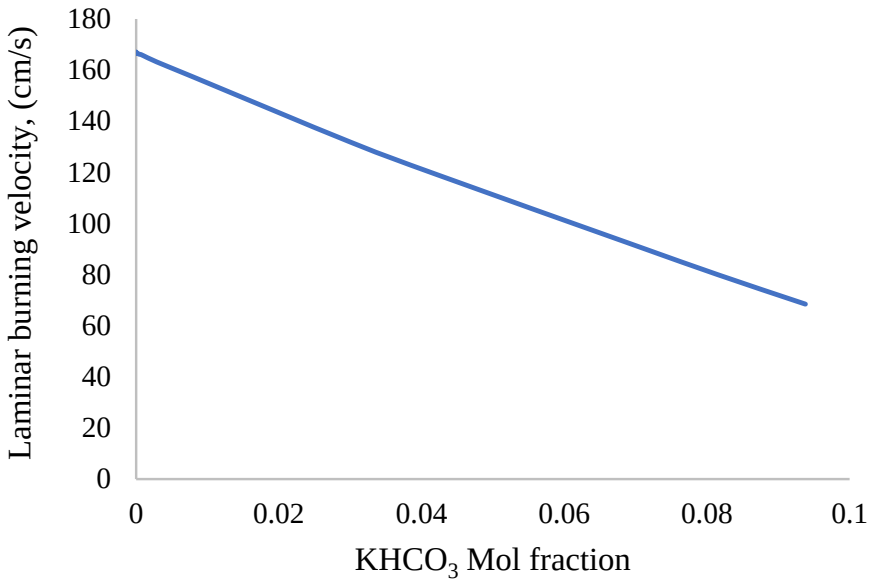
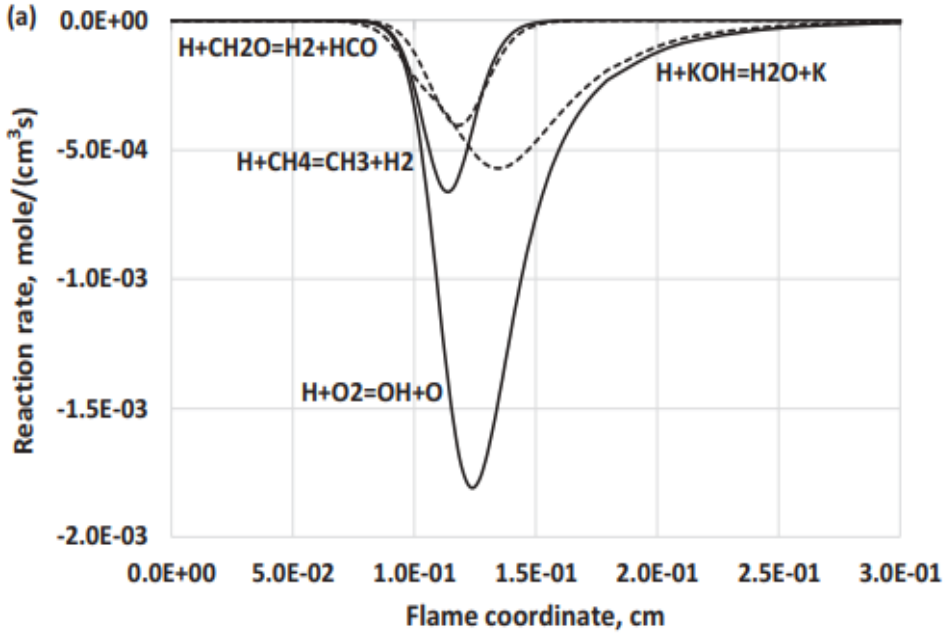
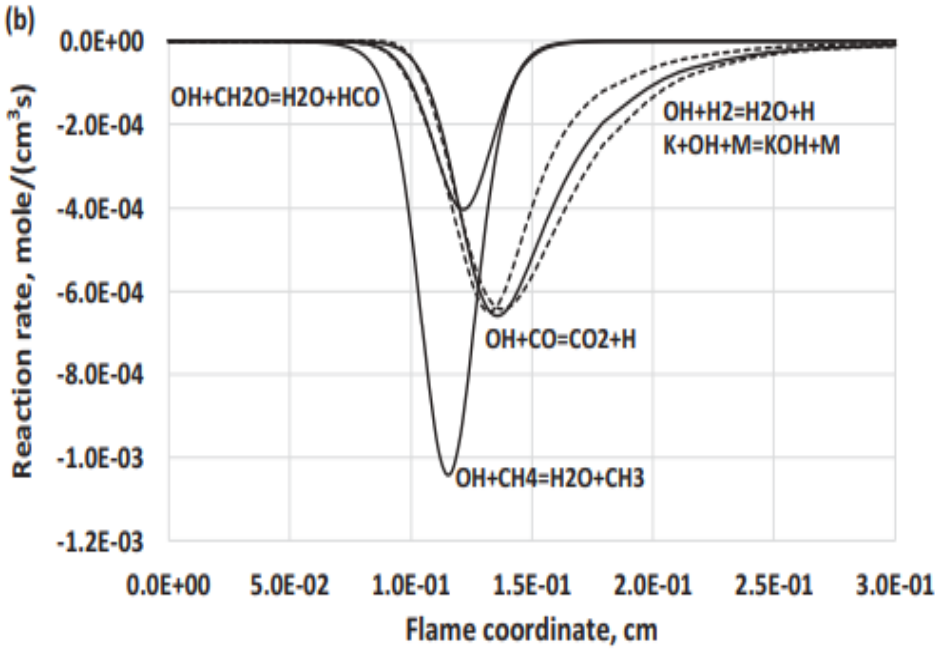


Figure 7.24: The laminar burning velocity of stoichiometric CH_4/air flame affected by $KHCO_3$ mole fraction at 673 K and 1 atm.

Based on Babushok et al. (2017), Figure 7.25 depicts the profiles of reaction rates for the primary reactions involving the consumption of H, OH radicals, and the main reactions responsible for the formation and consumption of potassium atoms in the primary reaction zone of the flame. They concluded that the key H atom scavenging reaction for potassium species is represented by KOH + H = H_2O + K, while the OH radical termination reaction is characterized by OH + K + M = KOH + M.

The main radical scavenging reactions involving potassium-containing species include K + OH + M = KOH + M and KOH + H = K + H_2O. This sequence of reactions delineates a relatively straightforward radical recombination cycle: the potassium atom predominantly recombines with the hydroxyl radical, resulting in the formation of potassium hydroxide. Subsequently, the reaction of potassium hydroxide with a hydrogen atom regenerates the potassium atom.


(a)
0.0E+00
-5.0E-04
-1.0E-03
-1.5E-03
-2.0E-03
Reaction rate, mole/(cm3s)
H+CH2O=H2+HCO
H+CH4=CH3+H2
H+O2=OH+O
H+KOH=H2O+K
0.0E+00
5.0E-02
1.0E-01
1.5E-01
2.0E-01
2.5E-01
3.0E-01
Flame coordinate, cm


(b)
0.0E+00
-2.0E-04
-4.0E-04
-6.0E-04
-8.0E-04
-1.0E-03
-1.2E-03
Reaction rate, mole/(cm3s)
OH+CH2O=H2O+HCO
OH+H2=H2O+H
K+OH+M=KOH+M
OH+CO=CO2+H
OH+CH4=H2O+CH3
0.0E+00
5.0E-02
1.0E-01
1.5E-01
2.0E-01
2.5E-01
3.0E-01
Flame coordinate, cm

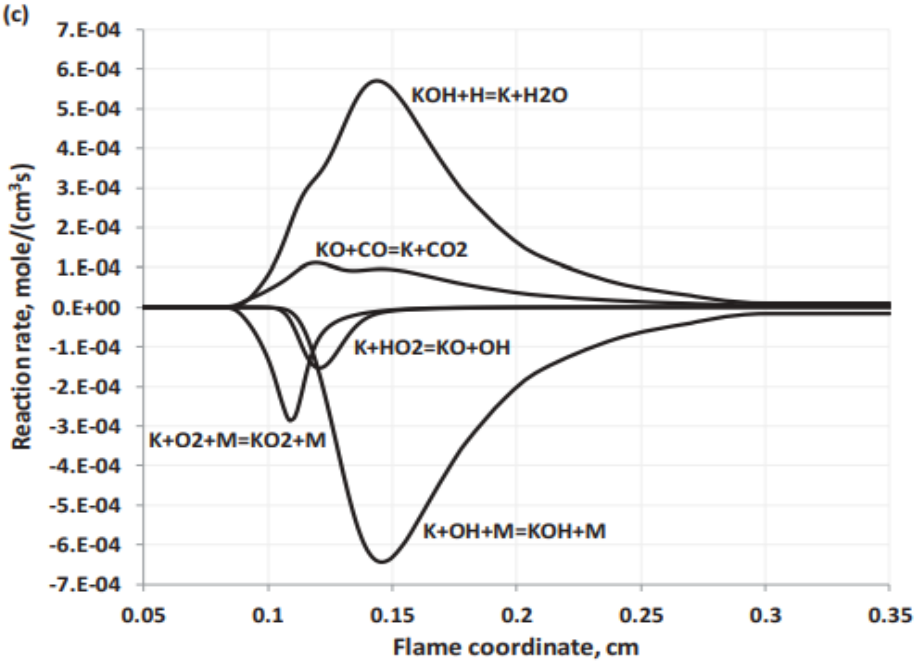
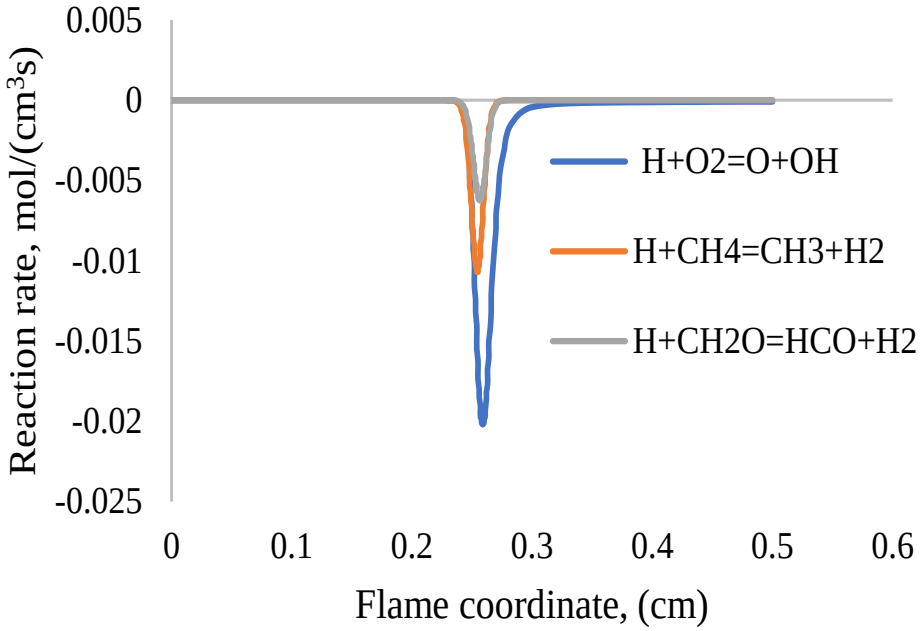


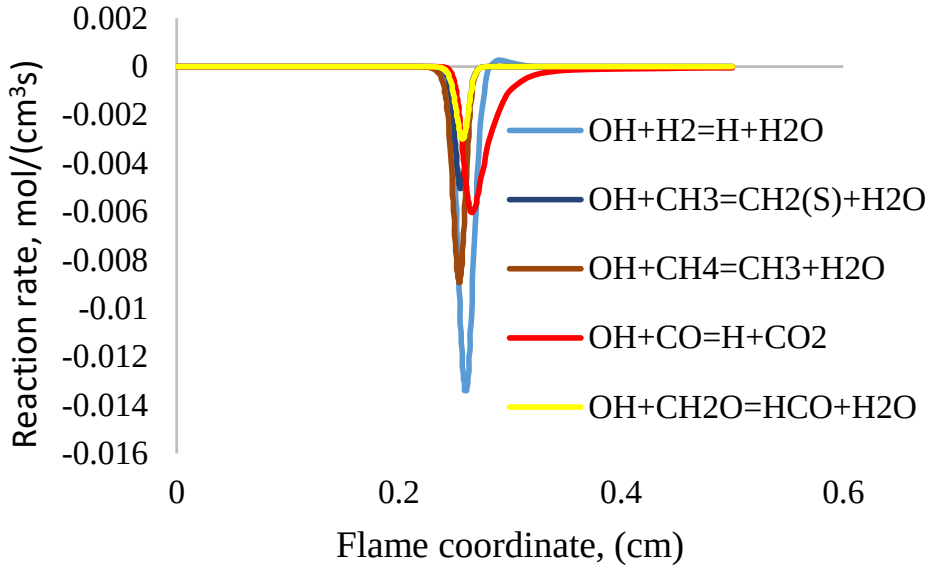
Figure 7.25: Reaction fluxes as a function of position in the flame, for the main reactions of: (a) H atom consumption atom, (b) OH radical consumption, and (c) formation and consumption of potassium atom (stoichiometric CH_4/air flame, 298 K, 1 atm, $KHCO_3$(s) mole fraction of 0.05% Babushok et al. (2017).

In this study using stoichiometric CH_4/air flame, 673 K, 1 atm, $KHCO_3$ mole fraction of 0.05% and due to differences in flame position, this study found that the reactions $KHCO_3$ + H = K +CO_2 + H_2O, K + OH = KOH, and KOH + H = K + H_2O were the main radical scavenging reactions as in Figure 7.26. As can be seen, for the reactions of potassium species, the H atom scavenging reactions are $KHCO_3$+H= K+CO_2+H_2O and KOH + H=H_2O + K. In addition, the OH radical termination reaction is OH + K=KOH.

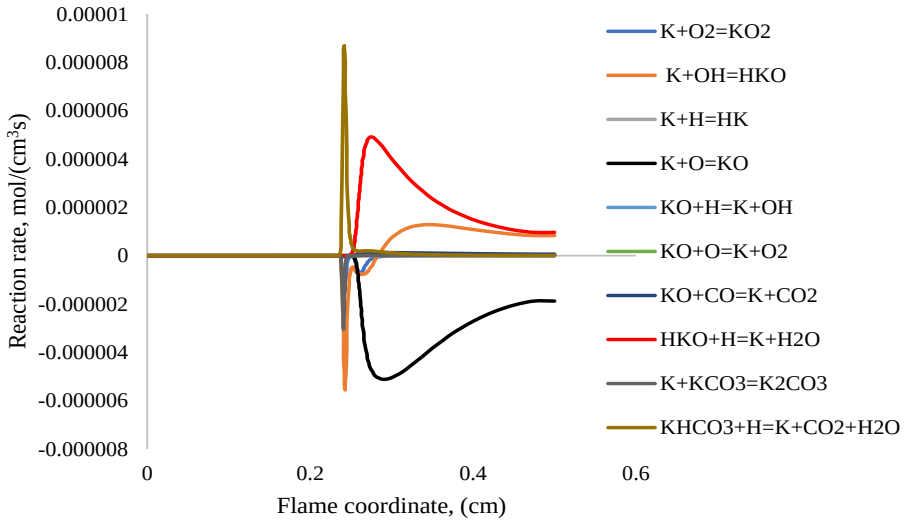
Figures 7.26a, and Figure 7.26b show that $KHCO_3$ do not significantly affect the concentrations of OH free radicals and H atoms, as they are primarily consumed by OH + H_2 = H + H_2O and H + O_2 = O + OH reactions, respectively. However, analyzing the formation and consumption of potassium atoms as presented in Figure 7.26c has helped to illustrate the interactions between K-species, OH, and H free radicals.


0.005
0
-0.005
-0.01
-0.015
-0.02
-0.025
Reaction rate, mol/(cm³s)
0
0.1
0.2
0.3
0.4
0.5
0.6
Flame coordinate, (cm)
H+O2=O+OH
H+CH4=CH3+H2
H+CH2O=HCO+H2

(a)


0.002
0
-0.002
-0.004
-0.006
-0.008
-0.01
-0.012
-0.014
-0.016
Reaction rate, mol/(cm³s)
0
0.2
0.4
0.6
Flame coordinate, (cm)
OH+H2=H+H2O
OH+CH3=CH2(S)+H2O
OH+CH4=CH3+H2O
OH+CO=H+CO2
OH+CH2O=HCO+H2O

(b)



(c)

Figure 7.26: Reaction fluxes as a function of position in the flame, for the main reactions of (a) H atom consumption atom (b) OH radical consumption, and (c) formation and consumption of potassium atom (stoichiometric CH_4/air flame, 673 K, 1 atm, $KHCO_3$ mole fraction of 0.05%).

In Figure 7.27, it is evident that when the $KHCO_3$ volume fraction is approximately 0.1%, the radical overshoot phenomenon diminishes, and the maximum hydroxyl concentration aligns with the equilibrium concentration of the flame. Subsequent addition of the agent results in a reduction of equilibrium concentration due to a decrease in the flame's equilibrium temperature. In contrast, the present study, as demonstrated in Figure 7.28, reveals that a higher mole fraction of $KHCO_3$ is required to eliminate the radical overshoot phenomenon.

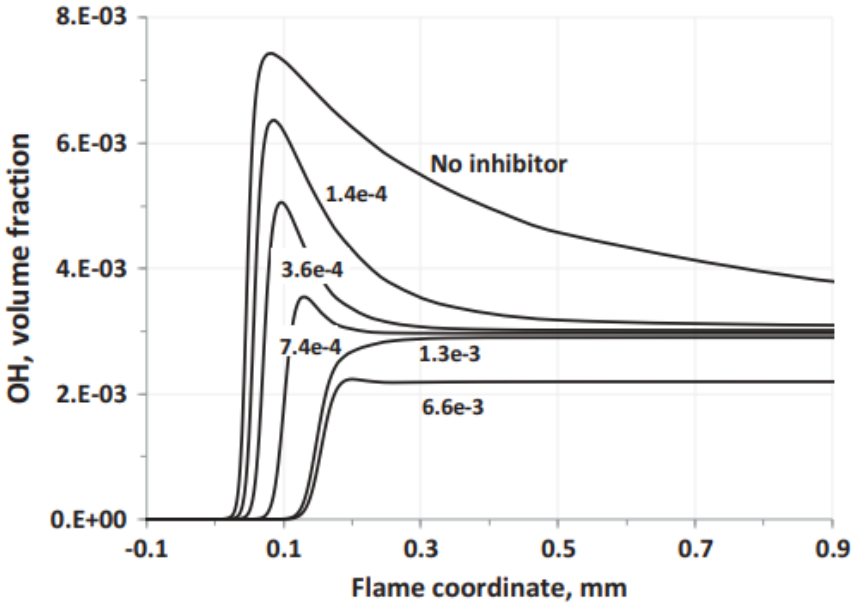


Figure 7.27: Flame concentration profiles of hydroxyl radical at different initial $KHCO_3$(s) loadings (stoichiometric CH_4/air flame, initial conditions: 298 K, 1 atm) Babushok et al. (2017).

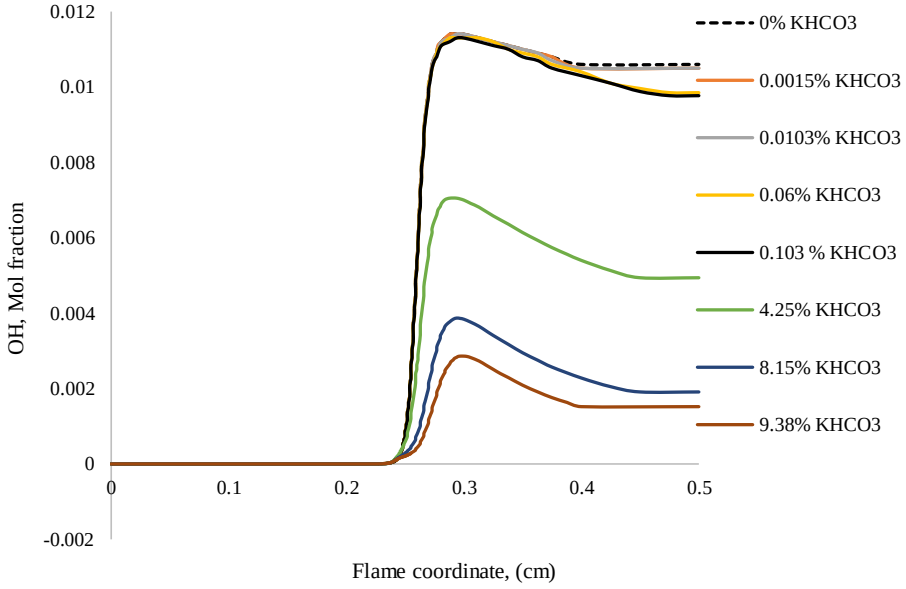


Figure 7.28: Flame concentration profiles of hydroxyl radical at different initial $KHCO_3$ loadings (stoichiometric CH_4/air flame, initial conditions: 673 K, 1 atm).

In Babushok et al. (2017)'s investigation of a stoichiometric CH_4/air flame at 298 K, 1 atm, inhibited by 0.036% mole fraction of $KHCO_3$, the primary potassium-containing species identified in the flame zone are potassium atoms and potassium hydroxide. In particular, a considerable concentration of KO_2 is observed in the lower temperature range, attributed to its rapid formation through the termolecular reaction $K + O_2 + M = KO_2 + M$. However, as the flame temperature increases, the concentration of KO_2 decreases, resulting in a reduced contribution to flame inhibition. Furthermore, a

relatively high concentration of KOH_2 is observed in the low-temperature region of the flame due to the association reaction $\mathrm{KOH} + \mathrm{KOH} = (\mathrm{KOH})_2$. However, in the higher temperature regions of the flame, the concentration of KOH_2 diminishes, and its reactions become less significant for flame inhibition, as evidenced by its absence in Figure 7.29.

In contrast, this study investigates the structure of the flame of a stoichiometric CH_4/air flame at 673 K, 1 atm, inhibited by the 0. 038% mole fraction of $\mathrm{KHCO_3}$. Here, the primary potassium species within the flame zone include KHO only, since the K atom is not observed, as shown in Figure 7.30. The concentrations of $\mathrm{KHCO_3}$, KHO, and $\mathrm{KCO_3}$ disappear, leading to a reduced contribution to flame inhibition.

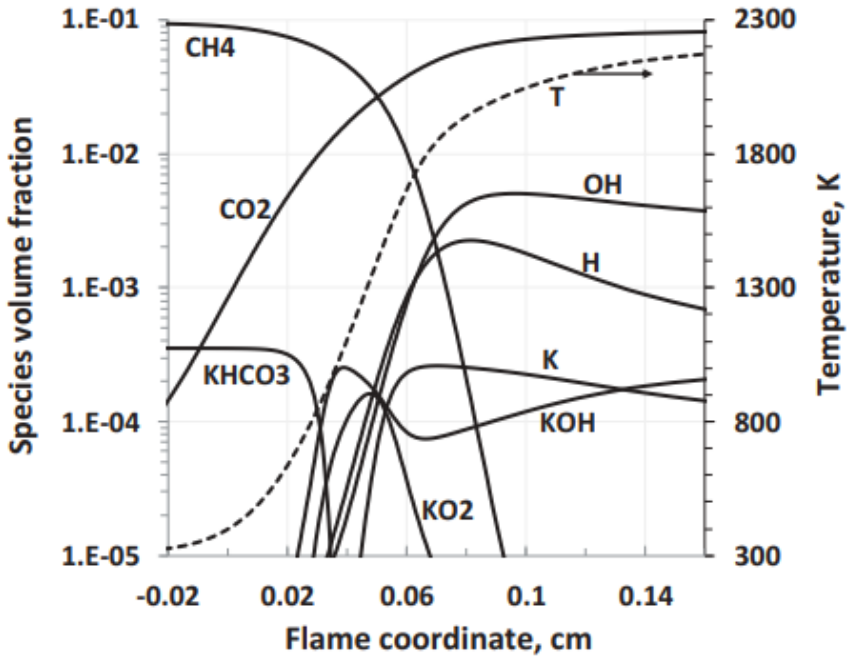


Figure 7.29: Flame structure of $KHCO_3$-inhibited stoichiometric $\mathrm{CH_4/air}$ (initial conditions: 298 K, 1 atm, $KHCO_3$(s) mole fraction of 0.036%) Babushok et al. (2017) .

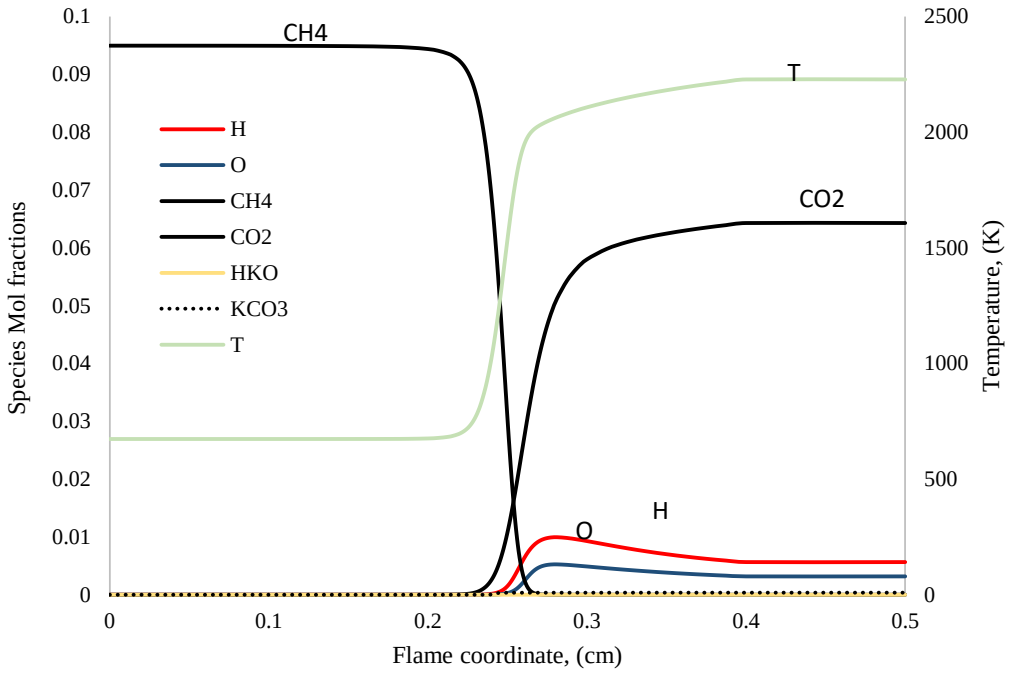


Figure 7.30: Flame structure of $KHCO_3$-inhibited stoichiometric CH_4/air (initial conditions: 673 K, 1 atm, $KHCO_3$ mole fraction of 0.038%).

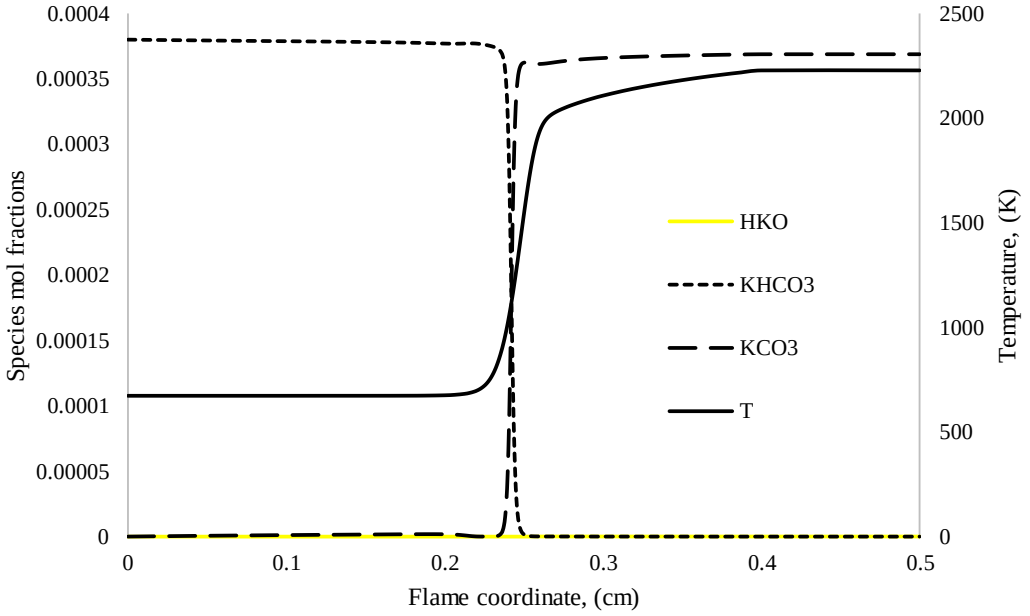


Figure 7.31: Zoomed the specific Distance to describe the flame structure of $KHCO_3$-inhibited stoichiometric CH_4/air (initial conditions: 673 K, 1atm, $KHCO_3$ mole fraction of 0.038%).

According to Babushok et al. (2017) and in the context of adding $KHCO_3$ to premixed CH_4/air flames ((ϕ)= 0.7, 1.0, and 1.34), the computations indicate a significant reduction in burning velocity with increasing $KHCO_3$ addition. The inhibition at low loading is less pronounced in richer premixed CH_4/air flames, aligning with findings from experimental studies.

On the contrary, the current study added $KHCO_3$ to premixed CH_4/air flames with varying equivalence ratios (0.9, 1.0, and 1.1). The results in Subsection 7.3 highlight a distinct observation: the inhibition effect of $KHCO_3$ is more prominent in rich mixtures compared to lean fuel mixtures.

7.7.2 Conclusion of Comparison of Potassium Species ($KHCO_3$) Impact on CH_4/air Mixture.

- The computed burning velocity of premixed CH_4/air flames with $KHCO_3$ addition resulted in a reduction in flame speed, consistent with Babushok's findings.
- The identified primary inhibition reactions, such as K + OH + M = KOH + M and H + KOH = K + H_2O, are in good agreement with the current study and Babushok's research. Due to differences in initial conditions, the reaction involving $KHCO_3$ + H = K + CO_2 + H_2O occurred in the current investigation.
- In contrast to Babushok's results, where the radical overshoot decreases at a volume fraction $KHCO_3$ of around 0.1%, aligning the hydroxyl concentration with the equilibrium concentration of the flame, this study observes that a higher mole fraction of $KHCO_3$ is needed to eliminate the radical overshoot.
- Unlike Babushok's findings suggesting $KHCO_3$ is more effective in lean mixtures than in rich fuel mixtures, this study, covering various equivalence ratios (0.9, 1, 1.1) for CH_4/air mixtures, indicates a different trend. The inhibition effectiveness of $KHCO_3$ is observed to be higher in rich mixtures compared to lean fuel mixtures.
- In the previous study conducted at 298K with a 0.036% mole fraction of $KHCO_3$ on the CH_4/air mixture, the primary potassium-containing species identified in the flame zone were potassium atoms and potassium hydroxide. However, in current simulations at 673 K, adding a 0.038% mole fraction of $KHCO_3$ shows no discernible effect on the CH_4 flame. The concentrations of potassium species are low and their reactions are not considered crucial to flame inhibition under these conditions.

7.8 Summary

- Applying a mole fraction of KO_2 increases the flame speed of a CH_4 flame. Using 20% KO_2 results in a significant increase in flame speed. This high concentration makes KO_2 an ineffective agent for suppressing CH_4 flames.
- There is no reduction in OH using KO_2 on CH_4 flames. The increase in OH levels ensures that the fundamental reaction pathways remain unaffected, allowing the combustion process to proceed efficiently even in the presence of KO_2.
- Apply $KHCO_3$ and KCO_3 mole fractions on CH_4 flame results in reducing the flame speed.
- The inhibitory efficacy of $KHCO_3$ is more pronounced in rich mixtures compared to lean fuel mixtures
- The reduction in OH by $KHCO_3$ is comparable to that of KCO_3. This similarity suggests that both compounds have similar abilities to influence the OH radicals in CH_4 flames.
- Limited mole fractions of KCO_3 could be employed to study its effect on CH_4 flame across a wide range of equivalence ratios.
- Both KCO_3 and $KHCO_3$ exhibit the same impact on the adiabatic flame temperature of the CH_4 flame.
- KCO_3 and $KHCO_3$ have different effect on the CH_4 pathway reactions, where $KHCO_3$ is more effective than KCO_3.
- The inhibition effect of KCO_3 on the flame of CH_4 is demonstrated by investigating the reactions of $KHCO_3$ with H and OH under conditions of high concentration and elevated temperature.
- The reaction rate profile for the main reactions of formation and consumption of K atom for CH_4 flame with 10% KCO_3 shows that K generated by HKO+H= K+ H_2O, $KHCO_3$+H= K+CO_2+H_2O, and consumed by K+OH= HKO.
- The main inhibition reaction of CH_4 flame affected by $KHCO_3$ are K + OH =KOH, H + KOH = K + H_2O, and $KHCO_3$+H= K+CO_2+H_2O.
- In real-world applications, $KHCO_3$ is the most effective agent for suppressing CH_4 flames compared to KCO_3 based on pathway analysis. Both $KHCO_3$ and KCO_3 are more effective than KO_2 in reducing flame speed and OH radicals. This effectiveness makes $KHCO_3$ a highly suitable choice for fires involving CH_4.

- $KHCO_3$ can be effectively used in industries such as chemical plants, refineries, and natural gas facilities where methane fires are a significant hazard. Its superior effectiveness ensures rapid suppression, minimising fire damage and improving overall safety.
- For household and commercial fire extinguishers, $KHCO_3$ offers a reliable option for dealing with methane-related fires, enhancing safety in environments where methane leaks may occur.
- A comparative numerical simulation analysis of the influence of $KHCO_3$ on the CH_4 flame demonstrated a good agreement with the findings documented in the literature review in terms of reducing the flame speed and identifying the inhibition reactions.

Chapter 8

Conclusion and Future Considerations

8.1 Conclusions

This study assesses the performance of K_2O in wood and pool fires. The impact of K_2O on the flames is analysed based on the test data. The kinetic effects of potassium species (KO_2, $KHCO_3$, and KCO_3) are determined through numerical modeling. Chemical kinetic mechanisms, thermodynamic, and transport data files are established for potassium species reactions. Various kinetic mechanisms are integrated with the potassium species mechanism using Chemkin software. Initial investigations into H_2 flames are based on established hydrocarbon /H_2 combustion mechanisms, specifically GRI-Mech and the Reduced mechanism of H_2 combustion from Hadi. Properties of the H_2 flame, including flame speed, adiabatic flame temperature, reaction pathway, and flammability limit, are then estimated through numerical methods and validated against existing literature data. These preliminary studies form the basis for ensuring the successful merging of different mechanisms. The merged mechanisms are tested, where the properties of the H_2 flame are determined and the results are compared with the initial H_2 flame study. Once the merged mechanism is prepared, the kinetic study of KO_2, $KHCO_3$, and KCO_3 on H_2 and CH_4 is determined through numerical modeling using different mole fractions at various equivalence ratios for H_2/air mixture or CH_4/air mixture.
The conclusions of the study are as follows.

- The tests demonstrate the effect of K_2O in suppressing various types of fires (wood, and pool fires), with a clear impact on flames.

- Selected H_2 combustion as a model fuel due to its well-described and relatively simple reaction mechanism. This choice allowed for a foundational understanding of combustion processes, enabling a clear investigation into the inhibition mechanisms of KO_2, $KHCO_3$, and KCO_3.

- Species pathway analysis has been employed for H_2 and CH_4 flames-based GRI-Mech mechanism. The main decomposition of H_2 occurs predominantly through reactions such as H_2+OH = H_2O+H and H_2+O=OH+H. For CH_4, the main

reaction pathways include CH_4+H=H_2+CH_3, CH_4+OH = H_2O+CH_3, and CH_4+O = OH+CH_3, leading to the formation of CH_3.

- H and OH are crucial contributors to the decomposition processes of CH_4 and CH_3 and these primary species are involved in the consumption of H_2.

- The study successfully incorporated reactions related to potassium species into established mechanisms and found that the numerical outcomes for the stoichiometric H_2 flame were within acceptable bounds. This finding indicates that the integration of potassium species reactions into the existing mechanisms did not substantially influence the properties of the H_2 flame. Thus, it confirms the validity and acceptability of the merged mechanisms.

- The impacts of KO_2, $KHCO_3$, and KCO_3 mole fractions on the properties of H_2 and CH_4 flames using numerical simulations facilitated by the Ansys Chemkin-Pro2019R2 software. Utilising a comprehensive reaction mechanism for hydrocarbon combustion, encompassing H_2, the study evaluates the influence of the specified potassium compounds on the reaction kinetics and species concentrations.

- For H_2 flame, the results demonstrate that KO_2 is the most potent agent affecting. At 8% concentration, KO_2 significantly reduces the flame speed under lean mixture conditions. In addition, reducing the OH concentration requires a low concentration of KO_2 compared with $KHCO_3$, and KCO_3.

- The pathway analysis was carried out using varying concentrations of KO_2, incorporating 0. 01%, 0. 147%, and 8% mole fractions in the numerical analysis. The results reveal a notable influence of K-species on the primary pathway reactions of H_2 flame at both low and high concentrations. Particularly, at 8% mole fraction of KO_2, the reactions involving KO_2 reacting with H and OH become distinctly evident.

- For CH_4 flame, the investigation identifies that both $KHCO_3$ and KCO_3 exhibit comparable performance as assessed through flame speed and when examining the impact on OH reduction.

- Concerning the impact of KCO_3 on the pathway reactions of CH_4 flames, simulation results indicate that KCO_3 has no clear effect on the primary free radicals (O, OH, and CH_3) or CH_4 itself in the combustion of CH_4 at low concentrations. However, at a high concentration (10% mole fraction) of KCO_3, the results show the influence of the K species on the reactions of the primary pathway of CH_4, especially on the H atom, where $KHCO_3$ reacts with H, producing K, CO_2 and H_2O. One important note is that at the maximum temperature based on simulation solutions, $KHCO_3$ will appear during the reaction $KHCO_3$+ OH = KCO_3+H_2O.

- A small amount of $KHCO_3$ has a clear effect on the CH_4 pathway reactions, whereas using KCO_3 with the same mole fraction does not affect the pathway reactions of CH_4.
- The comparison results of the $KHCO_3$ on CH_4/air mixture with previous study indicate a consistent reduction in flame speed. However, variations in initial conditions result in differences in the effective mol fraction of $KHCO_3$. At lower initial temperatures, a lesser amount of $KHCO_3$ is required to eliminate radical overshoot and manifest the effects of potassium species based on the flame structure. Additionally, studying reaction rate as a function of position in the flame at a higher initial temperature results in the production of more reactions that can impact flame propagation.
- In the context of CH_4 flames, the introduction of KO_2 as a fire suppression agent presents a distinctive set of challenges, particularly in the context of flame stability within numerical simulations.

8.2 Limitations and Suggested Future Work

- **Consider Foundational Postulation**: The foundational presumption underpinning this study posits that an assumption of uniform transport properties and the utilisation of polynomial coefficients to represent thermodynamic data for specific potassium species can serve as an initial assumption for investigation. This assumption enables preliminary inquiries. It is imperative to underscore that, as the research progresses and more precise empirical data becomes accessible, these underlying suppositions shall receive continual updates.
- **Exploration of Flammability Limits**: Explore the impact of inhibitors on flammability limits in various contexts.
- **Solid Phase Consideration**: Investigate the behavior of potassium species in the solid phase to better understand their impact on flames, considering that aerosol agents have both gas and solid phases.
- **Optimising Activation of Aerosol Systems**: Develop triggers inside aerosol generators to activate them at an earlier stage of a fire, enhancing fire suppression efficiency and minimising potential damage.
- **Particle Size and Dispersion Analysis**: Conduct further research on the concentration and dispersion of aerosol particles with varying sizes to understand their influence on fire suppression efficiency.
- **Diverse Fire Scenarios**: Expand the scope of future studies to encompass a wider range of fire scenarios, including different fuel types and fire sizes, to provide a

more comprehensive understanding of the applicability and limitations of potassium species.

- **Analysis of Released Gases**: Collect and analyse gases released during tests to understand their composition, toxicity, and potential risks. Additionally, measure pressure changes within the chamber to gain insights into pressure dynamics resulting from gas release.
- **Experimental Validation of Radical Interactions**: Experimentally test the interaction of critical radicals like OH, O, H, and HO_2 with potassium species in flame reaction zones to provide valuable insights into their consumption and production dynamics.

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Appendix:A

GRI-Mech Reaction Mechanism

```
! GRI-Mech Version 3.0 7/30/99  CHEMKIN format
! See README30 file at anonymous FTP site unix.sri.com, directory gri;
! WorldWideWeb home page http://www.me.berkeley.edu/gri_mech/ or
! through http://www.gri.org , under 'Basic  Research',
! for additional information, contacts, and disclaimer
ELEMENTS
O  H  C  N  AR
END
SPECIES
H2      H       O       O2      OH      H2O     HO2     H2O2
C       CH      CH2     CH2(S)  CH3     CH4     CO      CO2
HCO     CH2O    CH2OH   CH3O    CH3OH   C2H     C2H2    C2H3
C2H4    C2H5    C2H6    HCCO    CH2CO   HCCOH   N       NH
NH2     NH3     NNH     NO      NO2     N2O     HNO     CN
HCN     H2CN    HCNN    HCNO    HOCN    HNCO    NCO     N2
AR      C3H7    C3H8    CH2CHO  CH3CHO
!END
REACTIONS

Reactions                                 A           n          Ea (cal/mol)
2O+M<=>O2+M                              1.200E+17   -1.000        .00
H2/ 2.40/ H2O/15.40/ CH4/ 2.00/ CO/ 1.75/ CO2/ 3.60/ C2H6/ 3.00/ AR/  .83/
O+H+M<=>OH+M                             5.000E+17   -1.000        .00
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
O+H2<=>H+OH                              3.870E+04    2.700    6260.00
O+HO2<=>OH+O2                            2.000E+13     .000        .00
O+H2O2<=>OH+HO2                          9.630E+06    2.000    4000.00
O+CH<=>H+CO                              5.700E+13     .000        .00
O+CH2<=>H+HCO                            8.000E+13     .000        .00
O+CH2(S)<=>H2+CO                         1.500E+13     .000        .00
O+CH2(S)<=>H+HCO                         1.500E+13     .000        .00
O+CH3<=>H+CH2O                           5.060E+13     .000        .00
O+CH4<=>OH+CH3                           1.020E+09    1.500    8600.00
O+CO(+M)<=>CO2(+M)                       1.800E+10     .000    2385.00
   LOW/ 6.020E+14     .000    3000.00/
H2/2.00/ O2/6.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/3.50/ C2H6/3.00/ AR/ .50/
O+HCO<=>OH+CO                            3.000E+13     .000        .00
O+HCO<=>H+CO2                            3.000E+13     .000        .00
O+CH2O<=>OH+HCO                          3.900E+13     .000    3540.00
O+CH2OH<=>OH+CH2O                        1.000E+13     .000        .00
O+CH3O<=>OH+CH2O                         1.000E+13     .000        .00
O+CH3OH<=>OH+CH2OH                       3.880E+05    2.500    3100.00
O+CH3OH<=>OH+CH3O                        1.300E+05    2.500    5000.00
O+C2H<=>CH+CO                            5.000E+13     .000        .00
O+C2H2<=>H+HCCO                          1.350E+07    2.000    1900.00
O+C2H2<=>OH+C2H                          4.600E+19   -1.410   28950.00
O+C2H2<=>CO+CH2                          6.940E+06    2.000    1900.00
O+C2H3<=>H+CH2CO                         3.000E+13     .000        .00
O+C2H4<=>CH3+HCO                         1.250E+07    1.830     220.00
O+C2H5<=>CH3+CH2O                        2.240E+13     .000        .00
O+C2H6<=>OH+C2H5                         8.980E+07    1.920    5690.00
O+HCCO<=>H+2CO                           1.000E+14     .000        .00
O+CH2CO<=>OH+HCCO                        1.000E+13     .000    8000.00
O+CH2CO<=>CH2+CO2                        1.750E+12     .000    1350.00
O2+CO<=>O+CO2                            2.500E+12     .000   47800.00
O2+CH2O<=>HO2+HCO                        1.000E+14     .000   40000.00
H+O2+M<=>HO2+M                           2.800E+18    -.860        .00
O2/ .00/ H2O/ .00/ CO/ .75/ CO2/1.50/ C2H6/1.50/ N2/ .00/ AR/ .00/
H+2O2<=>HO2+O2                           2.080E+19   -1.240        .00
H+O2+H2O<=>HO2+H2O                       11.26E+18    -.760        .00
H+O2+N2<=>HO2+N2                         2.600E+19   -1.240        .00
H+O2+AR<=>HO2+AR                         7.000E+17    -.800        .00
H+O2<=>O+OH                              2.650E+16    -.6707  17041.00
2H+M<=>H2+M                              1.000E+18   -1.000        .00
```

```
H2/ .00/ H2O/ .00/ CH4/2.00/ CO2/ .00/ C2H6/3.00/ AR/ .63/
2H+H2<=>2H2                               9.000E+16    -.600        .00
2H+H2O<=>H2+H2O                           6.000E+19   -1.250        .00
2H+CO2<=>H2+CO2                           5.500E+20   -2.000        .00
H+OH+M<=>H2O+M                            2.200E+22   -2.000        .00
H2/ .73/ H2O/3.65/ CH4/2.00/ C2H6/3.00/ AR/ .38/
H+HO2<=>O+H2O                             3.970E+12     .000     671.00
H+HO2<=>O2+H2                             4.480E+13     .000    1068.00
H+HO2<=>2OH                               0.840E+14     .000     635.00
H+H2O2<=>HO2+H2                           1.210E+07    2.000    5200.00
H+H2O2<=>OH+H2O                           1.000E+13     .000    3600.00
H+CH<=>C+H2                               1.650E+14     .000        .00
H+CH2(+M)<=>CH3(+M)                       6.000E+14     .000        .00
     LOW  /  1.040E+26   -2.760   1600.00/
     TROE/   .5620  91.00  5836.00  8552.00/
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+CH2(S)<=>CH+H2                          3.000E+13     .000        .00
H+CH3(+M)<=>CH4(+M)                       13.90E+15    -.534     536.00
     LOW  /  2.620E+33   -4.760   2440.00/
     TROE/   .7830   74.00  2941.00  6964.00 /
H2/2.00/ H2O/6.00/ CH4/3.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+CH4<=>CH3+H2                            6.600E+08    1.620   10840.00
H+HCO(+M)<=>CH2O(+M)                      1.090E+12     .480    -260.00
     LOW  /  2.470E+24   -2.570    425.00/
     TROE/   .7824  271.00  2755.00  6570.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+HCO<=>H2+CO                             7.340E+13     .000        .00
H+CH2O(+M)<=>CH2OH(+M)                    5.400E+11     .454    3600.00
     LOW  /  1.270E+32   -4.820   6530.00/
     TROE/   .7187  103.00  1291.00  4160.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH2O(+M)<=>CH3O(+M)                     5.400E+11     .454    2600.00
     LOW  /  2.200E+30   -4.800   5560.00/
     TROE/   .7580   94.00  1555.00  4200.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH2O<=>HCO+H2                           5.740E+07    1.900    2742.00
H+CH2OH(+M)<=>CH3OH(+M)                   1.055E+12     .500      86.00
     LOW  /  4.360E+31   -4.650   5080.00/
     TROE/   .600  100.00  90000.0  10000.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH2OH<=>H2+CH2O                         2.000E+13     .000        .00
H+CH2OH<=>OH+CH3                          1.650E+11     .650    -284.00
H+CH2OH<=>CH2(S)+H2O                      3.280E+13    -.090     610.00
H+CH3O(+M)<=>CH3OH(+M)                    2.430E+12     .515      50.00
     LOW  /  4.660E+41   -7.440   14080.0/
     TROE/   .700  100.00  90000.0 10000.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH3O<=>H+CH2OH                          4.150E+07    1.630    1924.00
H+CH3O<=>H2+CH2O                          2.000E+13     .000        .00
H+CH3O<=>OH+CH3                           1.500E+12     .500    -110.00
H+CH3O<=>CH2(S)+H2O                       2.620E+14    -.230    1070.00
H+CH3OH<=>CH2OH+H2                        1.700E+07    2.100    4870.00
H+CH3OH<=>CH3O+H2                         4.200E+06    2.100    4870.00
H+C2H(+M)<=>C2H2(+M)                      1.000E+17   -1.000        .00
     LOW  /  3.750E+33   -4.800   1900.00/
     TROE/   .6464  132.00  1315.00  5566.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+C2H2(+M)<=>C2H3(+M)                     5.600E+12     .000    2400.00
     LOW  /  3.800E+40   -7.270   7220.00/
     TROE/   .7507   98.50  1302.00  4167.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+C2H3(+M)<=>C2H4(+M)                     6.080E+12     .270     280.00
     LOW  /  1.400E+30   -3.860   3320.00/
     TROE/   .7820  207.50  2663.00  6095.00 /
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H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+C2H3<=>H2+C2H2                          3.000E+13     .000        .00
H+C2H4(+M)<=>C2H5(+M)                     0.540E+12     .454    1820.00
     LOW  /  0.600E+42   -7.620   6970.00/
     TROE/   .9753  210.00   984.00  4374.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+C2H4<=>C2H3+H2                          1.325E+06    2.530   12240.00
H+C2H5(+M)<=>C2H6(+M)                     5.210E+17    -.990    1580.00
     LOW  /  1.990E+41   -7.080   6685.00/
     TROE/   .8422  125.00  2219.00  6882.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+C2H5<=>H2+C2H4                          2.000E+12     .000        .00
H+C2H6<=>C2H5+H2                          1.150E+08    1.900    7530.00
H+HCCO<=>CH2(S)+CO                        1.000E+14     .000        .00
H+CH2CO<=>HCCO+H2                         5.000E+13     .000    8000.00
H+CH2CO<=>CH3+CO                          1.130E+13     .000    3428.00
H+HCCOH<=>H+CH2CO                         1.000E+13     .000        .00
H2+CO(+M)<=>CH2O(+M)                      4.300E+07    1.500   79600.00
     LOW  /  5.070E+27   -3.420  84350.00/
     TROE/   .9320  197.00  1540.00 10300.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
OH+H2<=>H+H2O                             2.160E+08    1.510    3430.00
2OH(+M)<=>H2O2(+M)                        7.400E+13    -.370        .00
     LOW  /  2.300E+18    -.900  -1700.00/
     TROE/   .7346   94.00  1756.00  5182.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
2OH<=>O+H2O                               3.570E+04    2.400   -2110.00
OH+HO2<=>O2+H2O                           1.450E+13     .000    -500.00
 DUPLICATE
OH+H2O2<=>HO2+H2O                         2.000E+12     .000     427.00
 DUPLICATE
OH+H2O2<=>HO2+H2O                         1.700E+18     .000   29410.00
 DUPLICATE
OH+C<=>H+CO                               5.000E+13     .000        .00
OH+CH<=>H+HCO                             3.000E+13     .000        .00
OH+CH2<=>H+CH2O                           2.000E+13     .000        .00
OH+CH2<=>CH+H2O                           1.130E+07    2.000    3000.00
OH+CH2(S)<=>H+CH2O                        3.000E+13     .000        .00
OH+CH3(+M)<=>CH3OH(+M)                    2.790E+18   -1.430    1330.00
     LOW  /  4.000E+36   -5.920   3140.00/
     TROE/   .4120  195.0  5900.00  6394.00/
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
OH+CH3<=>CH2+H2O                          5.600E+07    1.600    5420.00
OH+CH3<=>CH2(S)+H2O                       6.440E+17   -1.340    1417.00
OH+CH4<=>CH3+H2O                          1.000E+08    1.600    3120.00
OH+CO<=>H+CO2                             4.760E+07    1.228      70.00
OH+HCO<=>H2O+CO                           5.000E+13     .000        .00
OH+CH2O<=>HCO+H2O                         3.430E+09    1.180    -447.00
OH+CH2OH<=>H2O+CH2O                       5.000E+12     .000        .00
OH+CH3O<=>H2O+CH2O                        5.000E+12     .000        .00
OH+CH3OH<=>CH2OH+H2O                      1.440E+06    2.000    -840.00
OH+CH3OH<=>CH3O+H2O                       6.300E+06    2.000    1500.00
OH+C2H<=>H+HCCO                           2.000E+13     .000        .00
OH+C2H2<=>H+CH2CO                         2.180E-04    4.500   -1000.00
OH+C2H2<=>H+HCCOH                         5.040E+05    2.300   13500.00
OH+C2H2<=>C2H+H2O                         3.370E+07    2.000   14000.00
OH+C2H2<=>CH3+CO                          4.830E-04    4.000   -2000.00
OH+C2H3<=>H2O+C2H2                        5.000E+12     .000        .00
OH+C2H4<=>C2H3+H2O                        3.600E+06    2.000    2500.00
OH+C2H6<=>C2H5+H2O                        3.540E+06    2.120     870.00
OH+CH2CO<=>HCCO+H2O                       7.500E+12     .000    2000.00
2HO2<=>O2+H2O2                            1.300E+11     .000   -1630.00
 DUPLICATE
2HO2<=>O2+H2O2                            4.200E+14     .000   12000.00
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 DUPLICATE
HO2+CH2<=>OH+CH2O                         2.000E+13     .000        .00
HO2+CH3<=>O2+CH4                          1.000E+12     .000        .00
HO2+CH3<=>OH+CH3O                         3.780E+13     .000        .00
HO2+CO<=>OH+CO2                           1.500E+14     .000   23600.00
HO2+CH2O<=>HCO+H2O2                       5.600E+06    2.000   12000.00
C+O2<=>O+CO                               5.800E+13     .000     576.00
C+CH2<=>H+C2H                             5.000E+13     .000        .00
C+CH3<=>H+C2H2                            5.000E+13     .000        .00
CH+O2<=>O+HCO                             6.710E+13     .000        .00
CH+H2<=>H+CH2                             1.080E+14     .000    3110.00
CH+H2O<=>H+CH2O                           5.710E+12     .000    -755.00
CH+CH2<=>H+C2H2                           4.000E+13     .000        .00
CH+CH3<=>H+C2H3                           3.000E+13     .000        .00
CH+CH4<=>H+C2H4                           6.000E+13     .000        .00
CH+CO(+M)<=>HCCO(+M)                      5.000E+13     .000        .00
     LOW  /  2.690E+28   -3.740   1936.00/
     TROE/   .5757  237.00  1652.00  5069.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
CH+CO2<=>HCO+CO                           1.900E+14     .000   15792.00
CH+CH2O<=>H+CH2CO                         9.460E+13     .000    -515.00
CH+HCCO<=>CO+C2H2                         5.000E+13     .000        .00
CH2+O2=>OH+H+CO                           5.000E+12     .000    1500.00
CH2+H2<=>H+CH3                            5.000E+05    2.000    7230.00
2CH2<=>H2+C2H2                            1.600E+15     .000   11944.00
CH2+CH3<=>H+C2H4                          4.000E+13     .000        .00
CH2+CH4<=>2CH3                            2.460E+06    2.000    8270.00
CH2+CO(+M)<=>CH2CO(+M)                    8.100E+11     .500    4510.00
     LOW  /  2.690E+33   -5.110   7095.00/
     TROE/   .5907  275.00  1226.00  5185.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
CH2+HCCO<=>C2H3+CO                        3.000E+13     .000        .00
CH2(S)+N2<=>CH2+N2                        1.500E+13     .000     600.00
CH2(S)+AR<=>CH2+AR                        9.000E+12     .000     600.00
CH2(S)+O2<=>H+OH+CO                       2.800E+13     .000        .00
CH2(S)+O2<=>CO+H2O                        1.200E+13     .000        .00
CH2(S)+H2<=>CH3+H                         7.000E+13     .000        .00
CH2(S)+H2O(+M)<=>CH3OH(+M)                4.820E+17   -1.160    1145.00
     LOW  /  1.880E+38   -6.360   5040.00/
     TROE/   .6027  208.00  3922.00  10180.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH2(S)+H2O<=>CH2+H2O                      3.000E+13     .000        .00
CH2(S)+CH3<=>H+C2H4                       1.200E+13     .000    -570.00
CH2(S)+CH4<=>2CH3                         1.600E+13     .000    -570.00
CH2(S)+CO<=>CH2+CO                        9.000E+12     .000        .00
CH2(S)+CO2<=>CH2+CO2                      7.000E+12     .000        .00
CH2(S)+CO2<=>CO+CH2O                      1.400E+13     .000        .00
CH2(S)+C2H6<=>CH3+C2H5                    4.000E+13     .000    -550.00
CH3+O2<=>O+CH3O                           3.560E+13     .000   30480.00
CH3+O2<=>OH+CH2O                          2.310E+12     .000   20315.00
CH3+H2O2<=>HO2+CH4                        2.450E+04    2.470    5180.00
2CH3(+M)<=>C2H6(+M)                       6.770E+16   -1.180     654.00
     LOW  /  3.400E+41   -7.030   2762.00/
     TROE/   .6190  73.20  1180.00  9999.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
2CH3<=>H+C2H5                             6.840E+12     .100   10600.00
CH3+HCO<=>CH4+CO                          2.648E+13     .000        .00
CH3+CH2O<=>HCO+CH4                        3.320E+03    2.810    5860.00
CH3+CH3OH<=>CH2OH+CH4                     3.000E+07    1.500    9940.00
CH3+CH3OH<=>CH3O+CH4                      1.000E+07    1.500    9940.00
CH3+C2H4<=>C2H3+CH4                       2.270E+05    2.000    9200.00
CH3+C2H6<=>C2H5+CH4                       6.140E+06    1.740   10450.00
HCO+H2O<=>H+CO+H2O                        1.500E+18   -1.000   17000.00
HCO+M<=>H+CO+M                            1.870E+17   -1.000   17000.00
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H2/2.00/ H2O/ .00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
HCO+O2<=>HO2+CO                          13.45E+12     .000     400.00
CH2OH+O2<=>HO2+CH2O                      1.800E+13     .000     900.00
CH3O+O2<=>HO2+CH2O                       4.280E-13    7.600   -3530.00
C2H+O2<=>HCO+CO                          1.000E+13     .000    -755.00
C2H+H2<=>H+C2H2                          5.680E+10    0.900    1993.00
C2H3+O2<=>HCO+CH2O                       4.580E+16   -1.390    1015.00
C2H4(+M)<=>H2+C2H2(+M)                   8.000E+12     .440   86770.00
     LOW  /  1.580E+51   -9.300  97800.00/
     TROE/   .7345  180.00  1035.00  5417.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
C2H5+O2<=>HO2+C2H4                       8.400E+11     .000    3875.00
HCCO+O2<=>OH+2CO                         3.200E+12     .000     854.00
2HCCO<=>2CO+C2H2                         1.000E+13     .000        .00
N+NO<=>N2+O                              2.700E+13     .000     355.00
N+O2<=>NO+O                              9.000E+09    1.000    6500.00
N+OH<=>NO+H                              3.360E+13     .000     385.00
N2O+O<=>N2+O2                            1.400E+12     .000   10810.00
N2O+O<=>2NO                              2.900E+13     .000   23150.00
N2O+H<=>N2+OH                            3.870E+14     .000   18880.00
N2O+OH<=>N2+HO2                          2.000E+12     .000   21060.00
N2O(+M)<=>N2+O(+M)                       7.910E+10     .000   56020.00
     LOW  /  6.370E+14     .000  56640.00/
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .625/
HO2+NO<=>NO2+OH                          2.110E+12     .000    -480.00
NO+O+M<=>NO2+M                           1.060E+20   -1.410        .00
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
NO2+O<=>NO+O2                            3.900E+12     .000    -240.00
NO2+H<=>NO+OH                            1.320E+14     .000     360.00
NH+O<=>NO+H                              4.000E+13     .000        .00
NH+H<=>N+H2                              3.200E+13     .000     330.00
NH+OH<=>HNO+H                            2.000E+13     .000        .00
NH+OH<=>N+H2O                            2.000E+09    1.200        .00
NH+O2<=>HNO+O                            4.610E+05    2.000    6500.00
NH+O2<=>NO+OH                            1.280E+06    1.500     100.00
NH+N<=>N2+H                              1.500E+13     .000        .00
NH+H2O<=>HNO+H2                          2.000E+13     .000   13850.00
NH+NO<=>N2+OH                            2.160E+13    -.230        .00
NH+NO<=>N2O+H                            3.650E+14    -.450        .00
NH2+O<=>OH+NH                            3.000E+12     .000        .00
NH2+O<=>H+HNO                            3.900E+13     .000        .00
NH2+H<=>NH+H2                            4.000E+13     .000    3650.00
NH2+OH<=>NH+H2O                          9.000E+07    1.500    -460.00
NNH<=>N2+H                               3.300E+08     .000        .00
NNH+M<=>N2+H+M                           1.300E+14    -.110    4980.00
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
NNH+O2<=>HO2+N2                          5.000E+12     .000        .00
NNH+O<=>OH+N2                            2.500E+13     .000        .00
NNH+O<=>NH+NO                            7.000E+13     .000        .00
NNH+H<=>H2+N2                            5.000E+13     .000        .00
NNH+OH<=>H2O+N2                          2.000E+13     .000        .00
NNH+CH3<=>CH4+N2                         2.500E+13     .000        .00
H+NO+M<=>HNO+M                           4.480E+19   -1.320     740.00
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
HNO+O<=>NO+OH                            2.500E+13     .000        .00
HNO+H<=>H2+NO                            9.000E+11     .720     660.00
HNO+OH<=>NO+H2O                          1.300E+07    1.900    -950.00
HNO+O2<=>HO2+NO                          1.000E+13     .000   13000.00
CN+O<=>CO+N                              7.700E+13     .000        .00
CN+OH<=>NCO+H                            4.000E+13     .000        .00
CN+H2O<=>HCN+OH                          8.000E+12     .000    7460.00
CN+O2<=>NCO+O                            6.140E+12     .000    -440.00
CN+H2<=>HCN+H                            2.950E+05    2.450    2240.00
NCO+O<=>NO+CO                            2.350E+13     .000        .00
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NCO+H<=>NH+CO                             5.400E+13     .000        .00
NCO+OH<=>NO+H+CO                          0.250E+13     .000        .00
NCO+N<=>N2+CO                             2.000E+13     .000        .00
NCO+O2<=>NO+CO2                           2.000E+12     .000   20000.00
NCO+M<=>N+CO+M                            3.100E+14     .000   54050.00
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
NCO+NO<=>N2O+CO                           1.900E+17   -1.520     740.00
NCO+NO<=>N2+CO2                           3.800E+18   -2.000     800.00
HCN+M<=>H+CN+M                            1.040E+29   -3.300  126600.00
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
HCN+O<=>NCO+H                             2.030E+04    2.640    4980.00
HCN+O<=>NH+CO                             5.070E+03    2.640    4980.00
HCN+O<=>CN+OH                             3.910E+09    1.580   26600.00
HCN+OH<=>HOCN+H                           1.100E+06    2.030   13370.00
HCN+OH<=>HNCO+H                           4.400E+03    2.260    6400.00
HCN+OH<=>NH2+CO                           1.600E+02    2.560    9000.00
H+HCN(+M)<=>H2CN(+M)                      3.300E+13     .000        .00
      LOW /  1.400E+26   -3.400    1900.00/
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H2CN+N<=>N2+CH2                           6.000E+13     .000     400.00
C+N2<=>CN+N                               6.300E+13     .000   46020.00
CH+N2<=>HCN+N                             3.120E+09    0.880   20130.00
CH+N2(+M)<=>HCNN(+M)                      3.100E+12     .150        .00
     LOW  /  1.300E+25   -3.160    740.00/
     TROE/   .6670  235.00  2117.00  4536.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ 1.0/
CH2+N2<=>HCN+NH                           1.000E+13     .000   74000.00
CH2(S)+N2<=>NH+HCN                        1.000E+11     .000   65000.00
C+NO<=>CN+O                               1.900E+13     .000        .00
C+NO<=>CO+N                               2.900E+13     .000        .00
CH+NO<=>HCN+O                             4.100E+13     .000        .00
CH+NO<=>H+NCO                             1.620E+13     .000        .00
CH+NO<=>N+HCO                             2.460E+13     .000        .00
CH2+NO<=>H+HNCO                           3.100E+17   -1.380    1270.00
CH2+NO<=>OH+HCN                           2.900E+14    -.690     760.00
CH2+NO<=>H+HCNO                           3.800E+13    -.360     580.00
CH2(S)+NO<=>H+HNCO                        3.100E+17   -1.380    1270.00
CH2(S)+NO<=>OH+HCN                        2.900E+14    -.690     760.00
CH2(S)+NO<=>H+HCNO                        3.800E+13    -.360     580.00
CH3+NO<=>HCN+H2O                          9.600E+13     .000   28800.00
CH3+NO<=>H2CN+OH                          1.000E+12     .000   21750.00
HCNN+O<=>CO+H+N2                          2.200E+13     .000        .00
HCNN+O<=>HCN+NO                           2.000E+12     .000        .00
HCNN+O2<=>O+HCO+N2                        1.200E+13     .000        .00
HCNN+OH<=>H+HCO+N2                        1.200E+13     .000        .00
HCNN+H<=>CH2+N2                           1.000E+14     .000        .00
HNCO+O<=>NH+CO2                           9.800E+07    1.410    8500.00
HNCO+O<=>HNO+CO                           1.500E+08    1.570   44000.00
HNCO+O<=>NCO+OH                           2.200E+06    2.110   11400.00
HNCO+H<=>NH2+CO                           2.250E+07    1.700    3800.00
HNCO+H<=>H2+NCO                           1.050E+05    2.500   13300.00
HNCO+OH<=>NCO+H2O                         3.300E+07    1.500    3600.00
HNCO+OH<=>NH2+CO2                         3.300E+06    1.500    3600.00
HNCO+M<=>NH+CO+M                          1.180E+16     .000   84720.00
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
HCNO+H<=>H+HNCO                           2.100E+15    -.690    2850.00
HCNO+H<=>OH+HCN                           2.700E+11     .180    2120.00
HCNO+H<=>NH2+CO                           1.700E+14    -.750    2890.00
HOCN+H<=>H+HNCO                           2.000E+07    2.000    2000.00
HCCO+NO<=>HCNO+CO                         0.900E+13     .000        .00
CH3+N<=>H2CN+H                            6.100E+14    -.310     290.00
CH3+N<=>HCN+H2                            3.700E+12     .150     -90.00
NH3+H<=>NH2+H2                            5.400E+05    2.400    9915.00
NH3+OH<=>NH2+H2O                          5.000E+07    1.600     955.00
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NH3+O<=>NH2+OH                          9.400E+06    1.940    6460.00
NH+CO2<=>HNO+CO                         1.000E+13     .000   14350.00
CN+NO2<=>NCO+NO                         6.160E+15   -0.752     345.00
NCO+NO2<=>N2O+CO2                       3.250E+12     .000    -705.00
N+CO2<=>NO+CO                           3.000E+12     .000   11300.00
O+CH3=>H+H2+CO                          3.370E+13     .000        .00
O+C2H4<=>H+CH2CHO                       6.700E+06    1.830     220.00
O+C2H5<=>H+CH3CHO                       1.096E+14     .000        .00
OH+HO2<=>O2+H2O                         0.500E+16     .000   17330.00
  DUPLICATE
OH+CH3=>H2+CH2O                         8.000E+09     .500   -1755.00
CH+H2(+M)<=>CH3(+M)                     1.970E+12     .430    -370.00
   LOW/ 4.820E+25  -2.80  590.0 /
   TROE/ .578  122.0  2535.0  9365.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
CH2+O2=>2H+CO2                          5.800E+12     .000    1500.00
CH2+O2<=>O+CH2O                         2.400E+12     .000    1500.00
CH2+CH2=>2H+C2H2                        2.000E+14     .000   10989.00
CH2(S)+H2O=>H2+CH2O                     6.820E+10     .250    -935.00
C2H3+O2<=>O+CH2CHO                      3.030E+11     .290      11.00
C2H3+O2<=>HO2+C2H2                      1.337E+06    1.610    -384.00
O+CH3CHO<=>OH+CH2CHO                    2.920E+12     .000    1808.00
O+CH3CHO=>OH+CH3+CO                     2.920E+12     .000    1808.00
O2+CH3CHO=>HO2+CH3+CO                   3.010E+13     .000   39150.00
H+CH3CHO<=>CH2CHO+H2                    2.050E+09    1.160    2405.00
H+CH3CHO=>CH3+H2+CO                     2.050E+09    1.160    2405.00
OH+CH3CHO=>CH3+H2O+CO                   2.343E+10    0.730   -1113.00
HO2+CH3CHO=>CH3+H2O2+CO                 3.010E+12     .000   11923.00
CH3+CH3CHO=>CH3+CH4+CO                  2.720E+06    1.770    5920.00
H+CH2CO(+M)<=>CH2CHO(+M)                4.865E+11    0.422   -1755.00
    LOW/ 1.012E+42  -7.63  3854.0/
    TROE/ 0.465  201.0  1773.0  5333.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
O+CH2CHO=>H+CH2+CO2                     1.500E+14     .000       .00
O2+CH2CHO=>OH+CO+CH2O                   1.810E+10     .000       .00
O2+CH2CHO=>OH+2HCO                      2.350E+10     .000       .00
H+CH2CHO<=>CH3+HCO                      2.200E+13     .000       .00
H+CH2CHO<=>CH2CO+H2                     1.100E+13     .000       .00
OH+CH2CHO<=>H2O+CH2CO                   1.200E+13     .000       .00
OH+CH2CHO<=>HCO+CH2OH                   3.010E+13     .000       .00
CH3+C2H5(+M)<=>C3H8(+M)                  .9430E+13     .000       .00
     LOW/ 2.710E+74  -16.82  13065.0 /
     TROE/ .1527  291.0  2742.0  7748.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
O+C3H8<=>OH+C3H7                        1.930E+05    2.680   3716.00
H+C3H8<=>C3H7+H2                        1.320E+06    2.540   6756.00
OH+C3H8<=>C3H7+H2O                      3.160E+07    1.800    934.00
C3H7+H2O2<=>HO2+C3H8                    3.780E+02    2.720   1500.00
CH3+C3H8<=>C3H7+CH4                     0.903E+00    3.650   7154.00
CH3+C2H4(+M)<=>C3H7(+M)                 2.550E+06    1.600   5700.00
      LOW/ 3.00E+63  -14.6  18170./
      TROE/ .1894  277.0  8748.0  7891.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
O+C3H7<=>C2H5+CH2O                      9.640E+13     .000       .00
H+C3H7(+M)<=>C3H8(+M)                   3.613E+13     .000       .00
      LOW/ 4.420E+61  -13.545  11357.0/
      TROE/ .315  369.0  3285.0  6667.0 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+C3H7<=>CH3+C2H5                       4.060E+06    2.190    890.00
OH+C3H7<=>C2H5+CH2OH                    2.410E+13     .000       .00
HO2+C3H7<=>O2+C3H8                      2.550E+10    0.255   -943.00
HO2+C3H7=>OH+C2H5+CH2O                  2.410E+13     .000       .00
CH3+C3H7<=>2C2H5                        1.927E+13   -0.320       .00
END
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GRI-Mech Thermodynamic Data File

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THERMO
   300.000  1000.000  5000.000
! GRI-Mech Version 3.0 Thermodynamics released 7/30/99
! NASA Polynomial format for CHEMKIN-II
! see README file for disclaimer
O                 L 1/90O   1               G   200.000  3500.000  1000.000    1
 2.56942078E+00-8.59741137E-05 4.19484589E-08-1.00177799E-11 1.22833691E-15    2
 2.92175791E+04 4.78433864E+00 3.16826710E+00-3.27931884E-03 6.64306396E-06    3
-6.12806624E-09 2.11265971E-12 2.91222592E+04 2.05193346E+00                   4
O2                TPIS89O   2               G   200.000  3500.000  1000.000    1
 3.28253784E+00 1.48308754E-03-7.57966669E-07 2.09470555E-10-2.16717794E-14    2
-1.08845772E+03 5.45323129E+00 3.78245636E+00-2.99673416E-03 9.84730201E-06    3
-9.68129509E-09 3.24372837E-12-1.06394356E+03 3.65767573E+00                   4
H                 L 7/88H   1               G   200.000  3500.000  1000.000    1
 2.50000001E+00-2.30842973E-11 1.61561948E-14-4.73515235E-18 4.98197357E-22    2
 2.54736599E+04-4.46682914E-01 2.50000000E+00 7.05332819E-13-1.99591964E-15    3
 2.30081632E-18-9.27732332E-22 2.54736599E+04-4.46682853E-01                   4
H2                TPIS78H   2               G   200.000  3500.000  1000.000    1
 3.33727920E+00-4.94024731E-05 4.99456778E-07-1.79566394E-10 2.00255376E-14    2
-9.50158922E+02-3.20502331E+00 2.34433112E+00 7.98052075E-03-1.94781510E-05    3
 2.01572094E-08-7.37611761E-12-9.17935173E+02 6.83010238E-01                   4
OH                RUS 78O   1H   1          G   200.000  3500.000  1000.000    1
 3.09288767E+00 5.48429716E-04 1.26505228E-07-8.79461556E-11 1.17412376E-14    2
 3.85865700E+03 4.47669610E+00 3.99201543E+00-2.40131752E-03 4.61793841E-06    3
-3.88113333E-09 1.36411470E-12 3.61508056E+03-1.03925458E-01                   4
H2O               L 8/89H   2O   1          G   200.000  3500.000  1000.000    1
 3.03399249E+00 2.17691804E-03-1.64072518E-07-9.70419870E-11 1.68200992E-14    2
-3.00042971E+04 4.96677010E+00 4.19864056E+00-2.03643410E-03 6.52040211E-06    3
-5.48797062E-09 1.77197817E-12-3.02937267E+04-8.49032208E-01                   4
HO2               L 5/89H   1O   2          G   200.000  3500.000  1000.000    1
 4.01721090E+00 2.23982013E-03-6.33658150E-07 1.14246370E-10-1.07908535E-14    2
 1.11856713E+02 3.78510215E+00 4.30179801E+00-4.74912051E-03 2.11582891E-05    3
-2.42763894E-08 9.29225124E-12 2.94808040E+02 3.71666245E+00                   4
H2O2              L 7/88H   2O   2          G   200.000  3500.000  1000.000    1
 4.16500285E+00 4.90831694E-03-1.90139225E-06 3.71185986E-10-2.87908305E-14    2
-1.78617877E+04 2.91615662E+00 4.27611269E+00-5.42822417E-04 1.67335701E-05    3
-2.15770813E-08 8.62454363E-12-1.77025821E+04 3.43505074E+00                   4
C                 L11/88C   1               G   200.000  3500.000  1000.000    1
 2.49266888E+00 4.79889284E-05-7.24335020E-08 3.74291029E-11-4.87277893E-15    2
 8.54512953E+04 4.80150373E+00 2.55423955E+00-3.21537724E-04 7.33792245E-07    3
-7.32234889E-10 2.66521446E-13 8.54438832E+04 4.53130848E+00                   4
CH                TPIS79C   1H   1          G   200.000  3500.000  1000.000    1
 2.87846473E+00 9.70913681E-04 1.44445655E-07-1.30687849E-10 1.76079383E-14    2
 7.10124364E+04 5.48497999E+00 3.48981665E+00 3.23835541E-04-1.68899065E-06    3
 3.16217327E-09-1.40609067E-12 7.07972934E+04 2.08401108E+00                   4
CH2               L S/93C   1H   2          G   200.000  3500.000  1000.000    1
 2.87410113E+00 3.65639292E-03-1.40894597E-06 2.60179549E-10-1.87727567E-14    2
 4.62636040E+04 6.17119324E+00 3.76267867E+00 9.68872143E-04 2.79489841E-06    3
-3.85091153E-09 1.68741719E-12 4.60040401E+04 1.56253185E+00                   4
CH2(S)            L S/93C   1H   2          G   200.000  3500.000  1000.000    1
 2.29203842E+00 4.65588637E-03-2.01191947E-06 4.17906000E-10-3.39716365E-14    2
 5.09259997E+04 8.62650169E+00 4.19860411E+00-2.36661419E-03 8.23296220E-06    3
-6.68815981E-09 1.94314737E-12 5.04968163E+04-7.69118967E-01                   4
CH3               L11/89C   1H   3          G   200.000  3500.000  1000.000    1
 2.28571772E+00 7.23990037E-03-2.98714348E-06 5.95684644E-10-4.67154394E-14    2
 1.67755843E+04 8.48007179E+00 3.67359040E+00 2.01095175E-03 5.73021856E-06    3
-6.87117425E-09 2.54385734E-12 1.64449988E+04 1.60456433E+00                   4
CH4               L 8/88C   1H   4          G   200.000  3500.000  1000.000    1
 7.48514950E-02 1.33909467E-02-5.73285809E-06 1.22292535E-09-1.01815230E-13    2
-9.46834459E+03 1.84373180E+01 5.14987613E+00-1.36709788E-02 4.91800599E-05    3
-4.84743026E-08 1.66693956E-11-1.02466476E+04-4.64130376E+00                   4
CO                TPIS79C   1O   1          G   200.000  3500.000  1000.000    1
 2.71518561E+00 2.06252743E-03-9.98825771E-07 2.30053008E-10-2.03647716E-14    2
-1.41518724E+04 7.81868772E+00 3.57953347E+00-6.10353680E-04 1.01681433E-06    3
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 9.07005884E-10-9.04424499E-13-1.43440860E+04 3.50840928E+00                   4
CO2               L 7/88C   1O   2          G   200.000  3500.000  1000.000    1
 3.85746029E+00 4.41437026E-03-2.21481404E-06 5.23490188E-10-4.72084164E-14    2
-4.87591660E+04 2.27163806E+00 2.35677352E+00 8.98459677E-03-7.12356269E-06    3
 2.45919022E-09-1.43699548E-13-4.83719697E+04 9.90105222E+00                   4
HCO               L12/89H   1C   1O   1     G   200.000  3500.000  1000.000    1
 2.77217438E+00 4.95695526E-03-2.48445613E-06 5.89161778E-10-5.33508711E-14    2
 4.01191815E+03 9.79834492E+00 4.22118584E+00-3.24392532E-03 1.37799446E-05    3
-1.33144093E-08 4.33768865E-12 3.83956496E+03 3.39437243E+00                   4
CH2O              L 8/88H   2C   1O   1     G   200.000  3500.000  1000.000    1
 1.76069008E+00 9.20000082E-03-4.42258813E-06 1.00641212E-09-8.83855640E-14    2
-1.39958323E+04 1.36563230E+01 4.79372315E+00-9.90833369E-03 3.73220008E-05    3
-3.79285261E-08 1.31772652E-11-1.43089567E+04 6.02812900E-01                   4
CH2OH             GUNL93C   1H   3O   1     G   200.000  3500.000  1000.000    1
 3.69266569E+00 8.64576797E-03-3.75101120E-06 7.87234636E-10-6.48554201E-14    2
-3.24250627E+03 5.81043215E+00 3.86388918E+00 5.59672304E-03 5.93271791E-06    3
-1.04532012E-08 4.36967278E-12-3.19391367E+03 5.47302243E+00                   4
CH3O              121686C   1H   3O   1     G   300.00   3000.00   1000.000    1
 0.03770799E+02 0.07871497E-01-0.02656384E-04 0.03944431E-08-0.02112616E-12    2
 0.12783252E+03 0.02929575E+02 0.02106204E+02 0.07216595E-01 0.05338472E-04    3
-0.07377636E-07 0.02075610E-10 0.09786011E+04 0.13152177E+02                   4
CH3OH             L 8/88C   1H   4O   1     G   200.000  3500.000  1000.000    1
 1.78970791E+00 1.40938292E-02-6.36500835E-06 1.38171085E-09-1.17060220E-13    2
-2.53748747E+04 1.45023623E+01 5.71539582E+00-1.52309129E-02 6.52441155E-05    3
-7.10806889E-08 2.61352698E-11-2.56427656E+04-1.50409823E+00                   4
C2H               L 1/91C   2H   1          G   200.000  3500.000  1000.000    1
 3.16780652E+00 4.75221902E-03-1.83787077E-06 3.04190252E-10-1.77232770E-14    2
 6.71210650E+04 6.63589475E+00 2.88965733E+00 1.34099611E-02-2.84769501E-05    3
 2.94791045E-08-1.09331511E-11 6.68393932E+04 6.22296438E+00                   4
C2H2              L 1/91C   2H   2          G   200.000  3500.000  1000.000    1
 4.14756964E+00 5.96166664E-03-2.37294852E-06 4.67412171E-10-3.61235213E-14    2
 2.59359992E+04-1.23028121E+00 8.08681094E-01 2.33615629E-02-3.55171815E-05    3
 2.80152437E-08-8.50072974E-12 2.64289807E+04 1.39397051E+01                   4
C2H3              L 2/92C   2H   3          G   200.000  3500.000  1000.000    1
 3.01672400E+00 1.03302292E-02-4.68082349E-06 1.01763288E-09-8.62607041E-14    2
 3.46128739E+04 7.78732378E+00 3.21246645E+00 1.51479162E-03 2.59209412E-05    3
-3.57657847E-08 1.47150873E-11 3.48598468E+04 8.51054025E+00                   4
C2H4              L 1/91C   2H   4          G   200.000  3500.000  1000.000    1
 2.03611116E+00 1.46454151E-02-6.71077915E-06 1.47222923E-09-1.25706061E-13    2
 4.93988614E+03 1.03053693E+01 3.95920148E+00-7.57052247E-03 5.70990292E-05    3
-6.91588753E-08 2.69884373E-11 5.08977593E+03 4.09733096E+00                   4
C2H5              L12/92C   2H   5          G   200.000  3500.000  1000.000    1
 1.95465642E+00 1.73972722E-02-7.98206668E-06 1.75217689E-09-1.49641576E-13    2
 1.28575200E+04 1.34624343E+01 4.30646568E+00-4.18658892E-03 4.97142807E-05    3
-5.99126606E-08 2.30509004E-11 1.28416265E+04 4.70720924E+00                   4
C2H6              L 8/88C   2H   6          G   200.000  3500.000  1000.000    1
 1.07188150E+00 2.16852677E-02-1.00256067E-05 2.21412001E-09-1.90002890E-13    2
-1.14263932E+04 1.51156107E+01 4.29142492E+00-5.50154270E-03 5.99438288E-05    3
-7.08466285E-08 2.68685771E-11-1.15222055E+04 2.66682316E+00                   4
CH2CO             L 5/90C   2H   2O   1     G   200.000  3500.000  1000.000    1
 4.51129732E+00 9.00359745E-03-4.16939635E-06 9.23345882E-10-7.94838201E-14    2
-7.55105311E+03 6.32247205E-01 2.13583630E+00 1.81188721E-02-1.73947474E-05    3
 9.34397568E-09-2.01457615E-12-7.04291804E+03 1.22156480E+01                   4
HCCO              SRIC91H   1C   2O   1     G   300.00   4000.00   1000.000    1
 0.56282058E+01 0.40853401E-02-0.15934547E-05 0.28626052E-09-0.19407832E-13    2
 0.19327215E+05-0.39302595E+01 0.22517214E+01 0.17655021E-01-0.23729101E-04    3
 0.17275759E-07-0.50664811E-11 0.20059449E+05 0.12490417E+02                   4
HCCOH              SRI91C   2O   1H   2     G   300.000  5000.000  1000.000    1
 0.59238291E+01 0.67923600E-02-0.25658564E-05 0.44987841E-09-0.29940101E-13    2
 0.72646260E+04-0.76017742E+01 0.12423733E+01 0.31072201E-01-0.50866864E-04    3
 0.43137131E-07-0.14014594E-10 0.80316143E+04 0.13874319E+02                   4
H2CN               41687H   2C   1N   1     G   300.00   4000.000  1000.000    1
 0.52097030E+01 0.29692911E-02-0.28555891E-06-0.16355500E-09 0.30432589E-13    2
 0.27677109E+05-0.44444780E+01 0.28516610E+01 0.56952331E-02 0.10711400E-05    3
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-0.16226120E-08-0.23511081E-12 0.28637820E+05 0.89927511E+01                   4
HCN               GRI/98H   1C   1N   1     G   200.000  6000.000  1000.000    1
 0.38022392E+01 0.31464228E-02-0.10632185E-05 0.16619757E-09-0.97997570E-14    2
 0.14407292E+05 0.15754601E+01 0.22589886E+01 0.10051170E-01-0.13351763E-04    3
 0.10092349E-07-0.30089028E-11 0.14712633E+05 0.89164419E+01                   4
HNO               And93 H   1N   1O   1     G   200.000  6000.000  1000.000    1
 0.29792509E+01 0.34944059E-02-0.78549778E-06 0.57479594E-10-0.19335916E-15    2
 0.11750582E+05 0.86063728E+01 0.45334916E+01-0.56696171E-02 0.18473207E-04    3
-0.17137094E-07 0.55454573E-11 0.11548297E+05 0.17498417E+01                   4
N                 L 6/88N   1               G   200.000  6000.000  1000.000    1
 0.24159429E+01 0.17489065E-03-0.11902369E-06 0.30226245E-10-0.20360982E-14    2
 0.56133773E+05 0.46496096E+01 0.25000000E+01 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 0.56104637E+05 0.41939087E+01                   4
NNH               T07/93N   2H   1          G   200.000  6000.000  1000.000    1
 0.37667544E+01 0.28915082E-02-0.10416620E-05 0.16842594E-09-0.10091896E-13    2
 0.28650697E+05 0.44705067E+01 0.43446927E+01-0.48497072E-02 0.20059459E-04    3
-0.21726464E-07 0.79469539E-11 0.28791973E+05 0.29779410E+01                   4
N2O               L 7/88N   2O   1          G   200.000  6000.000  1000.000    1
 0.48230729E+01 0.26270251E-02-0.95850874E-06 0.16000712E-09-0.97752303E-14    2
 0.80734048E+04-0.22017207E+01 0.22571502E+01 0.11304728E-01-0.13671319E-04    3
 0.96819806E-08-0.29307182E-11 0.87417744E+04 0.10757992E+02                   4
NH                And94 N   1H   1          G   200.000  6000.000  1000.000    1
 0.27836928E+01 0.13298430E-02-0.42478047E-06 0.78348501E-10-0.55044470E-14    2
 0.42120848E+05 0.57407799E+01 0.34929085E+01 0.31179198E-03-0.14890484E-05    3
 0.24816442E-08-0.10356967E-11 0.41880629E+05 0.18483278E+01                   4
NH2               And89 N   1H   2          G   200.000  6000.000  1000.000    1
 0.28347421E+01 0.32073082E-02-0.93390804E-06 0.13702953E-09-0.79206144E-14    2
 0.22171957E+05 0.65204163E+01 0.42040029E+01-0.21061385E-02 0.71068348E-05    3
-0.56115197E-08 0.16440717E-11 0.21885910E+05-0.14184248E+00                   4
NH3               J 6/77N   1H   3          G   200.000  6000.000  1000.000    1
 0.26344521E+01 0.56662560E-02-0.17278676E-05 0.23867161E-09-0.12578786E-13    2
-0.65446958E+04 0.65662928E+01 0.42860274E+01-0.46605230E-02 0.21718513E-04    3
-0.22808887E-07 0.82638046E-11-0.67417285E+04-0.62537277E+00                   4
NO                RUS 78N   1O   1          G   200.000  6000.000  1000.000    1
 0.32606056E+01 0.11911043E-02-0.42917048E-06 0.69457669E-10-0.40336099E-14    2
 0.99209746E+04 0.63693027E+01 0.42184763E+01-0.46389760E-02 0.11041022E-04    3
-0.93361354E-08 0.28035770E-11 0.98446230E+04 0.22808464E+01                   4
NO2               L 7/88N   1O   2          G   200.000  6000.000  1000.000    1
 0.48847542E+01 0.21723956E-02-0.82806906E-06 0.15747510E-09-0.10510895E-13    2
 0.23164983E+04-0.11741695E+00 0.39440312E+01-0.15854290E-02 0.16657812E-04    3
-0.20475426E-07 0.78350564E-11 0.28966179E+04 0.63119917E+01                   4
HCNO              BDEA94H   1N   1C   1O   1G   300.000  5000.000  1382.000    1
 6.59860456E+00 3.02778626E-03-1.07704346E-06 1.71666528E-10-1.01439391E-14    2
 1.79661339E+04-1.03306599E+01 2.64727989E+00 1.27505342E-02-1.04794236E-05    3
 4.41432836E-09-7.57521466E-13 1.92990252E+04 1.07332972E+01                   4
HOCN              BDEA94H   1N   1C   1O   1G   300.000  5000.000  1368.000    1
 5.89784885E+00 3.16789393E-03-1.11801064E-06 1.77243144E-10-1.04339177E-14    2
-3.70653331E+03-6.18167825E+00 3.78604952E+00 6.88667922E-03-3.21487864E-06    3
 5.17195767E-10 1.19360788E-14-2.82698400E+03 5.63292162E+00                   4
HNCO              BDEA94H   1N   1C   1O   1G   300.000  5000.000  1478.000    1
 6.22395134E+00 3.17864004E-03-1.09378755E-06 1.70735163E-10-9.95021955E-15    2
-1.66599344E+04-8.38224741E+00 3.63096317E+00 7.30282357E-03-2.28050003E-06    3
-6.61271298E-10 3.62235752E-13-1.55873636E+04 6.19457727E+00                   4
NCO               EA 93 N   1C   1O   1     G   200.000  6000.000  1000.000    1
 0.51521845E+01 0.23051761E-02-0.88033153E-06 0.14789098E-09-0.90977996E-14    2
 0.14004123E+05-0.25442660E+01 0.28269308E+01 0.88051688E-02-0.83866134E-05    3
 0.48016964E-08-0.13313595E-11 0.14682477E+05 0.95504646E+01                   4
CN                HBH92 C   1N   1          G   200.000  6000.000  1000.000    1
 0.37459805E+01 0.43450775E-04 0.29705984E-06-0.68651806E-10 0.44134173E-14    2
 0.51536188E+05 0.27867601E+01 0.36129351E+01-0.95551327E-03 0.21442977E-05    3
-0.31516323E-09-0.46430356E-12 0.51708340E+05 0.39804995E+01                   4
HCNN              SRI/94C   1N   2H   1     G   300.000  5000.000  1000.000    1
 0.58946362E+01 0.39895959E-02-0.15982380E-05 0.29249395E-09-0.20094686E-13    2
 0.53452941E+05-0.51030502E+01 0.25243194E+01 0.15960619E-01-0.18816354E-04    3
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 0.12125540E-07-0.32357378E-11 0.54261984E+05 0.11675870E+02                   4
N2                121286N   2               G   300.000  5000.000  1000.000    1
 0.02926640E+02 0.14879768E-02-0.05684760E-05 0.10097038E-09-0.06753351E-13    2
-0.09227977E+04 0.05980528E+02 0.03298677E+02 0.14082404E-02-0.03963222E-04    3
 0.05641515E-07-0.02444854E-10-0.10208999E+04 0.03950372E+02                   4
AR                120186AR  1               G   300.000  5000.000  1000.000    1
 0.02500000E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-0.07453750E+04 0.04366000E+02 0.02500000E+02 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-0.07453750E+04 0.04366000E+02                   4
C3H8              L 4/85C   3H   8          G   300.000  5000.000  1000.000    1
 0.75341368E+01 0.18872239E-01-0.62718491E-05 0.91475649E-09-0.47838069E-13    2
-0.16467516E+05-0.17892349E+02 0.93355381E+00 0.26424579E-01 0.61059727E-05    3
-0.21977499E-07 0.95149253E-11-0.13958520E+05 0.19201691E+02                   4
C3H7              L 9/84C   3H   7          G   300.000  5000.000  1000.000    1
 0.77026987E+01 0.16044203E-01-0.52833220E-05 0.76298590E-09-0.39392284E-13    2
 0.82984336E+04-0.15480180E+02 0.10515518E+01 0.25991980E-01 0.23800540E-05    3
-0.19609569E-07 0.93732470E-11 0.10631863E+05 0.21122559E+02                   4
CH3CHO            L 8/88C   2H   4O   1     G   200.000  6000.000  1000.000    1
 0.54041108E+01 0.11723059E-01-0.42263137E-05 0.68372451E-09-0.40984863E-13    2
-0.22593122E+05-0.34807917E+01 0.47294595E+01-0.31932858E-02 0.47534921E-04    3
-0.57458611E-07 0.21931112E-10-0.21572878E+05 0.41030159E+01                   4
CH2CHO            SAND86O   1H   3C   2     G   300.000  5000.000  1000.000    1
 0.05975670E+02 0.08130591E-01-0.02743624E-04 0.04070304E-08-0.02176017E-12    2
 0.04903218E+04-0.05045251E+02 0.03409062E+02 0.10738574E-01 0.01891492E-04    3
-0.07158583E-07 0.02867385E-10 0.15214766E+04 0.09558290E+02                   4
END
```

Species	Geometry	ε/kB	σ	μ	α	Zrot	
AR	0	136.500	3.330	0.000	0.000	0.000	
C	0	71.400	3.298	0.000	0.000	0.000	! *
C2	1	97.530	3.621	0.000	1.760	4.000	
C2O	1	232.400	3.828	0.000	0.000	1.000	! *
CN2	1	232.400	3.828	0.000	0.000	1.000	! OIS
C2H	1	209.000	4.100	0.000	0.000	2.500	
C2H2	1	209.000	4.100	0.000	0.000	2.500	
C2H2OH	2	224.700	4.162	0.000	0.000	1.000	! *
C2H3	2	209.000	4.100	0.000	0.000	1.000	! *
C2H4	2	280.800	3.971	0.000	0.000	1.500	
C2H5	2	252.300	4.302	0.000	0.000	1.500	
C2H6	2	252.300	4.302	0.000	0.000	1.500	
C2N	1	232.400	3.828	0.000	0.000	1.000	! OIS
C2N2	1	349.000	4.361	0.000	0.000	1.000	! OIS
C3H2	2	209.000	4.100	0.000	0.000	1.000	! *
C3H4	1	252.000	4.760	0.000	0.000	1.000	
C3H6	2	266.800	4.982	0.000	0.000	1.000	
C3H7	2	266.800	4.982	0.000	0.000	1.000	
C4H6	2	357.000	5.180	0.000	0.000	1.000	
I*C3H7	2	266.800	4.982	0.000	0.000	1.000	
N*C3H7	2	266.800	4.982	0.000	0.000	1.000	
C3H8	2	266.800	4.982	0.000	0.000	1.000	
C4H	1	357.000	5.180	0.000	0.000	1.000	
C4H2	1	357.000	5.180	0.000	0.000	1.000	
C4H2OH	2	224.700	4.162	0.000	0.000	1.000	! *
C4H8	2	357.000	5.176	0.000	0.000	1.000	
C4H9	2	357.000	5.176	0.000	0.000	1.000	
I*C4H9	2	357.000	5.176	0.000	0.000	1.000	
C5H2	1	357.000	5.180	0.000	0.000	1.000	
C5H3	1	357.000	5.180	0.000	0.000	1.000	
C6H2	1	357.000	5.180	0.000	0.000	1.000	
C6H5	2	412.300	5.349	0.000	0.000	1.000	! JAM
C6H5O	2	450.000	5.500	0.000	0.000	1.000	! JAM
C5H5OH	2	450.000	5.500	0.000	0.000	1.000	! JAM
C6H6	2	412.300	5.349	0.000	0.000	1.000	! SVE
C6H7	2	412.300	5.349	0.000	0.000	1.000	! JAM
CH	1	80.000	2.750	0.000	0.000	0.000	
CH2	1	144.000	3.800	0.000	0.000	0.000	
CH2(S)	1	144.000	3.800	0.000	0.000	0.000	
CH2*	1	144.000	3.800	0.000	0.000	0.000	
CH2CHCCH	2	357.000	5.180	0.000	0.000	1.000	! JAM
CH2CHCCH2	2	357.000	5.180	0.000	0.000	1.000	! JAM
CH2CHCH2	2	260.000	4.850	0.000	0.000	1.000	! JAM
CH2CHCHCH	2	357.000	5.180	0.000	0.000	1.000	! JAM
CH2CHCHCH2	2	357.000	5.180	0.000	0.000	1.000	! JAM
CH2CO	2	436.000	3.970	0.000	0.000	2.000	
CH2O	2	498.000	3.590	0.000	0.000	2.000	
CH2OH	2	417.000	3.690	1.700	0.000	2.000	
CH3	1	144.000	3.800	0.000	0.000	0.000	
CH3CC	2	252.000	4.760	0.000	0.000	1.000	! JAM
CH3CCCH2	2	357.000	5.180	0.000	0.000	1.000	! JAM
CH3CCCH3	2	357.000	5.180	0.000	0.000	1.000	! JAM
CH3CCH2	2	260.000	4.850	0.000	0.000	1.000	! JAM
CH3CHCH	2	260.000	4.850	0.000	0.000	1.000	! JAM
CH3CH2CCH	2	357.000	5.180	0.000	0.000	1.000	! JAM
CH3CHO	2	436.000	3.970	0.000	0.000	2.000	
CH2CHO	2	436.000	3.970	0.000	0.000	2.000	
CH3CO	2	436.000	3.970	0.000	0.000	2.000	
CH3O	2	417.000	3.690	1.700	0.000	2.000	
CH3OH	2	481.800	3.626	0.000	0.000	1.000	! SVE
CH4	2	141.400	3.746	0.000	2.600	13.000	
CH4O	2	417.000	3.690	1.700	0.000	2.000	
CN	1	75.000	3.856	0.000	0.000	1.000	! OIS

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CNC               1   232.400     3.828     0.000     0.000     1.000 ! OIS
CNN               1   232.400     3.828     0.000     0.000     1.000 ! OIS
CO                1    98.100     3.650     0.000     1.950     1.800
CO2               1   244.000     3.763     0.000     2.650     2.100
H                 0   145.000     2.050     0.000     0.000     0.000
H2C4O             2   357.000     5.180     0.000     0.000     1.000 ! JAM
H2                1    38.000     2.920     0.000     0.790   280.000
H2CCCCH           2   357.000     5.180     0.000     0.000     1.000 ! JAM
H2CCCCH2          2   357.000     5.180     0.000     0.000     1.000 ! JAM
H2CCCH            2   252.000     4.760     0.000     0.000     1.000 ! JAM
H2CN              1   569.000     3.630     0.000     0.000     1.000 ! os/jm
H2NO              2   116.700     3.492     0.000     0.000     1.000 ! JAM
H2O               2   572.400     2.605     1.844     0.000     4.000
H2O2              2   107.400     3.458     0.000     0.000     3.800
HC2N2             1   349.000     4.361     0.000     0.000     1.000 ! OIS
HCCHCCH           2   357.000     5.180     0.000     0.000     1.000 ! JAM
HCCO              2   150.000     2.500     0.000     0.000     1.000 ! *
HCNN              2   150.000     2.500     0.000     0.000     1.000 ! *
HCCOH             2   436.000     3.970     0.000     0.000     2.000
HCN               1   569.000     3.630     0.000     0.000     1.000 ! OIS
HCO               2   498.000     3.590     0.000     0.000     0.000
HE                0    10.200     2.576     0.000     0.000     0.000 ! *
HCNO              2   232.400     3.828     0.000     0.000     1.000 ! JAM
HOCN              2   232.400     3.828     0.000     0.000     1.000 ! JAM
HNCO              2   232.400     3.828     0.000     0.000     1.000 ! OIS
HNNO              2   232.400     3.828     0.000     0.000     1.000 ! *
HNO               2   116.700     3.492     0.000     0.000     1.000 ! *
HNOH              2   116.700     3.492     0.000     0.000     1.000 ! JAM
HO2               2   107.400     3.458     0.000     0.000     1.000 ! *
N                 0    71.400     3.298     0.000     0.000     0.000 ! *
N2                1    97.530     3.621     0.000     1.760     4.000
N2H2              2    71.400     3.798     0.000     0.000     1.000 ! *
N2H3              2   200.000     3.900     0.000     0.000     1.000 ! *
N2H4              2   205.000     4.230     0.000     4.260     1.500
N2O               1   232.400     3.828     0.000     0.000     1.000 ! *
NCN               1   232.400     3.828     0.000     0.000     1.000 ! OIS
NCO               1   232.400     3.828     0.000     0.000     1.000 ! OIS
NH                1    80.000     2.650     0.000     0.000     4.000
NH2               2    80.000     2.650     0.000     2.260     4.000
NH3               2   481.000     2.920     1.470     0.000    10.000
NNH               2    71.400     3.798     0.000     0.000     1.000 ! *
NO                1    97.530     3.621     0.000     1.760     4.000
NCNO              2   232.400     3.828     0.000     0.000     1.000 ! OIS
NO2               2   200.000     3.500     0.000     0.000     1.000 ! *
O                 0    80.000     2.750     0.000     0.000     0.000
O2                1   107.400     3.458     0.000     1.600     3.800
OH                1    80.000     2.750     0.000     0.000     0.000
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Appendix:B

Reduced Mechanism by Hadi Nozari

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!Reduced Mechanism by Hadi Nozari, H. Nozari and A. Karabeyoglu Fuel 2015
vol.159 223-233 DOI10.1016/j.fuel.2015.06.075
!High precision for H2 NH3 O2 N2 kinetics
!Source detailed Mechanism: Konnov

ELEM H O N !AR
END
SPECIES
H          H2         O          O2         OH         HO2        H2O
N          NH         NO
N2O        NH2
HNO        NO2        NNH        NH3        N2H2
N2       !AR
H2NO     N2H4       N2H3
END
       BASE M=N2

Reactions                          A             n       Ea (cal/mol)
H+H+M=H2+M                       7.000E+17     -1.0         0.0
 H2/0.0/ N2/0.0/ H/0.0/ H2O/14.3/

H+H+N2=H2+N2                     5.400E+18     -1.3         0.0
O+O+M=O2+M                       1.000E+17     -1.0         0.0
 O/71.0/ O2/20.0/ NO/5.0/ N2/5.0/ N/5.0/ H2O/5.0/

O+H2=OH+H                        5.060E+04      2.67     6290.0

H+O2=OH+O                        9.750E+13      0.0     14850.0

H+O2(+M)=HO2(+M)                 1.480E+12      0.6          0.0
    LOW /3.50E+16 -0.41 -1116.0/
    TROE /0.5 100000 10/
 H2O/10.6/ H2/1.5/!AR/0.0/
!H+O2(+AR)=HO2(+AR)               1.480E+12      0.6          0.0
!    LOW /7.00E+17 -0.8  0.0/
!    TROE /0.45 10 100000/
H+OH+M=H2O+M                     2.200E+22     -2.0          0.0
 H2O/6.4/ !AR/0.38/
H2+OH=H2O+H                      1.000E+08      1.6       3300.0
OH+OH=H2O+O                      1.500E+09      1.14       100.0
HO2+OH=H2O+O2                    2.890E+13      0.0       -500.0

HO2+O=OH+O2                      1.630E+13      0.0       -445.0
H+HO2=H2+O2                      4.280E+13      0.0       1411.0
H+HO2=OH+OH                      1.700E+14      0.0        875.0
H+HO2=H2O+O                      3.000E+13      0.0       1720.0

N2+O=NO+N                        1.800E+14      0.0      76100.0
NH3+M=NH2+H+M                    2.200E+16      0.0      93470.0
NH3+H=NH2+H2                     5.420E+05      2.4       9920.0
NH3+O=NH2+OH                     1.100E+06      2.1       5210.0
NH3+OH=NH2+H2O                   5.000E+07      1.6        950.0
NH3+NH=NH2+NH2                   3.160E+14      0.0      26770.0
NH2+M=NH+H+M                     3.160E+23     -2.0      91400.0

NH2+N=N2+H+H                     6.900E+13      0.0          0.0

NH2+NH=N2H2+H                    1.500E+15     -0.5          0.0
NH2+NH=NH3+N                     1.000E+13      0.0       2000.0
NH2+NH2=N2H2+H2                  1.000E+13      0.0       1500.0

NH2+O=H2+NO                      5.000E+12      0.0          0.0
NH2+O=HNO+H                      4.500E+13      0.0          0.0
NH2+O=NH+OH                      7.000E+12      0.0          0.0
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NH2+OH=NH+H2O                   9.000E+07      1.5      -460.0
NH2+HO2=HNO+H2O                 5.680E+15     -1.12      707.0
NH2+O2=HNO+OH                   1.000E+13      0.0     26290.0

NH2+NO=NNH+OH                   2.290E+10      0.425    -814.0
NH2+NO=N2+H2O                   2.770E+20     -2.65     1258.0
NH2+NO=H2+N2O                   1.000E+13      0.0     33700.0
NH2+NO2=N2O+H2O                 1.620E+16     -1.44      270.0

NH+H=N+H2                       3.200E+13      0.0       325.0
NH+N=N2+H                       9.000E+11      0.5         0.0
NH+NH=NNH+H                     5.100E+13      0.0         0.0
NH+O=NO+H                       7.000E+13      0.0         0.0
NH+O=N+OH                       7.000E+12      0.0         0.0
NH+OH=HNO+H                     2.000E+13      0.0         0.0
NH+OH=N+H2O                     2.000E+09      1.2         0.0
NH+OH=NO+H2                     2.000E+13      0.0         0.0

NH+O2=HNO+O                     4.000E+13      0.0     17880.0
NH+O2=NO+OH                     4.500E+08      0.79     1190.0
NH+H2O=HNO+H2                   2.000E+13      0.0     13850.0
NH+N2O=N2+HNO                   2.000E+12      0.0      6000.0
NH+NO=N2+OH                     6.100E+13     -0.50      120.0

N+OH=NO+H                       2.800E+13      0.0         0.0
N+O2=NO+O                       9.000E+09      1.0      6500.0

NO+O(+M)=NO2(+M)                1.300E+15     -0.75        0.0
    LOW /4.72E+24 -2.87 1551.0/
    TROE /0.962 10.0 7962.0 /
    NO2 /6.2/ NO /1.8/ O2 /0.8/ N2O /4.4/
    H2O /10.0/!AR /0.6/

H+NO(+M)=HNO(+M)                1.520E+15     -0.41        0.0
    LOW /4.00E+20 -1.75 0.0 /
    H2O/10.0/ O2/1.5/ H2/2.0/!AR/0.75/

N2O(+M)=N2+O(+M)                1.260E+12      0.0     62620.0
    LOW / 4.000E+14 0.0 56640.0/
   O2/1.4/ N2/1.7/ H2O/12.0/ NO/3.0/ N2O/3.5/

N2O+O=N2+O2                     1.000E+14      0.0     28200.0
N2O+O=NO+NO                     6.920E+13      0.0     26630.0

N2O+NO=N2+NO2                   2.750E+14      0.0     50000.0
N2O+H=N2+OH                     2.200E+14      0.0     16750.0
N2O+OH=N2+HO2                   1.000E+14      0.0     30000.0
NO2+O=NO+O2                     3.910E+12      0.0      -238.0

NO2+H=NO+OH                     1.320E+14      0.0       362.0
NO2+OH=HO2+NO                   1.810E+13      0.0      6676.0
HNO+H=NO+H2                     4.460E+11      0.72      655.0
HNO+OH=NO+H2O                   1.300E+07      1.88     -956.0
HNO+O=OH+NO                     5.000E+11      0.5      2000.0
HNO+NH2=NH3+NO                  2.000E+13      0.0      1000.0
NNH=N2+H                        3.000E+08      0.0         0.0
NNH+M=N2+H+M                    1.000E+13      0.5      3060.0
NNH+O=NH+NO                     2.000E+14      0.0      4000.0
NNH+O2=N2O+OH                   2.900E+11     -0.34      150.0
NNH+NO=N2+HNO                   5.000E+13      0.0         0.0
N2H2+M=NNH+H+M                  5.000E+16      0.0     50000.0
     H2O/15.0/ O2/2.0/ N2/2.0/ H2/2.0/

N2H2+H=NNH+H2                   8.500E+04      2.63     -230.0
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N2H2+NH2=NH3+NNH               8.800E-02      4.05    -1610.0

N2H2+O=NH2+NO                  1.000E+13      0.0        0.0
N2H2+O=NNH+OH                  2.000E+13      0.0     1000.0
N2H2+OH=NNH+H2O                5.920E+01      3.4     -1360.0
N2H2+NO=N2O+NH2                3.000E+10      0.0        0.0


!!last added by imp reacs prod/decomp imp radicsls
NH+H2=NH2+H                    1.000E+14      0.0     20070.0
N2O+H=NH+NO                    6.700E+22     -2.16    37155.0
!OH+OH(+H2O)=H2O2(+H2O)         7.200E+13     -0.37       0.0
!    LOW /1.45E+18 0.0 0.0/
H2NO+NO=HNO+HNO                2.000E+07      2.0     13000.0
NH2+HO2=H2NO+OH                2.910E+17     -1.32     1248.0
NH2+O2=H2NO+O                  6.000E+13      0.0     29880.0
H2NO+O=HNO+OH                  3.000E+07      2.0      2000.0
H2NO+H=HNO+H2                  3.000E+07      2.0      2000.0
HNO+NH=NH2+NO                  5.000E+11      0.5         0.0
H2NO+H=NH2+OH                  5.000E+13      0.0         0.0
N2H4(+M)=NH2+NH2(+M)           5.000E+14      0.0     60000.0
    LOW/1.50E+15 0.0 39000.0 /
  N2/2.4/ NH3/3.0/ N2H4/4.0/
N2H4+O=N2H2+H2O                8.500E+13      0.0      1200.0
NH3+NH2=N2H3+H2                1.000E+11      0.5     21600.0
N2H4+NH=NH2+N2H3               1.000E+09      1.5      2000.0
N2H3+M=N2H2+H+M                1.000E+16      0.0     37000.0
END
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THERMO ALL
 300.000  1000.000  5000.000
H                 L 6/94H   1O   00   00   0G   200.000  6000.00  1000.0      1
 0.25000000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 0.25473660E+05-0.44668285E+00 0.25000000E+01 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 0.25473660E+05-0.44668285E+00 0.26219035E+05    4
H2  REF ELEMENT   RUS 78H   20   00   00   0G   200.000  6000.00  1000.0      1
 0.29328305E+01 0.82659802E-03-0.14640057E-06 0.15409851E-10-0.68879615E-15    2
-0.81305582E+03-0.10243164E+01 0.23443029E+01 0.79804248E-02-0.19477917E-04    3
 0.20156967E-07-0.73760289E-11-0.91792413E+03 0.68300218E+00 0.00000000E+00    4
O                 L 1/90O   1O   00   00   0G   200.000  6000.00  1000.0      1
 2.54363697E+00-2.73162486E-05-4.19029520E-09 4.95481845E-12-4.79553694E-16    2
 2.92260120E+04 4.92229457E+00 3.16826710E+00-3.27931884E-03 6.64306396E-06    3
-6.12806624E-09 2.11265971E-12 2.91222592E+04 2.05193346E+00 2.99687009E+04    4
O2 REF ELEMENT    RUS 89O   20   00   00   0G   200.000  6000.00  1000.0      1
 3.66096083E+00 6.56365523E-04-1.41149485E-07 2.05797658E-11-1.29913248E-15    2
-1.21597725E+03 3.41536184E+00 3.78245636E+00-2.99673415E-03 9.84730200E-06    3
-9.68129508E-09 3.24372836E-12-1.06394356E+03 3.65767573E+00 0.00000000E+00    4
OH                RUS 78O   1H   10   00   0G   200.000  6000.00  1000.0      1
 2.83864607E+00 1.10725586E-03-2.93914978E-07 4.20524247E-11-2.42169092E-15    2
 3.94395852E+03 5.84452662E+00 3.99201543E+00-2.40131752E-03 4.61793841E-06    3
-3.88113333E-09 1.36411470E-12 3.61508056E+03-1.03925458E-01 4.73234213E+03    4
HO2               L 5/89H   1O   20   00   0G   200.000  6000.00  1000.0      1
 0.41722659E+01 0.18812098E-02-0.34629297E-06 0.19468516E-10 0.17609153E-15    2
 0.61818851E+02 0.29577974E+01 0.43017880E+01-0.47490201E-02 0.21157953E-04    3
-0.24275961E-07 0.92920670E-11 0.29480876E+03 0.37167010E+01 0.15096500E+04    4
H2O               L 5/89H   2O   10   00   0G   200.000  6000.00  1000.0      1
 0.26770389E+01 0.29731816E-02-0.77376889E-06 0.94433514E-10-0.42689991E-14    2
-0.29885894E+05 0.68825500E+01 0.41986352E+01-0.20364017E-02 0.65203416E-05    3
-0.54879269E-08 0.17719680E-11-0.30293726E+05-0.84900901E+00-0.29084817E+05    4
H2O2              L 2/93H   2O   20   00   0G   200.000  6000.00  1000.0      1
 4.57333537E+00 4.04984070E-03-1.29479479E-06 1.97281710E-10-1.13402846E-14    2
-1.80548121E+04 7.04278488E-01 4.27611269E+00-5.42822417E-04 1.67335701E-05    3
-2.15770813E-08 8.62454363E-12-1.77542989E+04 3.43505074E+00-1.63942313E+04    4
CO                RUS 79C   1O   10   00   0G   200.000  6000.00  1000.0      1
 0.30484859E+01 0.13517281E-02-0.48579405E-06 0.78853644E-10-0.46980746E-14    2
-0.14266117E+05 0.60170977E+01 0.35795335E+01-0.61035369E-03 0.10168143E-05    3
 0.90700586E-09-0.90442449E-12-0.14344086E+05 0.35084093E+01-0.13293628E+05    4
CO2               L 7/88C   1O   20   00   0G   200.000  6000.00  1000.0      1
 0.46365111E+01 0.27414569E-02-0.99589759E-06 0.16038666E-09-0.91619857E-14    2
-0.49024904E+05-0.19348955E+01 0.23568130E+01 0.89841299E-02-0.71220632E-05    3
 0.24573008E-08-0.14288548E-12-0.48371971E+05 0.99009035E+01-0.47328105E+05    4
HCO               L12/89H   1C   1O   10   0G   200.000  6000.00  1000.0      1
 3.64896209E+00 3.08090819E-03-1.12429876E-06 1.86308085E-10-1.13951828E-14    2
 3.71209048E+03 5.06147406E+00 4.22118584E+00-3.24392532E-03 1.37799446E-05    3
-1.33144093E-08 4.33768865E-12 3.83956496E+03 3.39437243E+00 5.05141013E+03    4
CH3               L 8/88C   1H   30   00   0G   200.000  6000.00  1000.0      1
 0.29669735E+01 0.57936672E-02-0.19694809E-05 0.30556936E-09-0.17767843E-13    2
 0.16537116E+05 0.47918803E+01 0.36733375E+01 0.20020559E-02 0.57853135E-05    3
-0.69873054E-08 0.26055599E-11 0.16440180E+05 0.16018315E+01 0.17662905E+05    4
CH4   ANHARMONIC  L 8/88C   1H   40   00   0G   200.000  6000.00  1000.0      1
 0.16354256E+01 0.10084431E-01-0.33692369E-05 0.53497280E-09-0.31552817E-13    2
-0.10005603E+05 0.99936953E+01 0.51498792E+01-0.13671008E-01 0.49180130E-04    3
-0.48474403E-07 0.16669441E-10-0.10246648E+05-0.46413244E+01-0.89722666E+04    4
C2H6      ETHANE  L 5/84C   2H   60   00   0G   300.000  5000.00  1000.0      1
 0.47028847E 01 0.14042635E-01-0.46469377E-05 0.67473738E-09-0.35089312E-13    2
-0.12671988E 05-0.45433950E 01 0.15395260E 01 0.15040841E-01 0.66847115E-05    3
-0.13382948E-07 0.48561398E-11-0.11248766E 05 0.14107375E 02-0.10085085E 05    4
CH2O              L 8/88H   2C   1O   10   0G   200.000  6000.00  1000.0      1
 0.31694807E+01 0.61932742E-02-0.22505981E-05 0.36598245E-09-0.22015410E-13    2
-0.14478425E+05 0.60423533E+01 0.47937036E+01-0.99081518E-02 0.37321459E-04    3
-0.37927902E-07 0.13177015E-10-0.14308955E+05 0.60288702E+00-0.13059098E+05    4
C2H5              T12/91C   2H   5    0    0G   200.000  6000.00  1000.0      1
 0.42878814E+01 0.12433893E-01-0.44139119E-05 0.70654102E-09-0.42035136E-13    2
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 0.12056455E+05 0.84602583E+00 0.43058580E+01-0.41833638E-02 0.49707270E-04    3
-0.59905874E-07 0.23048478E-10 0.12841714E+05 0.47100236E+01 0.14271225E+05    4
CH2      TRIPLET  RUS 79C   1H   2    0    0G   200.000  6000.00  1000.0      1
 0.25387122E+01 0.38225491E-02-0.12861304E-05 0.19800308E-09-0.11465743E-13    2
 0.46129253E+05 0.81054648E+01 0.41793655E+01-0.22178553E-02 0.79653602E-05    3
-0.69127339E-08 0.22475318E-11 0.45750857E+05-0.76113703E-02 0.46956131E+05    4
CH3O             L 8/88C   1H   3O   1    0G   200.000  6000.00  1000.0      1
 0.42653308E+01 0.78576406E-02-0.28410438E-05 0.46045190E-09-0.27631906E-13    2
 0.59351066E+02 0.39309947E+00 0.32652337E+01 0.33031665E-02 0.17048801E-04    3
-0.22709630E-07 0.88071768E-11 0.73229580E+03 0.74257357E+01 0.19625450E+04    4
CH2OH            T 9/92C   1H   3O   1    0G   200.000  6000.00  1000.0      1
 0.46776733E+01 0.65608772E-02-0.22636864E-05 0.35530469E-09-0.20842959E-13    2
-0.28928048E+04 0.48041879E+00 0.38644027E+01 0.55913161E-02 0.59514635E-05    3
-0.10477176E-07 0.43793199E-11-0.25050493E+04 0.54710652E+01-0.10704179E+04    4
CH               RUS 79C   1H   1    0    0G   200.000  6000.00  1000.0      1
 0.25209062E+01 0.17653726E-02-0.46147581E-06 0.59288567E-10-0.33473209E-14    2
 0.71134082E+05 0.74053223E+01 0.34898166E+01 0.32383554E-03-0.16889906E-05    3
 0.31621733E-08-0.14060907E-11 0.70799939E+05 0.20840111E+01 0.71845485E+05    4
C2H2             L 8/88C   2H   2    0    0G   200.000  6000.00  1000.0      1
 0.46587047E+01 0.48840949E-02-0.16083563E-05 0.24698787E-09-0.13861505E-13    2
 0.25663218E+05-0.39979074E+01 0.80869108E+00 0.23361395E-01-0.35516636E-04    3
 0.28014566E-07-0.85004459E-11 0.26332764E+05 0.13939671E+02 0.27349778E+05    4
C2H4    ETHYLENE  L 4/85C   2H   4    0    0G   300.000  5000.00  1000.0      1
 0.43985453E 01 0.96228607E-02-0.31663776E-05 0.45747628E-09-0.23659406E-13    2
 0.41153203E 04-0.24627438E 01 0.12176600E 01 0.13002675E-01 0.35037447E-05    3
-0.11155514E-07 0.47203222E-11 0.53373828E 04 0.15480169E 02 0.62902830E 04    4
C2H3             T06/93C   2H   3    0    0G   200.000  6000.00  1000.0      1
 0.47025310E+01 0.72642283E-02-0.25801992E-05 0.41319944E-09-0.24591492E-13    2
 0.34029675E+05-0.14293714E+01 0.30019602E+01 0.30304354E-02 0.24444315E-04    3
-0.35810242E-07 0.15108700E-10 0.34868173E+05 0.93304495E+01 0.36050230E+05    4
CH3OH            L 8/88C   1H   4O   1    0G   200.000  6000.00  1000.0      1
 0.36012593E+01 0.10243223E-01-0.35999217E-05 0.57251951E-09-0.33912719E-13    2
-0.25997155E+05 0.47056025E+01 0.57153948E+01-0.15230920E-01 0.65244182E-04    3
-0.71080873E-07 0.26135383E-10-0.25642765E+05-0.15040970E+01-0.24167389E+05    4
CH3HCO   ACETALDE L 8/88C   2H   4O   1    0G   200.000  6000.00  1000.0      1
 0.54041108E+01 0.11723059E-01-0.42263137E-05 0.68372451E-09-0.40984863E-13    2
-0.22593122E+05-0.34807917E+01 0.47294595E+01-0.31932858E-02 0.47534921E-04    3
-0.57458611E-07 0.21931112E-10-0.21572878E+05 0.41030159E+01-0.19987949E+05    4
C2H4O OXYRANE    L 8/88C   2H   4O   1    0G   200.000  6000.00  1000.0      1
 0.54887641E+01 0.12046190E-01-0.43336931E-05 0.70028311E-09-0.41949088E-13    2
-0.91804251E+04-0.70799605E+01 0.37590532E+01-0.94412180E-02 0.80309721E-04    3
-0.10080788E-06 0.40039921E-10-0.75608143E+04 0.78497475E+01-0.63304657E+04    4
C2H              T04/93C   2H   1    0    0G   200.000  6000.00  1000.0      1
 0.36646060E+01 0.38218694E-02-0.13650743E-05 0.21324828E-09-0.12309430E-13    2
 0.64597055E+05 0.39134973E+01 0.29018020E+01 0.13285982E-01-0.28050886E-04    3
 0.28930184E-07-0.10744742E-10 0.64490326E+05 0.61723506E+01 0.65750290E+05    4
CH2CO KETENE     T 6/94C   2H   2O   1    0G   200.000  6000.00  1000.0      1
 0.57577901E+01 0.63496507E-02-0.22584407E-05 0.36208462E-09-0.21569030E-13    2
-0.79786113E+04-0.61064037E+01 0.21401165E+01 0.18088368E-01-0.17324216E-04    3
 0.92767477E-08-0.19915011E-11-0.70430509E+04 0.12198699E+02-0.57366700E+04    4
HCCO             T 6/94C   2H   1O   1    0G   200.000  6000.00  1000.0      1
 0.58469006E+01 0.36405960E-02-0.12959007E-05 0.20796919E-09-0.12400022E-13    2
 0.19248496E+05-0.52916533E+01 0.23350118E+01 0.17010083E-01-0.22018867E-04    3
 0.15406447E-07-0.43455097E-11 0.20050299E+05 0.11976729E+02 0.21336387E+05    4
SCH2   SINGLET    C12/87C   1H   2    0     G   300.00   4000.00  1000.0      1
 0.03552888E+02 0.02066788E-01-0.01914116E-05-0.11046733E-09 0.02021349E-12    2
 0.04984975E+06 0.01686570E+02 0.03971265E+02-0.01699088E-02 0.10253689E-05    3
 0.02492550E-07-0.01981266E-10 0.04989367E+06 0.05753207E+00 0.51077663E+05    4
C2               RUS 79C   2    0    0    0G   200.000  6000.00  1000.0      1
 0.37913706E+01 0.51650473E-03-0.25486960E-07-0.82263554E-11 0.10086168E-14    2
 0.99023059E+05 0.28151802E+01 0.86470550E+00 0.39353120E-01-0.11981818E-03    3
 0.13908103E-06-0.55205503E-10 0.98731303E+05 0.11530141E+02 0.99928438E+05    4
C2O TRIPLET      110203C   2O   1    0    0G   300.000  4000.000 1000.00     1
 0.50266479E+01 0.28918227E-02-0.13913841E-05 0.30703546E-09-0.25567905E-13    2
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 0.44888900E+05-0.17853398E+01 0.29665556E+01 0.10513229E-01-0.13516489E-04    3
 0.99333965E-08-0.30881376E-11 0.45385915E+05 0.84432753E+01                   4
CH3CO             T 9/92C   2H   3O   1    0G   200.000  6000.00  1000.0      1
 0.59447731E+01 0.78667205E-02-0.28865882E-05 0.47270875E-09-0.28599861E-13    2
-0.37873075E+04-0.50136751E+01 0.41634257E+01-0.23261610E-03 0.34267820E-04    3
-0.44105227E-07 0.17275612E-10-0.26574529E+04 0.73468280E+01-0.12027167E+04    4
CH3CO3     4/24/92 THERMC   2H   3O   3    0G   300.000  5000.000 1575.000    21
 1.14020019E+01 8.59416721E-03-3.06838374E-06 4.90245722E-10-2.90175354E-14    2
-2.02745353E+04-3.30871657E+01 5.13747438E+00 1.59298658E-02-8.21627846E-07    3
-4.81982007E-09 1.57730795E-12-1.73772288E+04 3.13626395E+00                   4
CH3CO3H    4/24/92 THERMC   2H   4O   3    0G   300.000  5000.000 1374.000    21
 1.23794767E+01 1.00368883E-02-3.50324632E-06 5.51431811E-10-3.23046627E-14    2
-3.88133888E+04-3.71309181E+01 4.09002627E+00 2.54380593E-02-1.22828804E-05    3
 1.55365086E-09 2.77282260E-13-3.55663564E+04 8.74816008E+00                   4
CH3O2             L 1/84C   1H   3O   2    0G   300.000  5000.00   1000.0     1
 0.66812963E 01 0.80057271E-02-0.27188507E-05 0.40631365E-09-0.21927725E-13    2
 0.52621851E 03-0.99423847E 01 0.20986490E 01 0.15786357E-01 0.75683261E-07    3
-0.11274587E-07 0.56665133E-11 0.20695879E 04 0.15007068E 02 0.33715510E+04    4
CH3O2H            T11/96C   1H   4O   2    0G   200.000  6000.00  1000.0      1
 6.86907934E+00 1.00840883E-02-3.66515947E-06 5.96302681E-10-3.58894156E-14    2
-1.98402231E+04-1.24951986E+01 3.72654981E+00 7.51851847E-03 2.35970425E-05    3
-3.52694507E-08 1.42757614E-11-1.83982011E+04 6.52443362E+00-1.68074366E+04    4
C2H5O2H           T10/96C   2H   6O   2    0G   200.000  6000.00  1000.0      1
 9.99511555E+00 1.47311626E-02-5.30621235E-06 8.58442516E-10-5.14814807E-14    2
-2.53850722E+04-2.53504050E+01 4.37310002E+00 1.04422436E-02 4.63854723E-05    3
-7.02772770E-08 2.93034879E-11-2.29362227E+04 8.30134323E+00-2.08834916E+04    4
C2H5O2                 C   2H   5O   20   00   300.00   5000.00  1000.00     1
 0.78275410E+01 0.15347060E-01-0.58108700E-05 0.10465070E-08-0.71520540E-13    2
-0.45527100E+04-0.12726800E+02 0.39390180E+01 0.13991490E-01 0.21720800E-04    3
-0.36137480E-07 0.14824910E-10-0.28469040E+04 0.10394470E+02                   4
CH3CO2     4/24/92 THERMC   2H   3O   2    0G   300.000  5000.000 1482.000    11
 8.37781397E+00 7.83020766E-03-2.53555405E-06 3.78870534E-10-2.13859882E-14    2
-2.38389350E+04-1.58386711E+01 4.30690287E+00 1.70945538E-02-1.02260887E-05    3
 3.08829567E-09-3.50372173E-13-2.24325681E+04 6.05640546E+00                   4
CH3CO2H    4/24/92 THERMC   2H   4O   2    0G   300.000  5000.000 1997.000    21
 7.34453556E+00 1.17718973E-02-4.13228619E-06 6.55097801E-10-3.86190560E-14    2
-4.51365468E+04-1.26872633E+01 3.34602242E+00 1.84778690E-02-6.73574398E-06    3
 1.07401993E-10 2.97848907E-13-4.35715193E+04 9.61466866E+00                   4
C2H5O             T11/82O   1C   2H   5    0G   300.000  5000.0   1000.0     1
 0.60114346E+01 0.12165219E-01-0.40449604E-05 0.59076588E-09-0.30969595E-13    2
-0.49366992E+04-0.67901798E+01 0.17302504E+01 0.16908489E-01 0.39996221E-05    3
-0.13711180E-07 0.57643603E-11-0.32922483E+04 0.17336115E+02-0.20138288E+04    4
C2H5OH            L 8/88C   2H   6O   1    0G   200.000  6000.00  1000.0      1
 0.65624365E+01 0.15204222E-01-0.53896795E-05 0.86225011E-09-0.51289787E-13    2
-0.31525621E+05-0.94730202E+01 0.48586957E+01-0.37401726E-02 0.69555378E-04    3
-0.88654796E-07 0.35168835E-10-0.29996132E+05 0.48018545E+01-0.28257829E+05    4
SC2H5O            T 4/83C   2O   1H   5    0G   300.000  5000.00  1000.0      1
 0.67665424E+01 0.11634436E-01-0.37790651E-05 0.53828875E-09-0.27315345E-13    2
-0.56092969E+04-0.93980442E+01 0.24813328E+01 0.16790036E-01 0.37755499E-05    3
-0.13923497E-07 0.60095193E-11-0.40120054E+04 0.14581622E+02-0.25172860E+04    4
PC2H5O         T 4/83   C   2H   5O   10   0G   300.00   5000.0   1000.00     1
 0.75944014E+01 0.93229339E-02-0.30303854E-05 0.43216319E-09-0.21970039E-13    2
-0.57727852E+04-0.13968735E+02 0.14019508E+01 0.21543175E-01-0.22326512E-05    3
-0.14464092E-07 0.80488420E-11-0.38464519E+04 0.19135818E+02                   4
CH2HCO           T04/83 C   2H   3O   10   0G   300.00   5000.00  1000.00     1
 0.59756699E+01 0.81305914E-02-0.27436245E-05 0.40703041E-09-0.21760171E-13    2
 0.49032178E+03-0.50452509E+01 0.34090624E+01 0.10738574E-01 0.18914925E-05    3
-0.71585831E-08 0.28673851E-11 0.15214766E+04 0.95582905E+01                   4
CN                T 6/94C   1N   1    0    0G   200.000  6000.00  1000.0      1
 0.37459804E+01 0.43450773E-04 0.29705984E-06-0.68651804E-10 0.44134174E-14    2
 0.52353188E+05 0.27867600E+01 0.36129350E+01-0.95551327E-03 0.21442976E-05    3
-0.31516324E-09-0.46430356E-12 0.52525340E+05 0.39804995E+01 0.52571034E+05    4
H2CN RADICAL      T05/97H   2C   1N   1    0G   200.000  6000.00  1000.0      1
 3.80315523E+00 5.47197456E-03-1.95314927E-06 3.13362513E-10-1.86249463E-14    2
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 2.73218196E+04 3.31721893E+00 3.97799541E+00-3.43275678E-03 2.59134226E-05    3
-3.04692133E-08 1.16272702E-11 2.76769528E+04 4.43029598E+00 2.88846366E+04    4
N                 L 6/88N   1    0    0    0G   200.000  6000.00  1000.0      1
 0.24159429E+01 0.17489065E-03-0.11902369E-06 0.30226244E-10-0.20360983E-14    2
 0.56133775E+05 0.46496095E+01 0.25000000E+01 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 0.56104638E+05 0.41939088E+01 0.56850013E+05    4
NH                L11/89N   1H   1    0    0G   200.000  6000.00  1000.0      1
 0.27836929E+01 0.13298429E-02-0.42478047E-06 0.78348504E-10-0.55044470E-14    2
 0.42134514E+05 0.57407798E+01 0.34929084E+01 0.31179197E-03-0.14890484E-05    3
 0.24816442E-08-0.10356967E-11 0.41894294E+05 0.18483277E+01 0.42940822E+05    4
HCN               L 7/88H   1C   1N   1    0G   200.000  6000.00  1000.0      1
 0.38022392E+01 0.31464227E-02-0.10632185E-05 0.16619757E-09-0.97997567E-14    2
 0.14910512E+05 0.15754601E+01 0.22589885E+01 0.10051170E-01-0.13351763E-04    3
 0.10092349E-07-0.30089029E-11 0.15215853E+05 0.89164418E+01 0.16236675E+05    4
NO                RUS 89N   1O   1    0    0G   200.000  6000.00  1000.0      1
 3.26071234E+00 1.19101135E-03-4.29122646E-07 6.94481463E-11-4.03295681E-15    2
 9.92143132E+03 6.36900518E+00 4.21859896E+00-4.63988124E-03 1.10443049E-05    3
-9.34055507E-09 2.80554874E-12 9.84509964E+03 2.28061001E+00 1.09770882E+04    4
HCNO              120186H   1C   1N   1O   1G  0250.00   4000.00  1000.00     1
 0.06692412E+02 0.02368360E-01-0.02371510E-05-0.01275503E-08 0.02407137E-12    2
 0.01694737E+06-0.01245434E+03 0.03184859E+02 0.09752316E-01-0.01280203E-04    3
-0.06163104E-07 0.03226275E-10 0.01797907E+06 0.06123844E+02                   4
C                 L 7/88C   1    0    0    0G   200.000  6000.00  1000.0      1
 0.26055830E+01-0.19593434E-03 0.10673722E-06-0.16423940E-10 0.81870580E-15    2
 0.85411742E+05 0.41923868E+01 0.25542395E+01-0.32153772E-03 0.73379223E-06    3
-0.73223487E-09 0.26652144E-12 0.85442681E+05 0.45313085E+01 0.86195097E+05    4
HOCN              110193H   1C   1N   1O   1G   300.00   4000.00  1400.00     1
 0.06022112E+02 0.01929530E-01-0.01455029E-05-0.01045811E-08 0.01794814E-12    2
-0.04040321E+05-0.05866433E+02 0.03789424E+02 0.05387981E-01-0.06518270E-05    3
-0.01420164E-07 0.05367969E-11-0.03135335E+05 0.06667052E+02                   4
HNCO              T 6/94H   1N   1C   1O   1G   200.000  6000.00  1000.0      1
 0.52936894E+01 0.40307770E-02-0.14130589E-05 0.22445562E-09-0.13287683E-13    2
-0.15973489E+05-0.30864710E+01 0.22432188E+01 0.14491349E-01-0.15236174E-04    3
 0.83345851E-08-0.17104033E-11-0.15233708E+05 0.12157321E+02-0.14039745E+05    4
NCO               T 6/94C   1N   1O   1    0G   200.000  6000.00  1000.0      1
 0.51075979E+01 0.23371500E-02-0.88984637E-06 0.14920037E-09-0.91663122E-14    2
 0.14024945E+05-0.22908127E+01 0.27405490E+01 0.95089992E-02-0.10338762E-04    3
 0.68805052E-08-0.20963552E-11 0.14690320E+05 0.98908197E+01 0.15851325E+05    4
N2O               L 7/88N   2O   1    0    0G   200.000  6000.00  1000.0      1
 0.48230729E+01 0.26270251E-02-0.95850872E-06 0.16000712E-09-0.97752302E-14    2
 0.80734047E+04-0.22017208E+01 0.22571502E+01 0.11304728E-01-0.13671319E-04    3
 0.96819803E-08-0.29307182E-11 0.87417746E+04 0.10757992E+02 0.98141682E+04    4
NH2               L12/89N   1H   2    0    0G   200.000  6000.00  1000.0      1
 0.28476611E+01 0.31428453E-02-0.89866557E-06 0.13032357E-09-0.74885356E-14    2
 0.21823916E+05 0.64718133E+01 0.42055601E+01-0.21355282E-02 0.72682021E-05    3
-0.59302799E-08 0.18067218E-11 0.21535223E+05-0.14663231E+00 0.22747541E+05    4
HNO    WRA032498        H   1N   1O   1    0G   200.000  6000.00  1000.0      1
 3.16554762E+00 3.00005132E-03-3.94350282E-07-3.85787491E-11 7.08091931E-15    2
 1.18052184E+04 7.64764695E+00 4.53525882E+00-5.68546910E-03 1.85199976E-05    3
-1.71883674E-08 5.55833090E-12 1.16506820E+04 1.74314734E+00 1.28824477E+04    4
NO2               L 7/88N   1O   2    0    0G   200.000  6000.00  1000.0      1
 0.48847540E+01 0.21723955E-02-0.82806909E-06 0.15747510E-09-0.10510895E-13    2
 0.23164982E+04-0.11741695E+00 0.39440312E+01-0.15854290E-02 0.16657812E-04    3
-0.20475426E-07 0.78350564E-11 0.28966180E+04 0.63119919E+01 0.41124701E+04    4
C2N2              RUS 79C   2N   2    0    0G   200.000  6000.00  1000.0      1
 0.67055078E+01 0.36425829E-02-0.13094063E-05 0.21643797E-09-0.13121437E-13    2
 0.34860766E+05-0.10493904E+02 0.23292532E+01 0.26153785E-01-0.49000399E-04    3
 0.46191748E-07-0.16432385E-10 0.35668442E+05 0.98501993E+01 0.37175973E+05    4
NNH               T07/93N   2H   1    0    0G   200.000  6000.00  1000.0      1
 0.37667545E+01 0.28915081E-02-0.10416620E-05 0.16842594E-09-0.10091896E-13    2
 0.28650697E+05 0.44705068E+01 0.43446927E+01-0.48497072E-02 0.20059459E-04    3
-0.21726464E-07 0.79469538E-11 0.28791973E+05 0.29779411E+01 0.30009829E+05    4
NH3  AMONIA       RUS 89N   1H   3    0    0G   200.000  6000.00  1000.0      1
 2.71709692E+00 5.56856338E-03-1.76886396E-06 2.67417260E-10-1.52731419E-14    2
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-6.58451989E+03 6.09289837E+00 4.30177808E+00-4.77127330E-03 2.19341619E-05    3
-2.29856489E-08 8.28992268E-12-6.74806394E+03-6.90644393E-01-5.52528050E+03    4
N2H2              L 5/90N   2H   2    0    0G   200.000  6000.00  1000.0      1
 0.13111509E+01 0.90018727E-02-0.31491187E-05 0.48144969E-09-0.27189798E-13    2
 0.24786417E+05 0.16409109E+02 0.49106602E+01-0.10779187E-01 0.38651644E-04    3
-0.38650163E-07 0.13485210E-10 0.24224273E+05 0.91027970E-01 0.25480756E+05    4
CH2CHOW      cc       cc C   2H   3O   1    0G   300.000  5000.000 1389.000    01
 6.44647136E+00 7.67418446E-03-2.55298889E-06 3.88933291E-10-2.22665944E-14    2
 1.95121257E+04-7.93000911E+00 2.76406282E+00 1.50800828E-02-7.88093083E-06    3
 1.97116311E-09-1.74094646E-13 2.09267565E+04 1.22979303E+01                   4
C2H3O             T 9/92C   2H   3O   1    0G   298.150  3000.000  1000.0      1
 0.48131470E+00 0.20711914E-01-0.12693155E-04 0.34579642E-08-0.35399703E-12    2
 0.15648642E+05 0.34629876E+02 0.10854772E+01 0.12845259E-01 0.24138660E-05    3
-0.44642672E-08-0.29381916E-12 0.15910655E+05 0.33395312E+02 0.16817588E+05    4
CH3HCOW      cc       cc C   2H   4O   1    0G   300.000  5000.000 1376.000    11
 6.89091884E+00 9.95180916E-03-3.45461153E-06 5.41621230E-10-3.16369494E-14    2
 1.91997658E+04-1.23847501E+01 1.66831767E+00 1.89949607E-02-8.35817476E-06    3
 1.20243883E-09 6.37236161E-14 2.13971005E+04 1.68980856E+01                   4
C3H6OH     4/24/92 THERMC   3H   7O   1    0G   300.000  5000.000 1403.000    31
 1.09340809E+01 1.49384611E-02-4.97490474E-06 7.58435125E-10-4.34420191E-14    2
-1.15876725E+04-2.89343754E+01 1.65867207E-01 4.13141037E-02-2.99664397E-05    3
 1.16234591E-08-1.86270510E-12-7.97925983E+03 2.84481654E+01                   4
O2C3H6OH   4/24/92 THERMC   3H   7O   3    0G   300.000  5000.000 1380.000    41
 1.55655181E+01 1.68822736E-02-5.91144639E-06 9.32274430E-10-5.46815496E-14    2
-2.95301139E+04-5.17312137E+01 2.20217327E+00 4.59913087E-02-3.03766163E-05    3
 1.05366009E-08-1.55928684E-12-2.45762626E+04 2.09594636E+01                   4
C3H5O2     4/24/92 THERMC   3H   5O   2    0G   300.000  5000.000 1370.000    21
 1.27832465E+01 1.25399349E-02-4.43433905E-06 7.03952842E-10-4.14804136E-14    2
 5.58979899E+03-4.03574985E+01 2.65293041E+00 3.19993514E-02-1.73652420E-05    3
 4.00148647E-09-2.51071126E-13 9.58815244E+03 1.56431929E+01                   4
C3H5O2H    4/24/92 THERMC   3H   6O   2    0G   300.000  5000.000 1386.000    31
 1.39009363E+01 1.34732295E-02-4.70091523E-06 7.39632892E-10-4.33128479E-14    2
-1.29274765E+04-4.49719922E+01 1.75161845E+00 4.16542055E-02-3.01268606E-05    3
 1.14209488E-08-1.80624472E-12-8.64152220E+03 2.04277976E+01                   4
C3H5O      4/24/92 THERMC   3H   5O   1    0G   300.000  5000.000 1375.000    21
 9.93380796E+00 1.21383493E-02-4.23299952E-06 6.65805507E-10-3.89817563E-14    2
 6.20904655E+03-2.68841926E+01 1.48979417E+00 2.77306345E-02-1.35044719E-05    3
 2.24225811E-09 8.28232368E-14 9.58557792E+03 1.99841620E+01                   4
NC3H7O2    4/24/92 THERMC   3H   7O   2    0G   300.000  5000.000 1376.000    31
 1.39295562E+01 1.62109297E-02-5.69426414E-06 8.99917649E-10-5.28613664E-14    2
-1.09646348E+04-4.81871702E+01 1.65182379E+00 4.10402887E-02-2.41422856E-05    3
 6.91955127E-09-7.89713852E-13-6.22330250E+03 1.92752981E+01                   4
NC3H7O2H   4/24/92 THERMC   3H   8O   2    0G   300.000  5000.000 1392.000    31
 1.45695935E+01 1.77104023E-02-6.09654929E-06 9.50484279E-10-5.53030086E-14    2
-2.92401303E+04-4.99984239E+01 6.27002549E-01 5.14448631E-02-3.83791359E-05    3
 1.54653552E-08-2.61561123E-12-2.44385400E+04 2.45962330E+01                   4
IC3H7O2    4/24/92 THERMC   3H   7O   2    0G   300.000  5000.000 1382.000    31
 1.45333419E+01 1.56502508E-02-5.48993478E-06 8.66859600E-10-5.08886097E-14    2
-1.33000915E+04-5.13639953E+01 1.03606539E+00 4.57999209E-02-3.15792877E-05    3
 1.14069765E-08-1.73998862E-12-8.39327437E+03 2.17529616E+01                   4
IC3H7O2H   4/24/92 THERMC   3H   8O   2    0G   300.000  5000.000 1395.000    31
 1.51552007E+01 1.71807437E-02-5.90648731E-06 9.20033944E-10-5.34977754E-14    2
-3.15766321E+04-5.30871350E+01 1.35497567E-01 5.55626488E-02-4.48202480E-05    3
 1.93393698E-08-3.43326450E-12-2.66246790E+04 2.65182104E+01                   4
IC3H7O       cc       cc C   3H   7O   1    0G   300.000  5000.000 1379.000    21
 1.24938036E+01 1.42024822E-02-4.76949687E-06 7.32349424E-10-4.21933677E-14    2
-1.25023025E+04-4.32454233E+01-1.45132586E-01 4.09328495E-02-2.46708437E-05    3
 6.60628776E-09-5.34569348E-13-7.91212088E+03 2.54949227E+01                   4
NC3H7O N-PROPOXY  T 3/96C   3H   7O   1    0G   298.150  5000.00  1000.0      1
 0.84124958E+01 0.19520193E-01-0.71317071E-05 0.12393621E-08-0.82483889E-13    2
-0.87750718E+04-0.18293360E+02 0.91452571E+00 0.33601264E-01-0.12282254E-04    3
-0.10739947E-08 0.72924952E-12-0.61847956E+04 0.22563171E+02-0.45289500E+04    4
IC4H5            I-A 8/83C   4H   5    0    0G   300.00   3000.0   1000.0      1
 0.72559180E+01 0.17141310E-01-0.74350450E-05 0.16410520E-08-0.15360780E-12    2
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 0.36339860E+05-0.13420580E+02 0.10251400E+02-0.25627670E-01 0.10715090E-03    3
-0.11090190E-06 0.37550050E-10 0.37128550E+05-0.20574530E+02 0.39785870E+05    4
NC4H5           N-A 8/83C   4H   5    0    0G   300.0    3000.0   1000.0      1
 0.72559180E+01 0.17141310E-01-0.74350450E-05 0.16410520E-08-0.15360780E-12    2
 0.38227410E+05-0.12422830E+02-0.20329280E+01 0.53630530E-01-0.63382690E-04    3
 0.40641440E-07-0.10398020E-10 0.40219650E+05 0.32787830E+02 0.41505750E+05    4
C6H5  PHENYL RAD  L12/84C   6H   5    0    0G   300.000  5000.00  1000.0      1
 0.11431418E 02 0.17019045E-01-0.58387241E-05 0.88094687E-09-0.48050417E-13    2
 0.33942348E 05-0.38574219E 02-0.23405075E 01 0.42760305E-01-0.25518166E-05    3
-0.30668716E-07 0.16245519E-10 0.38376734E 05 0.35617355E 02 0.39502977E 05    4
C4H4 1-BUTEN-3YN  L 9/89C   4H   4    0    0G   200.000  6000.00  1000.0      1
 0.82948104E+01 0.11994381E-01-0.42624075E-05 0.68306978E-09-0.40680631E-13    2
 0.33550866E+05-0.18426826E+02 0.14049083E+01 0.29531073E-01-0.15596302E-04    3
-0.32142002E-08 0.45436937E-11 0.35507830E+05 0.17450183E+02 0.37097268E+05    4
C3H3 PROPARGYL    T 5/97C   3H   3    0    0G   200.000  6000.00  1000.0      1
 7.14221880E+00 7.61902005E-03-2.67459950E-06 4.24914801E-10-2.51475415E-14    2
 3.89087427E+04-6.82838123E+00 1.35110927E+00 3.27411223E-02-4.73827135E-05    3
 3.76309808E-08-1.18540923E-11 4.01057783E+04 2.09623551E+01 4.16139977E+04    4
C3H6   PROPYLENE  L 4/85C   3H   6    0    0G   300.000  5000.00  1000.0      1
 0.67213974E 01 0.14931757E-01-0.49652353E-05 0.72510753E-09-0.38001476E-13    2
-0.92453149E 03-0.12155617E 02 0.14575157E 01 0.21142263E-01 0.40468012E-05    3
-0.16319003E-07 0.70475153E-11 0.10740208E 04 0.17399460E 02 0.24557265E 04    4
C3H8     PROPANE  L 4/85C   3H   8    0    0G   300.000  5000.00  1000.0      1
 0.75341368E 01 0.18872239E-01-0.62718491E-05 0.91475649E-09-0.47838069E-13    2
-0.16467516E 05-0.17892349E 02 0.93355381E 00 0.26424579E-01 0.61059727E-05    3
-0.21977499E-07 0.95149253E-11-0.13958520E 05 0.19201691E 02-0.12489986E 05    4
IC3H7           I-L 9/84C   3H   7    0    0G   300.000  5000.00  1000.0      1
 0.65294638E 01 0.17193288E-01-0.57153220E-05 0.83408080E-09-0.43663532E-13    2
 0.77179102E 04-0.91399021E 01 0.14461584E 01 0.20988975E-01 0.77172672E-05    3
-0.18481391E-07 0.71269024E-11 0.98206094E 04 0.20108200E 02 0.11221480E 05    4
NC3H7           N-L 9/84C   3H   7    0    0G   300.000  5000.00  1000.0      1
 0.77026987E 01 0.16044203E-01-0.52833220E-05 0.76298590E-09-0.39392284E-13    2
 0.82984336E 04-0.15480180E 02 0.10515518E 01 0.25991980E-01 0.23800540E-05    3
-0.19609569E-07 0.93732470E-11 0.10631863E 05 0.21122559E 02 0.12087447E 05    4
SC3H5  CH3CH=CH*  T 6/96C   3H   5    0    0G   298.150  5000.00  1000.0      1
 0.61342175E+01 0.13325025E-01-0.48645230E-05 0.83773904E-09-0.55161424E-13    2
 0.28626198E+05-0.74112134E+01 0.22361012E+01 0.16387245E-01 0.76639733E-05    3
-0.19364818E-07 0.84155468E-11 0.30173536E+05 0.14806060E+02 0.31602007E+05    4
PC3H4     PROPYNE T 2/90H   4C   3    0    0G   200.000  6000.00  1000.0      1
 0.60252400E+01 0.11336542E-01-0.40223391E-05 0.64376063E-09-0.38299635E-13    2
 0.19620942E+05-0.86043785E+01 0.26803869E+01 0.15799651E-01 0.25070596E-05    3
-0.13657623E-07 0.66154285E-11 0.20802374E+05 0.98769351E+01 0.22302059E+05    4
TC3H5  CH3C*=CH2  T 6/96C   3H   5    0    0G   200.000  6000.00  1000.0      1
 0.61101805E+01 0.14673395E-01-0.53676822E-05 0.86904932E-09-0.51932006E-13    2
 0.25532442E+05-0.83555712E+01 0.25544033E+01 0.10986798E-01 0.30174305E-04    3
-0.47253568E-07 0.19771073E-10 0.27150242E+05 0.13207592E+02 0.28582707E+05    4
C3H6O PROPYLENE OX L9/85C   3H   6O   1    0G   300.000  5000.00  1000.0      1
 0.86900558E 01 0.16020987E-01-0.53971753E-05 0.79941542E-09-0.42656366E-13    2
-0.15420691E 05-0.22485016E 02 0.48733836E 00 0.28519690E-01 0.30096162E-05    3
-0.22652642E-07 0.10706728E-10-0.12556434E 05 0.22605270E 02-0.11156446E 05    4
C3H4CY            T12/81C   3H   4    0    0G   300.000  5000.00  1000.0      1
 0.66999931E+01 0.10357372E-01-0.34551167E-05 0.50652949E-09-0.26682276E-13    2
 0.30199051E+05-0.13378770E+02-0.24621047E-01 0.23197215E-01-0.18474357E-05    3
-0.15927593E-07 0.86846155E-11 0.32334137E+05 0.22729762E+02 0.3332728 E+05    4
C3H2 *HC=C=CH*    T 7/94C   3H   2    0    0G   298.150  5000.00  1000.0      1
 0.62476406E+01 0.56755154E-02-0.19541329E-05 0.31686787E-09-0.19722328E-13    2
 0.79187553E+05-0.63712327E+01 0.36613541E+01 0.89364130E-02 0.35404269E-05    3
-0.11072967E-07 0.52009416E-11 0.80115193E+05 0.79774693E+01 0.81616355E+05    4
C4H2              L 9/89C   4H   2    0    0G   200.000  6000.00  1000.0      1
 0.86670035E+01 0.67166371E-02-0.23544995E-05 0.37383079E-09-0.22118914E-13    2
 0.49856933E+05-0.21114205E+02-0.39518508E+00 0.51955813E-01-0.91786616E-04    3
 0.80523929E-07-0.26917088E-10 0.51451709E+05 0.20969101E+02 0.52978651E+05    4
C4H8    1-BUTENE  T 6/83C   4H   8    0    0G   300.000  5000.00  1000.0      1
 0.20535841E+01 0.34350507E-01-0.15883197E-04 0.33089662E-08-0.25361045E-12    2
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-0.21397231E+04 0.15556360E+02 0.11811380E+01 0.30853380E-01 0.50865247E-05    3
-0.24654888E-07 0.11110193E-10-0.17904004E+04 0.21075639E+02-0.06494670E+03    4
T2C4H8                  C   4H   80   00   0G   300.00   5000.00  1000.00     1
 0.82797676E+00 0.35864539E-01-0.16634498E-04 0.34732759E-08-0.26657398E-12    2
-0.30521033E+04 0.21342545E+02 0.12594252E+01 0.27808424E-01 0.87013932E-05    3
-0.24402205E-07 0.98977710E-11-0.29647742E+04 0.20501129E+02                   4
C2C4H8  C4H8CIS   T 6/83C   4H   8    0    0G   300.000  5000.00  1000.0      1
 0.11097383E+01 0.35542578E-01-0.16481703E-04 0.34412202E-08-0.26411468E-12    2
-0.26507607E+04 0.19366680E+02 0.24108791E+01 0.25147773E-01 0.98473047E-05    3
-0.22716758E-07 0.86585895E-11-0.27758694E+04 0.14097700E+02-0.89121300E+03    4
C4H5                    C   4H   50   00   0G   300.00   5000.00  1000.00     1
 0.52872400E+01 0.19416250E-01-0.75259100E-05 0.13124900E-08-0.84820000E-13    2
 0.38354600E+05-0.15660000E+01 0.27518800E+01 0.29092550E-01-0.23393090E-04    3
 0.14159370E-07-0.42054700E-11 0.38953300E+05 0.10953000E+02                   4
C4H               T12/91C   4H   1    0    0G   200.000  6000.00  1000.0      1
 0.77680939E+01 0.49850386E-02-0.17648839E-05 0.28217408E-09-0.16779623E-13    2
 0.93912126E+05-0.14159577E+02 0.13210657E+01 0.38562824E-01-0.71343174E-04    3
 0.65319977E-07-0.22607050E-10 0.95021629E+05 0.15554575E+02 0.96617600E+05    4
C6H6    BENZENE   L12/84C   6H   6    0    0G   300.000  5000.00  1000.0      1
 0.11815166E 02 0.19169778E-01-0.65425238E-05 0.98228425E-09-0.53280361E-13    2
 0.40707441E 04-0.43973511E 02-0.32181215E 01 0.47168836E-01-0.21254918E-05    3
-0.34879005E-07 0.18425386E-10 0.89017773E 04 0.36999313E 02 0.99586128E 04    4
C3H5 SYMMETRIC    T 9/96C   3H   5    0    0G   200.000  6000.00  1000.0      1
 0.70094568D+01 0.13106629D-01-0.46533442D-05 0.74514323D-09-0.44350051D-13    2
 0.16412909D+05-0.13946114D+02 0.14698036D+01 0.19034365D-01 0.14480425D-04    3
-0.35468652D-07 0.16647594D-10 0.18325831D+05 0.16724114D+02 0.19675772D+05    4
C3H4      ALLENE  L 8/89C   3H   4    0    0G   200.000  6000.00  1000.0      1
 0.63168722E+01 0.11133728E-01-0.39629378E-05 0.63564238E-09-0.37875540E-13    2
 0.20117495E+05-0.10995766E+02 0.26130445E+01 0.12122575E-01 0.18539880E-04    3
-0.34525149E-07 0.15335079E-10 0.21541567E+05 0.10226139E+02 0.22962267E+05    4
C4H6    1,3-Bdiene      C   4H   60   00   0G   300.00   3000.00  1000.00     1
 0.7130943E 01  0.2064008E-01 -0.9323906E-05  0.2147307E-08 -0.2061361E-12    2
 0.9612654E 04 -0.1417222E 02 -0.2530900E 01  0.5387969E-01 -0.5173933E-04    3
 0.2510720E-07 -0.4324726E-11  0.1187691E 05  0.3391388E 02  0.1333562E+05    4
IC4H3                   C   4H   30   00   0G   300.00   5000.00  1000.00     1
 0.97570450E+01 0.88991060E-02-0.36321540E-05 0.67966640E-09-0.47498080E-13    2
 0.52220940E+05-0.22567330E+02 0.92063570E+01-0.68412580E-02 0.49426770E-04    3
-0.57756540E-07 0.21620850E-10 0.53230880E+05-0.15490760E+02                   4
NC4H3                   C   4H   30   00   0G   300.00   5000.00  1000.00     1
 0.91143560E+01 0.95471120E-02-0.38843590E-05 0.72623270E-09-0.50737070E-13    2
 0.61621520E+05-0.21296650E+02 0.56986800E+01 0.60107180E-02 0.28706380E-04    3
-0.41907200E-07 0.16944030E-10 0.63201220E+05-0.49851380E+00                   4
H2C4O             120189H   2C   4O   1     G  0300.00   4000.00  1000.00     1
 0.10268878E+02 0.04896164E-01-0.04885080E-05-0.02708566E-08 0.05107013E-12    2
 0.02346902E+06-0.02815985E+03 0.04810971E+02 0.13139988E-01 0.09865073E-05    3
-0.06120720E-07 0.16400028E-11 0.02545803E+06 0.02113424E+02                   4
C6H5O       PHENOXY RAD C   6H   5O   10   0G   300.00   5000.00  1000.00     1
 0.13833984E+02 0.17618403E-01-0.60696257E-05 0.91988173E-09-0.50449181E-13    2
-0.69212549E+03-0.50392990E+02-0.18219433E+01 0.48122510E-01-0.46792302E-05    3
-0.34018594E-07 0.18649637E-10 0.42429180E+04 0.33526199E+02                   4
CH3NO3     T05/98       C   1H   3O   3N   1G   200.000  6000.000  1000.0     1
 9.77845489E+00 1.10069541E-02-4.25928645E-06 7.18198185E-10-4.42041793E-14    2
-1.88804487E+04-2.39163197E+01 3.91363583E+00 1.52137945E-02 1.73479131E-05    3
-3.37074473E-08 1.44322204E-11-1.66103232E+04 9.44208392E+00-1.46737980E+04    4
CH2NO3     T05/98       C   1H   2O   3N   1G   200.000  6000.000  1000.0     1
 1.03913885E+01 7.66103917E-03-3.02728077E-06 5.16124915E-10-3.19767406E-14    2
 7.78486241E+03-2.54151556E+01 2.98654023E+00 2.47990510E-02-1.17175684E-05    3
-5.36820166E-09 4.80947389E-12 1.00202588E+04 1.36939353E+01 1.19010741E+04    4
HONO         HNO2 RUS 89H   1N   1O   2    0G   200.000  6000.000  1000.0     1
 0.57919018E+01 0.36515212E-02-0.12928936E-05 0.20688716E-09-0.12315254E-13    2
-0.11565589E+05-0.40558233E+01 0.32141709E+01 0.81276869E-02 0.16602559E-05    3
-0.95285182E-08 0.48715058E-11-0.10753237E+05 0.98219504E+01-0.94355439E+04    4
AR REF ELEMENT    L 6/88AR  1    0    0    0G   200.000  6000.00  1000.0      1
 0.25000000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
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-0.74537500E+03 0.43796749E+01 0.25000000E+01 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-0.74537500E+03 0.43796749E+01 0.00000000E+00    4
N2  REF ELEMENT    RUS 78N   2    0    0    0G   200.000  6000.00  1000.0      1
 0.29525407E+01 0.13968838E-02-0.49262577E-06 0.78600091E-10-0.46074978E-14    2
-0.92393753E+03 0.58718221E+01 0.35309628E+01-0.12365950E-03-0.50299339E-06    3
 0.24352768E-08-0.14087954E-11-0.10469637E+04 0.29674391E+01 0.00000000E+00    4
NO3                J12/64N   1O   3    0    0G   200.000  6000.00  1000.0      1
 7.48347734E+00 2.57772041E-03-1.00945831E-06 1.72314072E-10-1.07154015E-14    2
 5.70919428E+03-1.41618155E+01 2.17359310E+00 1.04902697E-02 1.10472650E-05    3
-2.81561854E-08 1.36583958E-11 7.39219877E+03 1.46022098E+01 8.55492386E+03    4
HNO3               L 4/90H   1N   1O   3    0G   200.000  6000.00  1000.0      1
 0.80037397E+01 0.44984461E-02-0.17365219E-05 0.29369198E-09-0.18148285E-13    2
-0.19256280E+05-0.16098258E+02 0.17449337E+01 0.18804057E-01-0.81595875E-05    3
-0.57859036E-08 0.44377077E-11-0.17380530E+05 0.16954532E+02-0.16105924E+05    4
N2H3               T 7/93H   3N   2    0    0G   200.000  6000.00  1000.0      1
 0.43414654E+01 0.75280979E-02-0.27478351E-05 0.44688178E-09-0.26846990E-13    2
 0.25176779E+05 0.98835045E+00 0.33151120E+01 0.21514763E-02 0.21849694E-04    3
-0.29813376E-07 0.12038856E-10 0.25844190E+05 0.82263324E+01 0.27068024E+05    4
N2H4 HYDRAZINE     L 5/90N   2H   4    0    0G   200.000  6000.00  1000.0      1
 4.93957357E+00 8.75017187E-03-2.99399058E-06 4.67278418E-10-2.73068599E-14    2
 9.28265548E+03-2.69439772E+00 3.83472149E+00-6.49129555E-04 3.76848463E-05    3
-5.00709182E-08 2.03362064E-11 1.00893925E+04 5.75272030E+00 1.14474575E+04    4
CNN                RUS 79C   1N   2    0    0G   200.000  6000.00  1000.0      1
 0.41398983E+01 0.38071002E-02-0.14753456E-05 0.24441991E-09-0.14746300E-13    2
 0.46790796E+05 0.32444306E+01 0.27584988E+01 0.12901042E-01-0.22802003E-04    3
 0.21393697E-07-0.75499090E-11 0.46953824E+05 0.91902188E+01 0.48186940E+05    4
HCNN               SRI/94C   1N   2H   10   0G   300.000  5000.000  1000.000    1
 0.58946362E+01 0.39895959E-02-0.15982380E-05 0.29249395E-09-0.20094686E-13    2
 0.53452941E+05-0.51030502E+01 0.25243194E+01 0.15960619E-01-0.18816354E-04    3
 0.12125540E-07-0.32357378E-11 0.54261984E+05 0.11675870E+02                  4
HCCOH              T 4/93C   2H   2O   1    0G   200.000  6000.000  1000.0     1
 0.63660255E+01 0.55038729E-02-0.18851901E-05 0.29446414E-09-0.17218598E-13    2
 0.89184965E+04-0.82504705E+01 0.19654173E+01 0.25585205E-01-0.38773334E-04    3
 0.31566335E-07-0.10081670E-10 0.97694090E+04 0.12602749E+02 0.11207642E+05    4
N2O4               RUS 89N   2O   4    0    0G   200.000  6000.000  1000.0     1
 1.15752899E+01 4.01616086E-03-1.57178323E-06 2.68274309E-10-1.66922019E-14    2
-2.92191226E+03-3.19488439E+01 3.02002308E+00 2.95904321E-02-3.01342458E-05    3
 1.42360407E-08-2.44100049E-12-6.40040162E+02 1.18059606E+01 1.33632866E+03    4
N2O3               L 4/90N   2O   3    0    0G   200.000  6000.000  1000.0     1
 9.08583845E+00 3.37756330E-03-1.31583890E-06 2.30762329E-10-1.47151267E-14    2
 7.27160146E+03-1.55361904E+01 5.81083964E+00 1.43330962E-02-1.96208597E-05    3
 1.73060735E-08-6.46553954E-12 8.19184453E+03 1.20461321E+00 1.04192062E+04    4
N2O5               L 4/90N   2O   5    0    0G   200.000  6000.000  1000.0     1
 1.31108082E+01 4.87435791E-03-1.87548389E-06 3.16374121E-10-1.95926845E-14    2
-3.11634700E+03-3.46877692E+01 3.68767444E+00 3.92120798E-02-5.53770029E-05    3
 4.20097833E-08-1.31260710E-11-8.30291184E+02 1.21967866E+01 1.59961321E+03    4
NH2OH  WRA032798         N   1H   3O   1    0G   200.000  6000.000  1000.0     1
 3.98241375E+00 7.99825642E-03-2.74883544E-06 4.22874218E-10-2.42498273E-14    2
-6.44279418E+03 3.22666600E+00 2.67285464E+00 1.13645347E-02-4.92179546E-06    3
-9.18041765E-11 6.06669407E-13-6.08956846E+03 1.00068112E+01-4.83091791E+00    4
HNOH               102290H   2N   1O   1     G  0300.00   4000.00  1500.00     1
 0.06396134E+02 0.01821067E-01-0.01870891E-05-0.07844471E-09 0.14448555E-13    2
 0.07859615E+05-0.10404785E+02 0.02125274E+02 0.10662818E-01-0.07602588E-04    3
 0.03081641E-07-0.05726498E-11 0.09553544E+05 0.13096718E+02                  4
H2NO               102290H   2N   1O   1     G  0300.00   4000.00  1500.00     1
 0.05673346E+02 0.02298836E-01-0.01774445E-05-0.11034818E-09 0.01859762E-12    2
 0.05569325E+05-0.06153540E+02 0.02530589E+02 0.08596035E-01-0.05471030E-04    3
 0.02276249E-07-0.04648073E-11 0.06868030E+05 0.11266506E+02                  4
HNNO               103190H   1N   2O   1     G  0300.00   4000.00  1500.00     1
 0.06991217E+02 0.01875970E-01-0.02124584E-05-0.06710472E-09 0.12305080E-13    2
 0.02497566E+06-0.11235229E+02 0.02238298E+02 0.13591997E-01-0.11798728E-04    3
 0.05392970E-07-0.10108589E-11 0.02660258E+06 0.14136789E+02                  4
C2H5CHO            T 9/92C   3H   6O   1    0G   273.150  5000.000 1500.00     1
 0.33137982E+01 0.26619606E-01-0.10475596E-04 0.18815334E-08-0.12761310E-12    2
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-0.25459603E+05 0.96608447E+01 0.76044596E+01-0.86403564E-02 0.73930097E-04    3
-0.79687398E-07 0.28004927E-10-0.25489789E+05-0.67643691E+01-0.23097645E+05    4
C2H5CO            T 9/92C   3H   5O   1    0G   298.150  5000.000 1500.00     1
 0.30445698E+01 0.23236429E-01-0.86317936E-05 0.14799550E-08-0.96860829E-13    2
-0.61787211E+04 0.13122302E+02 0.67368294E+01-0.26945299E-02 0.49927017E-04    3
-0.50025808E-07 0.15011503E-10-0.65703366E+04-0.23398732E+01-0.43321855E+04    4
H2CNO H2C*N=O     T 9/96H   2C   1N   1O   1G   200.000  6000.000 1500.       1
 0.54028152E+01 0.69057001E-02-0.25162977E-05 0.41014066E-09-0.24718300E-13    2
 0.24528690E+05-0.44574262E+01 0.38781858E+01-0.66530886E-02 0.53947610E-04    3
-0.68176813E-07 0.27181746E-10 0.25716857E+05 0.74618774E+01 0.26932156E+05    4
CH3NO             T12/92C   1H   3N   1O   1G   200.000  6000.000 1500.       1
 0.50677397E+01 0.93871079E-02-0.33958317E-05 0.55076729E-09-0.33095301E-13    2
 0.71852464E+04-0.10709779E+01 0.52463494E+01-0.68175691E-02 0.46713959E-04    3
-0.53482743E-07 0.19916692E-10 0.79241319E+04 0.18687355E+01 0.95017371E+04    4
HCNH cis          T05/97H   2C   1N   1    0G   200.000  6000.000 1500.       1
 4.21964804E+00 5.00385006E-03-1.76392053E-06 2.80725924E-10-1.65851919E-14    2
 3.67706419E+04 1.67138658E+00 3.68324269E+00-1.38553482E-03 2.40042191E-05    3
-3.11573905E-08 1.25791818E-11 3.72527355E+04 6.21248890E+00 3.84457533E+04    4
HNCN              101104H   1C   1N   2    0G   300.000  4000.000 1000.00    0 1
 0.52750960E+01 0.48693948E-02-0.21552530E-05 0.44936888E-09-0.35961378E-13    2
 0.36546125E+05-0.18901038E+01 0.27948119E+01 0.13672404E-01-0.14937082E-04    3
 0.95251352E-08-0.26526239E-11 0.37139905E+05 0.10459907E+02                   4
NCN               ATCT/AN   2C   1.   0.   0G   200.000  6000.000  1000.00     1
 5.68743460E+00 1.82663439E-03-7.07551130E-07 1.19517763E-10-7.31862017E-15    2
 5.40184049E+04-6.31950475E+00 2.79807986E+00 1.00008861E-02-9.59242059E-06    3
 4.75565678E-09-1.04348512E-12 5.48304555E+04 8.62129570E+00 5.60333682E+04    4
HE                120186HE  1               g  0300.00   5000.00  1000.00     1
 0.02500000e+02 0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00    2
-0.07453750e+04 0.09153489e+01 0.02500000e+02 0.00000000e+00 0.00000000e+00    3
 0.00000000e+00 0.00000000e+00-0.07453750e+04 0.09153488e+01                   4
END
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Species	Geometry	ε/kB	σ	μ	α	Zrot	
AR	0	136.500	3.330	0.000	0.000	0.000	
C	0	71.400	3.298	0.000	0.000	0.000	!(*)
C2	1	97.530	3.621	0.000	1.760	4.000	
C2O	1	232.400	3.828	0.000	0.000	1.000	! *
CN2	1	232.400	3.828	0.000	0.000	1.000	! OIS
C2H	1	209.000	4.100	0.000	0.000	2.500	
C2H2	1	209.000	4.100	0.000	0.000	2.500	
C2H2OH	2	224.700	4.162	0.000	0.000	1.000	!(*)
CH2OH	2	417.000	3.690	1.700	0.000	2.000	
C2H3	2	209.000	4.100	0.000	0.000	1.000	!(*)
C2H4	2	280.800	3.971	0.000	0.000	1.500	
C2H5	2	252.300	4.302	0.000	0.000	1.500	
C2H6	2	252.300	4.302	0.000	0.000	1.500	
C2N	1	232.400	3.828	0.000	0.000	1.000	! OIS
C2N2	1	349.000	4.361	0.000	0.000	1.000	!(OIS)
C3H2	2	209.000	4.100	0.000	0.000	1.000	!(*)
C3H3	1	252.000	4.760	0.000	0.000	1.000	
C3H4	1	252.000	4.760	0.000	0.000	1.000	
C3H4P	1	252.000	4.760	0.000	0.000	1.000	! JAM
PC3H4	1	252.000	4.760	0.000	0.000	1.000	! JAM
C3H6	2	266.800	4.982	0.000	0.000	1.000	
C3H7	2	266.800	4.982	0.000	0.000	1.000	
C4H6	2	357.000	5.180	0.000	0.000	1.000	
IC3H7	2	266.800	4.982	0.000	0.000	1.000	
NC3H7	2	266.800	4.982	0.000	0.000	1.000	
C3H8	2	266.800	4.982	0.000	0.000	1.000	
C4H	1	357.000	5.180	0.000	0.000	1.000	
C4H2	1	357.000	5.180	0.000	0.000	1.000	
C4H2OH	2	224.700	4.162	0.000	0.000	1.000	!(*)
C4H3	1	357.000	5.180	0.000	0.000	1.000	
C4H4	1	357.000	5.180	0.000	0.000	1.000	
C4H8	2	357.000	5.176	0.000	0.000	1.000	
T2C4H8	2	357.000	5.176	0.000	0.000	1.000	!=C4H8
C2C4H8	2	357.000	5.176	0.000	0.000	1.000	!=C4H8
NC3H7O	2	357.000	5.176	0.000	0.000	1.000	!=C4H8
IC3H7O	2	357.000	5.176	0.000	0.000	1.000	!=C4H8
IC3H7O2H	2	357.000	5.176	0.000	0.000	1.000	!=C4H8
IC3H7O2	2	357.000	5.176	0.000	0.000	1.000	!=C4H8
NC3H7O2H	2	357.000	5.176	0.000	0.000	1.000	!=C4H8
NC3H7O2	2	357.000	5.176	0.000	0.000	1.000	!=C4H8
IC4H7	2	357.000	5.176	0.000	0.000	1.000	!=C4H8
TC4H7	2	357.000	5.176	0.000	0.000	1.000	!=C4H8
C3H5O2	2	357.000	5.176	0.000	0.000	1.000	!=C4H8
C3H5O2H	2	357.000	5.176	0.000	0.000	1.000	!=C4H8
C3H5O	2	357.000	5.176	0.000	0.000	1.000	!=C4H8
C3H6OH	2	357.000	5.176	0.000	0.000	1.000	!=C4H8
O2C3H6OH	2	357.000	5.176	0.000	0.000	1.000	!=C4H8
CH3CO2H	2	357.000	5.176	0.000	0.000	1.000	!=C4H8
CH3CO2	2	357.000	5.176	0.000	0.000	1.000	!=C4H8
CH3CO3	2	357.000	5.176	0.000	0.000	1.000	!=C4H8
CH3CO3H	2	357.000	5.176	0.000	0.000	1.000	!=C4H8
C2H5CHO	2	357.000	5.176	0.000	0.000	1.000	!=C4H8
C2H5CO	2	357.000	5.176	0.000	0.000	1.000	!=C4H8
C4H9	2	357.000	5.176	0.000	0.000	1.000	
S*C4H9	2	357.000	5.176	0.000	0.000	1.000	
C4H9	2	357.000	5.176	0.000	0.000	1.000	
I*C4H9	2	357.000	5.176	0.000	0.000	1.000	
C5H2	1	357.000	5.180	0.000	0.000	1.000	
C5H3	1	357.000	5.180	0.000	0.000	1.000	
C6H2	1	357.000	5.180	0.000	0.000	1.000	
C6H5	2	412.300	5.349	0.000	0.000	1.000	! JAM
C6H5(L)	2	412.300	5.349	0.000	0.000	1.000	! JAM
C6H5O	2	450.000	5.500	0.000	0.000	1.000	! JAM

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C5H5OH              2   450.000     5.500     0.000     0.000     1.000 ! JAM
C6H6                2   412.300     5.349     0.000     0.000     1.000 ! SVE
C6H7                2   412.300     5.349     0.000     0.000     1.000 ! JAM
CH                  1    80.000     2.750     0.000     0.000     0.000
CH2                 1   144.000     3.800     0.000     0.000     0.000
CH2(S)              1   144.000     3.800     0.000     0.000     0.000
CH2(SING)           1   144.000     3.800     0.000     0.000     0.000
SCH2                1   144.000     3.800     0.000     0.000     0.000
CH2CHCCH            2   357.000     5.180     0.000     0.000     1.000 ! JAM
CH2CHCCH2           2   357.000     5.180     0.000     0.000     1.000 ! JAM
CH2CHCH2            2   260.000     4.850     0.000     0.000     1.000 ! JAM
C3H5                2   260.000     4.850     0.000     0.000     1.000 ! JAM
CH2CHCHCH           2   357.000     5.180     0.000     0.000     1.000 ! JAM
CH2CHCHCH2          2   357.000     5.180     0.000     0.000     1.000 ! JAM
IC4H5               2   357.000     5.180     0.000     0.000     1.000
NC4H5               2   357.000     5.180     0.000     0.000     1.000
CH2CO               2   436.000     3.970     0.000     0.000     2.000
CH2O                2   498.000     3.590     0.000     0.000     2.000
CH3                 1   144.000     3.800     0.000     0.000     0.000
CH3CC               2   252.000     4.760     0.000     0.000     1.000 ! JAM
CH3CCCH2            2   357.000     5.180     0.000     0.000     1.000 ! JAM
CH3CCCH3            2   357.000     5.180     0.000     0.000     1.000 ! JAM
IC4H3               2   357.000     5.180     0.000     0.000     1.000
NC4H3               2   357.000     5.180     0.000     0.000     1.000
CH3CCH2             2   260.000     4.850     0.000     0.000     1.000 ! JAM
TC3H5               2   260.000     4.850     0.000     0.000     1.000 ! JAM
CH3CHCH             2   260.000     4.850     0.000     0.000     1.000 ! JAM
SC3H5               2   260.000     4.850     0.000     0.000     1.000 ! JAM
CH3CH2CCH           2   357.000     5.180     0.000     0.000     1.000 ! JAM
CH3HCO              2   436.000     3.970     0.000     0.000     2.000
CH3HCOW             2   436.000     3.970     0.000     0.000     2.000 !=AA
C2H4O               2   436.000     3.970     0.000     0.000     2.000 !=AA
C2H3O               2   436.000     3.970     0.000     0.000     2.000 !=AA
C3H6O               2   436.000     3.970     0.000     0.000     2.000 !=AA
CH3CO               2   436.000     3.970     0.000     0.000     2.000
CH3O                2   417.000     3.690     1.700     0.000     2.000
CH3OH               2   481.800     3.626     0.000     0.000     1.000 ! SVE
CH4                 2   141.400     3.746     0.000     2.600    13.000
CH4O                2   417.000     3.690     1.700     0.000     2.000
CN                  1    75.000     3.856     0.000     0.000     1.000  !(OIS)
CNC                 1   232.400     3.828     0.000     0.000     1.000 ! OIS
CNN                 1   232.400     3.828     0.000     0.000     1.000 ! OIS
HCNN                1   232.400     3.828     0.000     0.000     1.000 !=CNN
NCN                 1   232.400     3.828     0.000     0.000     1.000 !=CNN
HNCN                1   232.400     3.828     0.000     0.000     1.000 !=CNN
CO                  1    98.100     3.650     0.000     1.950     1.800
CO2                 1   244.000     3.763     0.000     2.650     2.100
H                   0   145.000     2.050     0.000     0.000     0.000
H2C4O               2   357.000     5.180     0.000     0.000     1.000 ! JAM
H2                  1    38.000     2.920     0.000     0.790   280.000
H2CCCCH             2   357.000     5.180     0.000     0.000     1.000 ! JAM
H2CCCCH2            2   357.000     5.180     0.000     0.000     1.000 ! JAM
H2CCCH              2   252.000     4.760     0.000     0.000     1.000 ! JAM
H2CN                1   569.000     3.630     0.000     0.000     1.000 ! os/jm
H2NO                2   116.700     3.492     0.000     0.000     1.000 ! JAM
H2O                 2   572.400     2.605     1.844     0.000     4.000
H2O2                2   107.400     3.458     0.000     0.000     3.800
H2S                 2   301.000     3.600     0.000     0.000     1.000  !(OIS)
HC2N2               1   349.000     4.361     0.000     0.000     1.000 ! OIS
HCCHCCH             2   357.000     5.180     0.000     0.000     1.000 ! JAM
HCCO                2   150.000     2.500     0.000     0.000     1.000  !(*)
HCCOH               2   436.000     3.970     0.000     0.000     2.000
HCN                 1   569.000     3.630     0.000     0.000     1.000  !(OIS)
HCNO                2   232.400     3.828     0.000     0.000     1.000 ! JAM
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H2CNO              2   232.400     3.828     0.000     0.000     1.000 !=HCNO
CH3NO              2   232.400     3.828     0.000     0.000     1.000 !=HCNO
HCNH               2   232.400     3.828     0.000     0.000     1.000 !=HCNO
HCO                2   498.000     3.590     0.000     0.000     0.000
HCO+               1   498.000     3.590     0.000     0.000     0.000
CH2HCO             2   436.000     3.970     0.000     0.000     2.000
CH2CHOW            2   436.000     3.970     0.000     0.000     2.000 !=CH2HCO
HOCN               2   232.400     3.828     0.000     0.000     1.000  !(JAM)
HNCO               2   232.400     3.828     0.000     0.000     1.000  !(OIS)
HNNO               2   232.400     3.828     0.000     0.000     1.000  !(*)
HONO               2   232.400     3.828     0.000     0.000     1.000  !=HNNO
HNO                2   116.700     3.492     0.000     0.000     1.000  !(*)
HNOH               2   116.700     3.492     0.000     0.000     1.000 ! JAM
NH2OH              2   116.700     3.492     0.000     0.000     1.000 !=HNOH
HO2                2   107.400     3.458     0.000     0.000     1.000  !(*)
HSO2               2   252.000     4.290     0.000     0.000     1.000  !(OIS)
HE                 0    10.200     2.576     0.000     0.000     0.000  !(*)
N                  0    71.400     3.298     0.000     0.000     0.000  !(*)
N2                 1    97.530     3.621     0.000     1.760     4.000
N2H2               2    71.400     3.798     0.000     0.000     1.000  !(*)
N2H3               2   200.000     3.900     0.000     0.000     1.000  !(*)
N2H4               2   205.000     4.230     0.000     4.260     1.500
N2O                1   232.400     3.828     0.000     0.000     1.000  !(*)
NCN                1   232.400     3.828     0.000     0.000     1.000 ! OIS
NCO                1   232.400     3.828     0.000     0.000     1.000  !(OIS)
NH                 1    80.000     2.650     0.000     0.000     4.000
NH2                2    80.000     2.650     0.000     2.260     4.000
NH3                2   481.000     2.920     1.470     0.000    10.000
NNH                2    71.400     3.798     0.000     0.000     1.000  !(*)
NO                 1    97.530     3.621     0.000     1.760     4.000
NCNO               2   232.400     3.828     0.000     0.000     1.000 ! OIS
NO2                2   200.000     3.500     0.000     0.000     1.000  !(*)
CH3O2              2   200.000     3.500     0.000     0.000     1.000  !=NO2
CH3O2H             2   200.000     3.500     0.000     0.000     1.000  !=NO2
SO2                2   252.000     4.290     0.000     0.000     1.000  !(OIS)
SO3                2   378.400     4.175     0.000     0.000     1.000  !(OIS)
NO3                2   378.400     4.175     0.000     0.000     1.000  !=SO3
HNO3               2   378.400     4.175     0.000     0.000     1.000  !=SO3
O                  0    80.000     2.750     0.000     0.000     0.000
O2                 1   107.400     3.458     0.000     1.600     3.800
O3                 2   180.000     4.100     0.000     0.000     2.000
OH                 1    80.000     2.750     0.000     0.000     0.000
C2H5OH             2   362.6       4.53      0.000     0.000     1.000  !(sve)
PC2H5O             2   362.6       4.53      0.000     0.000     1.000  !=C2H5OH
SC2H5O             2   362.6       4.53      0.000     0.000     1.000  !=C2H5OH
C2H5O              2   362.6       4.53      0.000     0.000     1.000  !=C2H5OH
C2H5O2H            2   362.6       4.53      0.000     0.000     1.000  !=C2H5OH
C2H5O2             2   362.6       4.53      0.000     0.000     1.000  !=C2H5OH
C2F4               2   202.6       5.164     0.000     0.000     1.000  !(mec)
N2O4               2   202.6       5.164     0.000     0.000     1.000  !=C2F4
N2O3               2   202.6       5.164     0.000     0.000     1.000  !=C2F4
CH3CHO             2   436.000     3.970     0.000     0.000     2.000
CH2CHO             2   436.000     3.970     0.000     0.000     2.000
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Appendix:C

Thermodynamic Data File of the Reactions of K-species

!Kee et al. (1990); Glarborg and Marshall (2005);
!Chemkin file janaf$_t herm.datV.4.0March2004$; $Babushoketal.(2017)$;
!this file therm.dat 2021;
!The polynomial coefficients representing thermodynamic
THERMO
300.000 1000.000 5000.000
! Species: C2H CAS Number: 2122-48-7
! Name: Ethynyl Radical
! Source: SNLL fit to 1986 JANAF tables, 8/11/93
! H0(298K) = 135.000 (Kcal/mole), S0(298K) = 51.1000 (cal/mole-K)
C2H 81193C 2H 1 G 300.000 4000.000 1000.00 1
3.98636700e+00 3.14312300e-03-1.26724300e-06 2.92436300e-10-2.71632000e-14 2
6.65588400e+04 1.19106300e+00 2.73770400e+00 8.04844600e-03-9.24431000e-06 3
6.52525900e-09-1.93958000e-12 6.68381300e+04 7.30022000e+00 4
!
! Species: C2H2 CAS Number: 74-86-2
! Name: Acetylene
! Source: SNLL fit to 1986 JANAF tables, 12/13/86
! H0(298K) = 54.1900 (Kcal/mole), S0(298K) = 48.0000 (cal/mole-K)
C2H2 121386C 2H 2 G 300.000 5000.000 1000.00 1
4.43677000e+00 5.37603900e-03-1.91281700e-06 3.28637900e-10-2.15671000e-14 2
2.56676600e+04-2.80033800e+00 2.01356200e+00 1.51904500e-02-1.61631900e-05 3
9.07899200e-09-1.91274600e-12 2.61244400e+04 8.80537800e+00 4
!
! Species: C2H3 CAS Number: 2669-89-8
! Name: Vinyl Radical
! Source: Recalc. OF Burcat fit (Technion), H298=68.4 per Miller, 1/27/87
! H0(298K) = 68.4000 (Kcal/mole), S0(298K) = 55.3000 (cal/mole-K)
C2H3 12787C 2H 3 G 300.000 5000.000 1000.00 1
5.93346800e+00 4.01774600e-03-3.96674000e-07-1.44126700e-10 2.37864400e-14 2
3.18543500e+04-8.53031300e+00 2.45927600e+00 7.37147600e-03 2.10987300e-06 3
-1.32164200e-09-1.18478400e-12 3.33522500e+04 1.15562000e+01 4
!
! Species: C2H4 CAS Number: 74-85-1
! Name: Ethylene
! Source: SNLL fit to 1986 JANAF tables, 12/12/86
! H0(298K) = 12.5400 (Kcal/mole), S0(298K) = 52.4000 (cal/mole-K)
C2H4 121286C 2H 4 G 300.000 5000.000 1000.00 1
3.52841900e+00 1.14851800e-02-4.41838500e-06 7.84460100e-10-5.26684800e-14 2

4.42828900e+03 2.23038900e+00-8.61488000e-01 2.79616300e-02-3.38867700e-05 3
2.78515200e-08-9.73787900e-12 5.57304600e+03 2.42114900e+01 4
!
! Species: C2H5 CAS Number: 2025-56-1
! Name: Ethyl Radical
! Source: Recalc. OF Burcat fit (TSIV tables), H298=28 per Miller, 1/23/87
! H0(298K) = 28.0000 (Kcal/mole), S0(298K) = 60.1000 (cal/mole-K)
C2H5 12387C 2H 5 G 300.000 5000.000 1000.00 1
7.19048000e+00 6.48407700e-03-6.42806500e-07-2.34787900e-10 3.88087700e-14 2
1.06745500e+04-1.47808900e+01 2.69070200e+00 8.71913300e-03 4.41983900e-06 3
9.33870300e-10-3.92777300e-12 1.28704000e+04 1.21382000e+01 4
!
! Species: C2H6 CAS Number: 74-84-0
! Name: Ethane
! Source: Burcat (Technion Reports), 12/16/86
! H0(298K) = -20.0000 (Kcal/mole), S0(298K) = 60.1000 (cal/mole-K)
C2H6 121686C 2H 6 G 300.000 4000.000 1000.00 1
4.82593800e+00 1.38404300e-02-4.55725900e-06 6.72496700e-10-3.59816100e-14 2
-1.27177900e+04-5.23950700e+00 1.46253900e+00 1.54946700e-02 5.78050700e-06 3
-1.25783200e-08 4.58626700e-12-1.12391800e+04 1.44322900e+01 4
!
C3H7 L 9/84C 3H 7 G 300.000 5000.000 1000.000 1
0.77026987E+01 0.16044203E-01-0.52833220E-05 0.76298590E-09-0.39392284E-13 2
0.82984336E+04-0.15480180E+02 0.10515518E+01 0.25991980E-01 0.23800540E-05 3
-0.19609569E-07 0.93732470E-11 0.10631863E+05 0.21122559E+02 4
!
! Species: C3H8 CAS Number: 74-98-6
! Name: Propane
! Source: Burcat (NASA Lewis tables), 12/01/86
! H0(298K) = -24.8000 (Kcal/mole), S0(298K) = 64.6000 (cal/mole-K)
C3H8 120186C 3H 8 G 300.000 5000.000 1000.00 1
7.52521700e+00 1.88903400e-02-6.28392400e-06 9.17937300e-10-4.81241000e-14 2
-1.64645500e+04-1.78439000e+01 8.96920800e-01 2.66898600e-02 5.43142500e-06 3
-2.12600100e-08 9.24333000e-12-1.39549200e+04 1.93553300e+01 4
!
! Species: CH2O CAS Number: 50-00-0
! Name: Formaldehyde
! Source: SNLL fit to 1986 JANAF tables, 12/12/86
! H0(298K) = -27.7000 (Kcal/mole), S0(298K) = 52.2600 (cal/mole-K)
CH2O 121286C 1H 2O 1 G 300.000 5000.000 1000.00 1
2.99560600e+00 6.68132100e-03-2.62895500e-06 4.73715300e-10-3.21251700e-14 2
-1.53203700e+04 6.91257200e+00 1.65273100e+00 1.26314400e-02-1.88816800e-05 3

2.05003100e-08-8.41323700e-12-1.48654000e+04 1.37848200e+01 4
!
! Species: CH3 CAS Number: 2229-07-4
! Name: Methyl Radical
! Source: SNLL fit to 1986 JANAF tables, 12/12/86
! H0(298K) = 34.8200 (Kcal/mole), S0(298K) = 46.3800 (cal/mole-K)
CH3 121286C 1H 3 G 300.000 5000.000 1000.00 1
2.84405200e+00 6.13797400e-03-2.23034500e-06 3.78516100e-10-2.45215900e-14 2
1.64378100e+04 5.45269700e+00 2.43044300e+00 1.11241000e-02-1.68022000e-05 3
1.62182900e-08-5.86495300e-12 1.64237800e+04 6.78979400e+00 4
!
! Species: CH3O CAS Number: 2143-68-2
! Name: Methyloxide (Methoxy Radical)
! Source: Burcat (LSU calculations), 12/16/86
! H0(298K) = 3.90000 (Kcal/mole), S0(298K) = 54.6000 (cal/mole-K)
CH3O 121686C 1H 3O 1 G 300.000 3000.000 1000.00 1
3.77080000e+00 7.87149700e-03-2.65638400e-06 3.94443100e-10-2.11261600e-14 2
1.27832500e+02 2.92957500e+00 2.10620400e+00 7.21659500e-03 5.33847200e-06 3
-7.37763600e-09 2.07561100e-12 9.78601100e+02 1.31521800e+01 4
!
! Species: CH3OH CAS Number: 67-56-1
! Name: Methanol
! Source: Burcat (CH4O) (Technion Reports), 12/16/86
! H0(298K) = -48.0000 (Kcal/mole), S0(298K) = 57.3000 (cal/mole-K)
CH3OH 121686C 1H 4O 1 G 300.000 5000.000 1000.00 1
4.02906100e+00 9.37659300e-03-3.05025400e-06 4.35879300e-10-2.22472300e-14 2
-2.61579100e+04 2.37819600e+00 2.66011500e+00 7.34150800e-03 7.17005100e-06 3
-8.79319400e-09 2.39057000e-12-2.53534800e+04 1.12326300e+01 4
!
! Species: CH4 CAS Number: 74-82-8
! Name: Methane
! Source: SNLL fit to 1986 JANAF tables, 12/12/86
! H0(298K) = -17.9000 (Kcal/mole), S0(298K) = 44.4900 (cal/mole-K)
CH4 121286C 1H 4 G 300.000 5000.000 1000.00 1
1.68347900e+00 1.02372400e-02-3.87512900e-06 6.78558500e-10-4.50342300e-14 2
-1.00807900e+04 9.62339500e+00 7.78741500e-01 1.74766800e-02-2.78340900e-05 3
3.04970800e-08-1.22393100e-11-9.82522900e+03 1.37221900e+01 4
!
! Species: CO CAS Number: 630-08-0
! Name: Carbon Monoxide
! Source: SNLL fit to 1986 JANAF tables, 12/12/86
! H0(298K) = -26.4200 (Kcal/mole), S0(298K) = 47.2100 (cal/mole-K)

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CO 121286C 1O 1 G 300.000 5000.000 1000.00 1
3.02507800e+00 1.44268900e-03-5.63082800e-07 1.01858100e-10-6.91095200e-15 2
-1.42683500e+04 6.10821800e+00 3.26245200e+00 1.51194100e-03-3.88175500e-06 3
5.58194400e-09-2.47495100e-12-1.43105400e+04 4.84889700e+00 4
!
! Species: CO2 CAS Number: 124-38-9
! Name: Carbon Dioxide
! Source: SNLL fit to 1986 JANAF tables, 12/12/86
! H0(298K) = -94.0500 (Kcal/mole), S0(298K) = 51.0700 (cal/mole-K)
CO2 121286C 1O 2 G 300.000 5000.000 1000.00 1
4.45362300e+00 3.14016900e-03-1.27841100e-06 2.39399700e-10-1.66903300e-14 2
-4.89669600e+04-9.55395900e-01 2.27572500e+00 9.92207200e-03-1.04091100e-05 3
6.86668700e-09-2.11728000e-12-4.83731400e+04 1.01884900e+01 4
!
! Species: H CAS Number: 12385-13-6
! Name: Hydrogen Monatomic
! Source: NASA fit to 1986 JANAF tables, 12/01/86
! H0(298K) = 52.1000 (Kcal/mole), S0(298K) = 27.3900 (cal/mole-K)
H 120186H 1 G 300.000 5000.000 1000.00 1
2.50000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00 2
2.54716300e+04-4.60117600e-01 2.50000000e+00 0.00000000e+00 0.00000000e+00 3
0.00000000e+00 0.00000000e+00 2.54716300e+04-4.60117600e-01 4
!
! Species: H2 CAS Number: 1333-74-0
! Name: Hydrogen Diatomic (Ref St)
! Source: SNLL fit to 1986 JANAF tables, 12/12/86
! H0(298K) = 0.00000 (Kcal/mole), S0(298K) = 31.2100 (cal/mole-K)
H2 121286H 2 G 300.000 5000.000 1000.00 1
2.99142300e+00 7.00064400e-04-5.63382900e-08-9.23157800e-12 1.58275200e-15 2
-8.35034000e+02-1.35511000e+00 3.29812400e+00 8.24944200e-04-8.14301500e-07 3
-9.47543400e-11 4.13487200e-13-1.01252100e+03-3.29409400e+00 4
!
! Species: H2O CAS Number: 7732-18-5
! Name: Water
! Source: SNLL fit to 1986 JANAF tables, 2/03/87
! H0(298K) = -57.8000 (Kcal/mole), S0(298K) = 45.1100 (cal/mole-K)
H2O 20387H 2O 1 G 300.000 5000.000 1000.00 1
2.67214600e+00 3.05629300e-03-8.73026000e-07 1.20099600e-10-6.39161800e-15 2
-2.98992100e+04 6.86281700e+00 3.38684200e+00 3.47498200e-03-6.35469600e-06 3
6.96858100e-09-2.50658800e-12-3.02081100e+04 2.59023300e+00 4
!
! Species: H2O2 CAS Number: 7722-84-1
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! Name: Hydrogen Peroxide
! Source: NASA fit to NASA-Lewis data, 12/01/86
! H0(298K) = -32.5000 (Kcal/mole), S0(298K) = 55.6600 (cal/mole-K)
H2O2 120186H 2O 2 G 300.000 5000.000 1000.00 1
4.57316700e+00 4.33613600e-03-1.47468900e-06 2.34890400e-10-1.43165400e-14 2
-1.80069600e+04 5.01137000e-01 3.38875400e+00 6.56922600e-03-1.48501300e-07 3
-4.62580600e-09 2.47151500e-12-1.76631500e+04 6.78536300e+00 4
!
! Species: HCO CAS Number: 2597-44-6
! Name: Formyl Radical
! Source: SNLL fit to 1986 JANAF tables (CHO), 12/12/86
! H0(298K) = 10.4000 (Kcal/mole), S0(298K) = 53.6700 (cal/mole-K)
HCO 121286H 1C 1O 1 G 300.000 5000.000 1000.00 1
3.55727100e+00 3.34557300e-03-1.33500600e-06 2.47057300e-10-1.71385100e-14 2
3.91632400e+03 5.55229900e+00 2.89833000e+00 6.19914700e-03-9.62308400e-06 3
1.08982500e-08-4.57488500e-12 4.15992200e+03 8.98361400e+00 4
!
! Species: HO2 CAS Number: 3170-83-0
! Name: Hydroperoxyl Radical
! Source: SNLL fit to 1986 JANAF tables with H298=2.5 per Miller, 2/03/87
! H0(298K) = 2.50000 (Kcal/mole), S0(298K) = 54.7300 (cal/mole-K)
HO2 20387H 1O 2 G 300.000 5000.000 1000.00 1
4.07219100e+00 2.13129600e-03-5.30814500e-07 6.11226900e-11-2.84116500e-15 2
-1.57972700e+02 3.47602900e+00 2.97996300e+00 4.99669700e-03-3.79099700e-06 3
2.35419200e-09-8.08902400e-13 1.76227400e+02 9.22272400e+00 4
!
! Species: K CAS Number: 7440-09-7
! Name: Potassium Monatomic
! Source: SNLL fit to 1986 JANAF data, 8/10/92
! H0(298K) = 21.3100 (Kcal/mole), S0(298K) = 38.3000 (cal/mole-K)
K 81092K 1 G 300.000 5000.000 1000.00 1
2.56372000e+00-1.45365600e-04 1.22379400e-07-5.33779700e-11 1.19625100e-14 2
9.95893300e+03 4.68909000e+00 2.59939500e+00-6.66519200e-04 1.53741900e-06 3
-1.46270100e-09 4.91722600e-13 9.96853400e+03 4.60612500e+00 4
!
! Species: K2O CAS Number: 12136-45-7
! Name: Potassium Oxide
! Source: SNLL fit to 1986 JANAF data, 8/10/92
! H0(298K) = -86.8000 (Kcal/mole), S0(298K) = 22.5000 (cal/mole-K)
K2O 81092K 2O 1 S 300.000 2000.000 1000.00 1
9.20010900e+00 4.81352900e-03-1.01865600e-06 8.97297300e-10-2.12141700e-13 2
-4.67115400e+04-4.26414200e+01 2.64031500e+00 4.57722500e-02-9.34935700e-05 3
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8.92101200e-08-3.04489800e-11-4.58369700e+04-1.39276300e+01 4
!
! Species: K2O2 CAS Number: 17014-71-0
! Name: Potassium Peroxide
! Source: SNLL fit to 1986 JANAF data, 8/10/92
! H0(298K) = -118.500 (Kcal/mole), S0(298K) = 27.0000 (cal/mole-K)
K2O2 81092K 2O 2 S 300.000 2000.000 1000.00 1
1.09413800e+01 6.10230900e-03 8.63995100e-07-2.38397800e-10 1.02195900e-14 2
-6.33511400e+04-5.09944700e+01 8.94002400e+00 1.22501400e-02-8.06536500e-06 3
7.18227100e-09-2.62756100e-12-6.27748500e+04-4.06668300e+01 4
!
! Species: K2H2O2 CAS Number: 12395-66-3
! Name: Potassium Hydroxide, Dimeric
! Source: SNLL fit to 1986 JANAF data, 8/12/92
! H0(298K) = -156.500 (Kcal/mole), S0(298K) = 78.3700 (cal/mole-K)
K2H2O2 81292H 2K 2O 2 G 300.000 5000.000 1000.00 1
9.47600700e+00 5.52001200e-03-2.00351200e-06 3.41698400e-10-2.23008900e-14 2
-8.20478600e+04-1.66554600e+01 6.06965700e+00 1.65715900e-02-1.64113400e-05 3
9.62801200e-09-2.54601300e-12-8.11815200e+04 5.62592900e-01 4
!
! Species: HK CAS Number: 7693-26-7
! Name: Potassium Hydride
! Source: SNLL fit to 1986 JANAF data, 8/10/92
! H0(298K) = 29.4000 (Kcal/mole), S0(298K) = 47.3000 (cal/mole-K)
HK 81092H 1K 1 G 300.000 5000.000 1000.00 1
3.96813800e+00 7.08692400e-04-2.61851700e-07 5.09604400e-11-3.65545200e-15 2
1.35012000e+04 8.02741300e-01 2.90012100e+00 3.51831700e-03-2.54477400e-06 3
4.59996100e-10 1.28622900e-13 1.37966700e+04 6.34276600e+00 4
!
! Species: KO CAS Number: 12401-70-6
! Name: Potassium Monoxide
! Source: SNLL fit to 1986 JANAF data, 8/10/92
! H0(298K) = 17.0000 (Kcal/mole), S0(298K) = 56.8600 (cal/mole-K)
KO 81092K 1O 1 G 300.000 5000.000 1000.00 1
4.40029100e+00 2.38678700e-04-5.88004700e-08 1.20671300e-11-9.00696100e-16 2
7.21711000e+03 3.43477500e+00 3.98533300e+00 1.46935300e-03-9.47905400e-07 3
-2.41914100e-10 3.26470000e-13 7.31112000e+03 5.51790200e+00 4
!
! Species: KO2 CAS Number: 12030-88-5
! Name: Potassium Superoxide
! Source: SNLL fit to 1986 JANAF data, 8/10/92
! H0(298K) = -68.0000 (Kcal/mole), S0(298K) = 29.2800 (cal/mole-K)

KO2 81092K 1O 2 S 300.000 1500.000 1000.00 1
1.04931000e+01 1.39761800e-03-6.97664300e-07 3.47742700e-10-1.22270800e-13 2
-3.76751600e+04-4.60732100e+01 4.02324400e+00 2.90356100e-02-4.81241600e-05 3
3.81661300e-08-1.16823100e-11-3.63580500e+04-1.50219100e+01 4
!
! Species: HKO CAS Number: 1310-58-3
! Name: Potassium Hydroxide
! Source: ReactionDesign fit to 1986 JANAF tables, J622
! H0(298K) = -55.5700 (Kcal/mole), S0(298K) = 56.4700 (cal/mole-K)
HKO J622 H 1K 1O 1 G 200.000 6000.000 700.00 1
5.72919876e+00 1.13238275e-03-3.00385838e-07 3.65979074e-11-1.68011958e-15 2
-2.97307715e+04-4.57882868e+00 2.25503887e+00 2.39627570e-02-5.56041134e-05 3
5.87844310e-08-2.31536263e-11-2.93173509e+04 1.04216832e+01 4
!
! Species: O CAS Number: 17778-80-2
! Name: Oxygen Monatomic
! Source: NASA fit to 1986 JANAF tables, 12/01/86
! H0(298K) = 59.5500 (Kcal/mole), S0(298K) = 38.4700 (cal/mole-K)
O 120186O 1 G 300.000 5000.000 1000.00 1
2.54206000e+00-2.75506200e-05-3.10280300e-09 4.55106700e-12-4.36805200e-16 2
2.92308000e+04 4.92030800e+00 2.94642900e+00-1.63816600e-03 2.42103200e-06 3
-1.60284300e-09 3.89069600e-13 2.91476400e+04 2.96399500e+00 4
!
! Species: O2 CAS Number: 7782-44-7
! Name: Oxygen Diatomic (Ref St)
! Source: SNLL fit to 1986 JANAF tables, 12/13/86
! H0(298K) = 0.00000 (Kcal/mole), S0(298K) = 49.0100 (cal/mole-K)
O2 121386O 2 G 300.000 5000.000 1000.00 1
3.69757800e+00 6.13519700e-04-1.25884200e-07 1.77528100e-11-1.13643500e-15 2
-1.23393000e+03 3.18916600e+00 3.21293600e+00 1.12748600e-03-5.75615000e-07 3
1.31387700e-09-8.76855400e-13-1.00524900e+03 6.03473800e+00 4
!
! Species: OH CAS Number: 3352-57-6
! Name: Hydroxyl Radical
! Source: SNLL fit to 1986 JANAF tables, 12/12/86
! H0(298K) = 9.32000 (Kcal/mole), S0(298K) = 43.8800 (cal/mole-K)
OH 121286O 1H 1 G 300.000 5000.000 1000.00 1
2.88273000e+00 1.01397400e-03-2.27687700e-07 2.17468400e-11-5.12630500e-16 2
3.88688800e+03 5.59571200e+00 3.63726600e+00 1.85091000e-04-1.67616500e-06 3
2.38720300e-09-8.43144200e-13 3.60678200e+03 1.35886000e+00 4
!
! Species: N2 CAS Number: 7727-37-9

! Name: Nitrogen Diatomic (Ref St)
! Source: SNLL fit to 1986 JANAF tables, 12/12/86
! H0(298K) = 0.00000 (Kcal/mole), S0(298K) = 45.7700 (cal/mole-K)
N2 121286N 2 G 300.000 5000.000 1000.00 1
2.92664000e+00 1.48797700e-03-5.68476100e-07 1.00970400e-10-6.75335100e-15 2
-9.22797700e+02 5.98052800e+00 3.29867700e+00 1.40824000e-03-3.96322200e-06 3
5.64151500e-09-2.44485500e-12-1.02090000e+03 3.95037200e+00 4
!
! Species: KO3 CAS Number: 12030-89-6
! Name: Potassium Ozonide
! Source: Babushok et al. (2017);
! H0(298K) = -18.39 (Kcal/mole), S0(298K) = 68.26(cal/mole-K)
KO3 81092K 1O 3 S 300.000 1500.000 1000.00 1
1.04931000e+01 1.39761800e-03-6.97664300e-07 3.47742700e-10-1.22270800e-13 2
-3.76751600e+04-4.60732100e+01 4.02324400e+00 2.90356100e-02-4.81241600e-05 3
3.81661300e-08-1.16823100e-11-3.63580500e+04-1.50219100e+01 4
!
! Species: K2CO3 CAS Number: 584-08-7
! Name: Potassium Carbonate
! Source: SNL fit to 1986 JANAF data, 8/12/92
! H0(298K) = -274.900 (Kcal/mole), S0(298K) = 37.1700 (cal/mole-K)
K2CO3 81298C 1K 2O 3 S 300.000 2000.000 1000.00 1
1.17093500e+01 1.04161900e-02 1.02081200e-06-5.15567000e-10 9.38847200e-14 2
-1.42467000e+05-5.15489900e+01 6.68049500e+00 3.15487500e-02-3.25834800e-05 3
2.34108000e-08-6.33188200e-12-1.41499400e+05-2.75103100e+01 4
!
! Species: KHCO3 CAS Number: 298-14-6
! Name: Potassium Bicarbonate
! Source: Babushok et al. (2017);
! H0(298K) = -230 (Kcal/mole), S0(298K) = 37.16(cal/mole-K)
KHCO3 81298C 1H 1K 1O 3S 300.000 5000.000 1500.00 1
1.17093500e+01 1.04161900e-02 1.02081200e-06-5.15567000e-10 9.38847200e-14 2
-1.42467000e+05-5.15489900e+01 6.68049500e+00 3.15487500e-02-3.25834800e-05 3
2.34108000e-08-6.33188200e-12-1.41499400e+05-2.75103100e+01 4
!
! Species: KCO3 CAS Number: 584-08-7
! Name: Potassium Carbonate Radical
! Source: Babushok et al. (2017);
! H0(298K) = -124.900 (Kcal/mole), S0(298K) = 74.300 (cal/mole-K)
KCO3 81298C 1K 1O 3 G 300.000 2000.000 1000.00 1
1.17093500e+01 1.04161900e-02 1.02081200e-06-5.15567000e-10 9.38847200e-14 2
-1.42467000e+05-5.15489900e+01 6.68049500e+00 3.15487500e-02-3.25834800e-05 3

2.34108000e-08-6.33188200e-12-1.41499400e+05-2.75103100e+01 4

Table 1: Transport Data File of the Reactions of K-species

Species	Geometry	ε/kB	σ	μ	α	Zrot
C_2H	1	209.000	4.100	0.000	0.000	2.500
C_2H_2	1	209.000	4.100	0.000	0.000	2.500
CH_2OH	2	417.000	3.690	1.700	0.000	2.000
C_2H_3	2	209.000	4.100	0.000	0.000	1.000!(*)
C_2H_4	2	280.800	3.971	0.000	0.000	1.500
C_2H_5	2	252.300	4.302	0.000	0.000	1.500
C_2H_6	2	252.300	4.302	0.000	0.000	1.500
C_3H_7	2	266.800	4.982	0.000	0.000	1.000
C_3H_8	2	266.800	4.982	0.000	0.000	1.000
CH_2O	2	498.000	3.590	0.000	0.000	2.000
CH_3	1	144.000	3.800	0.000	0.000	0.000
CH_3O	2	417.000	3.690	1.700	0.000	2.000
CH_3OH	2	481.800	3.626	0.000	0.000	1.000 ! SVE
CH_4	2	141.400	3.746	0.000	2.600	13.000
CO	1	98.100	3.650	0.000	1.950	1.800
CO_2	1	244.000	3.763	0.000	2.650	2.100
H	0	145.000	2.050	0.000	0.000	0.000
H_2	1	38.000	2.920	0.000	0.790	280.000
H_2O	2	572.400	2.605	1.844	0.000	4.000
H_2O_2	2	107.400	3.458	0.000	0.000	3.800
HCO	2	498.000	3.590	0.000	0.000	0.000
K	0	850.	4.25	0.000	0.000	1.000 !(singh)
KO	1	383.0	3.812	0.000	0.000	1.000 !(singh)
HKO	2	1213.	4.52	0.000	0.000	1.000 !(singh)
KO_2	2	1213.	4.69	0.000	0.000	1.000 !(singh)
HK	1	93.3	3.542	0.000	0.000	1.000 !(singh)
O	0	80.000	2.750	0.000	0.000	0.000
O_2	1	107.400	3.458	0.000	1.600	3.800
OH	1	80.000	2.750	0.000	0.000	0.000
HO_2	2	107.400	3.458	0.000	0.000	1.000 !(*)
N_2	1	97.530	3.621	0.000	1.760	4.000
K_2O	2	1213.0	4.69	0.000	0.000	1.000
K_2O_2	2	1213.0	4.69	0.000	0.000	1.000
K_2CO_3	2	1213.0	4.69	0.000	0.000	1.000
$K_2H_2O_2$	2	1213.0	4.69	0.000	0.000	1.000
KO_3	2	1213.0	4.69	0.000	0.000	1.000
$KHCO_3$	2	1213.0	4.69	0.000	0.000	1.000
KCO_3	2	1213.0	4.69	0.000	0.000	1.000

Appendix:D

a. Premix Laminar Flame Model for H_2/air Mixtures Developed by GRI-Mech Mechanism at 298K

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*****************************************************************
*                    ANSYS Chemkin-Pro 2019 R2                  *
*                       PREMIX Application                      *
*                  PREMIXED LAMINAR FLAME MODEL                 *
*****************************************************************

     KEYWORD INPUT

     !
     ! problem type definition
     !
     ENRG   ! Solve Gas Energy Equation
     FLUX   ! Flux Balance for Inlet Species
     FREE   ! Freely Propagating Flame
     MIX   ! Use Mixture-averaged Transport
     !
     ! physical property
     !
     EQUI 1.0   ! Equivalence Ratio
     FLRT 1.0   ! Mass Flow Rate (g/cm2-sec)
     PRES 1.0   ! Pressure (atm)
     QLOS 0.0   ! Heat Flux Per Unit Length (cal/cm-sec)
     TINF 298.0   ! Ambient Temperature (K)
     TUNBURNT 298.0   ! Unburnt Gas Temperature (K)
     !
     ! reactor dimension definition
     !
     CURV 0.5   ! Adaptive Grid Control Based On Solution Curvature
     GRAD 0.1   ! Adaptive Grid Control Based On Solution Gradient
     NADP 10   ! Number of Adaptive Grid Points
     NPTS 6   ! Number of Uniform Grid Points
     NTOT 250   ! Maximum Number of Grid Points Allowed
     XEND 0.5   ! Ending Axial Position (cm)
     XSTR 0.0   ! Starting Axial Position (cm)
     !
     ! species property
     !
     CPROD H2O   ! Complete-Combustion Products
     CPROD N2   ! Complete-Combustion Products
     FUEL H2 0.295   ! Fuel Fraction of Total Fuel Species (mole fraction)
     MOLE   ! Print Mole Fractions
     OXID N2 0.556   ! Oxidizer Fraction of Total Oxidizer Species (mole fraction)
     OXID O2 0.1479   ! Oxidizer Fraction of Total Oxidizer Species (mole fraction)
     PRMN 0.0   ! Minimum for Product Estimates (mole fraction)
     XIMN 0.0   ! Minimum for Estimated Intermediate Fraction (mole fraction)
     !
     ! solver control
     !
     !USE_ADVANCED_TECHNIQUE   ! Advanced Solution Technique (Default)
     ATIM 1.0E-9   ! Absolute Tolerance for Pseudo Timestepping
     ATOL 1.0E-9   ! Absolute Tolerance
     DTMN 1.0E-10   ! Minimum Pseudo Time Step (sec)
     DTMX 0.01   ! Maximum Pseudo Time Step (sec)
     IRET 25   ! Number Time Steps Before Increasing
     ISTP 0   ! Number of Initial Pseudo Time Steps
     MAXTIME 100   ! Maximum Number of Pseudo Time Stepping Operations Allowed
     NDPR 100   ! Output Frequency during Integration
     NJAC 20   ! Number of Iterations before Updating Jacobian
     RTIM 0.0001   ! Relative Tolerance for Pseudo Timestepping
     RTOL 0.0001   ! Relative Tolerance
     SFLR -0.001   ! Minimum Bounds on Species Fractions
     SPOS 0.0   ! Positive Value to Reset Species Fractions
     SSMAXITER 100   ! Maximum Number of Iterations per Steady State Search
     TIM1 100.0 5.0E-7   ! Pseudo Time Steps (Fixed Temperature) (none, sec)
     TIM2 200.0 1.0E-6   ! Pseudo Time Steps (Energy Equation) (none, sec)
     TJAC 20   ! Number of Transient Iterations before Updating Jacobian
     TPROF   ! Automatic Estimated Temperature Profile
     grid count !   6
     TRMAXITER 25   ! Maximum Number of Iterations per Pseudo Time Step
     WDIF   ! Windward Differencing
     !
     ! output control and other misc. property
     !
     ASEN H2   ! A-factor Sensitivity
     DFAC 2.0   ! Time Step Decrement Factor
     EPSS 0.001   ! Threshold for Species Sensitivity
     FLT_NPOINTS 50   ! Flamelet Grid Points
     GFAC 1.0   ! Gas Reaction Rate Multiplier
```

```
HSEN H2   ! Heat of Formation Sensitivity
PRNT 1   ! Print Level Control
SIZE 100000000   ! Solution Data Block Size (bytes)
UFAC 2.0   ! Time Step Increment Factor
! Number of Continuation 0   ! Continuation Count
END
```

FIRST SOLUTION ESTIMATE IS EQUILIBRIUM

INFO...using default f(Tequilibrium) fixed temperature: 1338.95909350755

TWOPNT: SOLVE THE PROBLEM.

TASK	LOG10 NORM F	LOG10 COND J	REMARK
START	4.31		7 GRID POINTS
SEARCH	-3.07	0.00	22 SEARCH STEPS
REFINE	-3.07		1.00 AND 1.00 RATIOS, 13 GRID POINTS
SEARCH	-4.67	0.00	18 SEARCH STEPS
REFINE	-4.67		1.00 AND 1.00 RATIOS, 21 GRID POINTS
SEARCH	-4.80	0.00	32 SEARCH STEPS
REFINE	-4.80		0.83 AND 1.00 RATIOS, 30 GRID POINTS
SEARCH	-4.91	0.00	18 SEARCH STEPS
REFINE	-4.91		0.72 AND 0.65 RATIOS, 40 GRID POINTS
SEARCH	-3.21	0.00	12 SEARCH STEPS
REFINE	-3.21		0.46 AND 0.79 RATIOS, 50 GRID POINTS
SEARCH	-4.19	0.00	16 SEARCH STEPS
REFINE	-4.19		0.31 AND 0.48 RATIOS, 60 GRID POINTS
SEARCH	-3.32	0.00	9 SEARCH STEPS
REFINE	-3.32		0.23 AND 0.43 RATIOS, 70 GRID POINTS
SEARCH	-3.28	0.00	9 SEARCH STEPS
REFINE	-3.28		0.15 AND 0.27 RATIOS, 76 GRID POINTS
SEARCH	-2.90	0.00	8 SEARCH STEPS
REFINE	-2.90		0.10 AND 0.23 RATIOS, 77 GRID POINTS
SEARCH	-3.15	0.00	7 SEARCH STEPS
REFINE	-3.15		0.10 AND 0.19 RATIOS

TWOPNT: FINAL SOLUTION:

	X(cm)	T(K)	AREA(cm^2)	V(cm/s)	RHO(g/cm^3)	HDOT(cal/s/cm^3)
1	0.0000	2.9800E+002	1.0000E+000	2.3622E+002	8.5513E-004	6.1179E-014
2	0.0500	2.9800E+002	1.0000E+000	2.3622E+002	8.5513E-004	6.2491E-013
3	0.1000	2.9800E+002	1.0000E+000	2.3622E+002	8.5513E-004	1.9803E-011
4	0.1500	2.9800E+002	1.0000E+000	2.3622E+002	8.5513E-004	8.7716E-010
5	0.1750	2.9800E+002	1.0000E+000	2.3622E+002	8.5515E-004	4.2164E-008
6	0.2000	2.9802E+002	1.0000E+000	2.3620E+002	8.5521E-004	3.0771E-006
7	0.2063	2.9806E+002	1.0000E+000	2.3619E+002	8.5525E-004	4.2588E-005
8	0.2125	2.9821E+002	1.0000E+000	2.3620E+002	8.5521E-004	4.0848E-004
9	0.2156	2.9848E+002	1.0000E+000	2.3628E+002	8.5492E-004	1.7828E-003
10	0.2188	2.9918E+002	1.0000E+000	2.3659E+002	8.5382E-004	7.9235E-003
11	0.2219	3.0098E+002	1.0000E+000	2.3755E+002	8.5034E-004	3.8850E-002
12	0.2234	3.0297E+002	1.0000E+000	2.3874E+002	8.4611E-004	1.1114E-001
13	0.2250	3.0652E+002	1.0000E+000	2.4100E+002	8.3817E-004	3.7758E-001
14	0.2266	3.1286E+002	1.0000E+000	2.4522E+002	8.2377E-004	1.5944E+000
15	0.2273	3.1786E+002	1.0000E+000	2.4863E+002	8.1245E-004	4.0861E+000
16	0.2281	3.2473E+002	1.0000E+000	2.5342E+002	7.9712E-004	1.0553E+001
17	0.2285	3.2912E+002	1.0000E+000	2.5650E+002	7.8754E-004	1.7685E+001
18	0.2289	3.3429E+002	1.0000E+000	2.6016E+002	7.7647E-004	2.9217E+001
19	0.2293	3.4036E+002	1.0000E+000	2.6448E+002	7.6378E-004	4.7666E+001
20	0.2297	3.4746E+002	1.0000E+000	2.6955E+002	7.4940E-004	7.6572E+001
21	0.2301	3.5570E+002	1.0000E+000	2.7547E+002	7.3330E-004	1.2065E+002
22	0.2305	3.6520E+002	1.0000E+000	2.8232E+002	7.1551E-004	1.8572E+002
23	0.2309	3.7607E+002	1.0000E+000	2.9017E+002	6.9614E-004	2.7827E+002
24	0.2313	3.8838E+002	1.0000E+000	2.9909E+002	6.7539E-004	4.0450E+002
25	0.2316	4.0218E+002	1.0000E+000	3.0910E+002	6.5352E-004	5.6894E+002
26	0.2320	4.1747E+002	1.0000E+000	3.2020E+002	6.3087E-004	7.7286E+002
27	0.2324	4.3420E+002	1.0000E+000	3.3235E+002	6.0781E-004	1.0132E+003
28	0.2328	4.5230E+002	1.0000E+000	3.4548E+002	5.8470E-004	1.2825E+003
29	0.2332	4.7163E+002	1.0000E+000	3.5950E+002	5.6190E-004	1.5700E+003

30	0.2336	4.9205E+002	1.0000E+000	3.7429E+002	5.3969E-004	1.8634E+003
31	0.2344	5.3559E+002	1.0000E+000	4.0576E+002	4.9783E-004	2.4113E+003
32	0.2352	5.8140E+002	1.0000E+000	4.3871E+002	4.6045E-004	2.8775E+003
33	0.2359	6.2843E+002	1.0000E+000	4.7236E+002	4.2765E-004	3.2393E+003
34	0.2367	6.7591E+002	1.0000E+000	5.0613E+002	3.9911E-004	3.5013E+003
35	0.2375	7.2330E+002	1.0000E+000	5.3963E+002	3.7434E-004	3.6811E+003
36	0.2383	7.7023E+002	1.0000E+000	5.7261E+002	3.5278E-004	3.7990E+003
37	0.2387	7.9343E+002	1.0000E+000	5.8885E+002	3.4305E-004	3.8410E+003
38	0.2391	8.1643E+002	1.0000E+000	6.0491E+002	3.3394E-004	3.8746E+003
39	0.2395	8.3922E+002	1.0000E+000	6.2078E+002	3.2540E-004	3.9014E+003
40	0.2398	8.6177E+002	1.0000E+000	6.3646E+002	3.1738E-004	3.9227E+003
41	0.2406	9.0615E+002	1.0000E+000	6.6723E+002	3.0275E-004	3.9529E+003
42	0.2414	9.4952E+002	1.0000E+000	6.9721E+002	2.8973E-004	3.9693E+003
43	0.2422	9.9179E+002	1.0000E+000	7.2637E+002	2.7810E-004	3.9759E+003
44	0.2430	1.0329E+003	1.0000E+000	7.5470E+002	2.6766E-004	3.9741E+003
45	0.2437	1.0727E+003	1.0000E+000	7.8216E+002	2.5826E-004	3.9637E+003
46	0.2445	1.1113E+003	1.0000E+000	8.0872E+002	2.4978E-004	3.9432E+003
47	0.2453	1.1484E+003	1.0000E+000	8.3434E+002	2.4211E-004	3.9110E+003
48	0.2461	1.1841E+003	1.0000E+000	8.5899E+002	2.3516E-004	3.8651E+003
49	0.2469	1.2182E+003	1.0000E+000	8.8263E+002	2.2887E-004	3.8041E+003
50	0.2477	1.2508E+003	1.0000E+000	9.0521E+002	2.2316E-004	3.7272E+003
51	0.2484	1.2818E+003	1.0000E+000	9.2672E+002	2.1798E-004	3.6347E+003
52	0.2492	1.3112E+003	1.0000E+000	9.4714E+002	2.1328E-004	3.5273E+003
53	0.2500	1.3390E+003	1.0000E+000	9.6645E+002	2.0901E-004	3.4070E+003
54	0.2508	1.3651E+003	1.0000E+000	9.8467E+002	2.0515E-004	3.2759E+003
55	0.2516	1.3898E+003	1.0000E+000	1.0018E+003	2.0164E-004	3.1369E+003
56	0.2531	1.4346E+003	1.0000E+000	1.0329E+003	1.9557E-004	2.8482E+003
57	0.2547	1.4743E+003	1.0000E+000	1.0604E+003	1.9050E-004	2.5568E+003
58	0.2562	1.5094E+003	1.0000E+000	1.0846E+003	1.8624E-004	2.2797E+003
59	0.2578	1.5406E+003	1.0000E+000	1.1060E+003	1.8264E-004	2.0276E+003
60	0.2594	1.5684E+003	1.0000E+000	1.1250E+003	1.7956E-004	1.8050E+003
61	0.2625	1.6154E+003	1.0000E+000	1.1567E+003	1.7464E-004	1.4574E+003
62	0.2656	1.6549E+003	1.0000E+000	1.1830E+003	1.7076E-004	1.2038E+003
63	0.2688	1.6888E+003	1.0000E+000	1.2053E+003	1.6760E-004	1.0194E+003
64	0.2719	1.7184E+003	1.0000E+000	1.2246E+003	1.6495E-004	8.8278E+002
65	0.2750	1.7447E+003	1.0000E+000	1.2416E+003	1.6269E-004	7.7839E+002
66	0.2812	1.7888E+003	1.0000E+000	1.2698E+003	1.5908E-004	6.3247E+002
67	0.2875	1.8261E+003	1.0000E+000	1.2934E+003	1.5618E-004	5.3061E+002
68	0.2938	1.8581E+003	1.0000E+000	1.3136E+003	1.5378E-004	4.5515E+002
69	0.3000	1.8861E+003	1.0000E+000	1.3310E+003	1.5177E-004	3.9712E+002
70	0.3125	1.9314E+003	1.0000E+000	1.3590E+003	1.4864E-004	3.1508E+002
71	0.3250	1.9686E+003	1.0000E+000	1.3817E+003	1.4620E-004	2.5850E+002
72	0.3500	2.0237E+003	1.0000E+000	1.4149E+003	1.4277E-004	1.8834E+002
73	0.3750	2.0662E+003	1.0000E+000	1.4402E+003	1.4026E-004	1.4491E+002
74	0.4000	2.1002E+003	1.0000E+000	1.4605E+003	1.3831E-004	1.1587E+002
75	0.4250	2.1280E+003	1.0000E+000	1.4771E+003	1.3675E-004	9.5693E+001
76	0.4500	2.1498E+003	1.0000E+000	1.4905E+003	1.3552E-004	8.2128E+001
77	0.5000	2.1498E+003	1.0000E+000	1.4905E+003	1.3552E-004	8.2128E+001

b. Premix Laminar Flame Model for H_2/air Mixtures Developed by Reduced Mechanism at 298K

```
*****************************************************************
*                    ANSYS Chemkin-Pro 2019 R2                  *
*                       PREMIX Application                      *
*                  PREMIXED LAMINAR FLAME MODEL                 *
*****************************************************************

     KEYWORD INPUT

     !
     ! problem type definition
     !
     ENRG   ! Solve Gas Energy Equation
     FLUX   ! Flux Balance for Inlet Species
     FREE   ! Freely Propagating Flame
     MIX   ! Use Mixture-averaged Transport
     !
     ! physical property
     !
     EQUI 1.0   ! Equivalence Ratio
     FLRT 1.0   ! Mass Flow Rate (g/cm2-sec)
     PRES 1.0   ! Pressure (atm)
     QLOS 0.0   ! Heat Flux Per Unit Length (cal/cm-sec)
     TINF 298.0   ! Ambient Temperature (K)
     TUNBURNT 298.0   ! Unburnt Gas Temperature (K)
     !
     ! reactor dimension definition
     !
     CURV 0.5   ! Adaptive Grid Control Based On Solution Curvature
     GRAD 0.1   ! Adaptive Grid Control Based On Solution Gradient
     NADP 10   ! Number of Adaptive Grid Points
     NPTS 6   ! Number of Uniform Grid Points
     NTOT 250   ! Maximum Number of Grid Points Allowed
     XEND 0.5   ! Ending Axial Position (cm)
     XSTR 0.0   ! Starting Axial Position (cm)
     !
     ! species property
     !
     CPROD H2O   ! Complete-Combustion Products
     CPROD N2   ! Complete-Combustion Products
     FUEL H2 0.295   ! Fuel Fraction of Total Fuel Species (mole fraction)
     MOLE   ! Print Mole Fractions
     OXID N2 0.556   ! Oxidizer Fraction of Total Oxidizer Species (mole fraction)
     OXID O2 0.1479   ! Oxidizer Fraction of Total Oxidizer Species (mole fraction)
     PRMN 0.0   ! Minimum for Product Estimates (mole fraction)
     XIMN 0.0   ! Minimum for Estimated Intermediate Fraction (mole fraction)
     !
     ! solver control
     !
     !USE_ADVANCED_TECHNIQUE   ! Advanced Solution Technique (Default)
     ATIM 1.0E-9   ! Absolute Tolerance for Pseudo Timestepping
     ATOL 1.0E-9   ! Absolute Tolerance
     DTMN 1.0E-10   ! Minimum Pseudo Time Step (sec)
     DTMX 0.01   ! Maximum Pseudo Time Step (sec)
     IRET 25   ! Number Time Steps Before Increasing
     ISTP 0   ! Number of Initial Pseudo Time Steps
     MAXTIME 100   ! Maximum Number of Pseudo Time Stepping Operations Allowed
     NDPR 100   ! Output Frequency during Integration
     NJAC 20   ! Number of Iterations before Updating Jacobian
     RTIM 0.0001   ! Relative Tolerance for Pseudo Timestepping
     RTOL 0.0001   ! Relative Tolerance
     SFLR -0.001   ! Minimum Bounds on Species Fractions
     SPOS 0.0   ! Positive Value to Reset Species Fractions
     SSMAXITER 100   ! Maximum Number of Iterations per Steady State Search
     TIM1 100.0 1.0E-6   ! Pseudo Time Steps (Fixed Temperature) (none, sec)
     TIM2 100.0 1.0E-6   ! Pseudo Time Steps (Energy Equation) (none, sec)
     TJAC 20   ! Number of Transient Iterations before Updating Jacobian
     TPROF   ! Automatic Estimated Temperature Profile
     A uniform grid with given NPTS grid count! 6
     TRMAXITER 25   ! Maximum Number of Iterations per Pseudo Time Step
     WDIF   ! Windward Differencing
     !
     ! output control and other misc. property
     !
     ASEN H2   ! A-factor Sensitivity
     DFAC 2.0   ! Time Step Decrement Factor
     EPSS 0.001   ! Threshold for Species Sensitivity
     FLT_NPOINTS 50   ! Flamelet Grid Points
     GFAC 1.0   ! Gas Reaction Rate Multiplier
```

```
          HSEN H2   ! Heat of Formation Sensitivity
          PRNT 1   ! Print Level Control
          SIZE 100000000   ! Solution Data Block Size (bytes)
          UFAC 2.0   ! Time Step Increment Factor
          ! Number of Continuation 0   ! Continuation Count
          END
TWOPNT:   SOLVE THE PROBLEM.

                      LOG10    LOG10
             TASK    NORM F   COND J    REMARK

            START      4.31             7 GRID POINTS
           SEARCH     -3.53     0.00    17 SEARCH STEPS

           REFINE     -3.53             1.00 AND 1.00 RATIOS, 13 GRID POINTS
           SEARCH     -0.64     0.00    DIVERGING
           EVOLVE      1.74     0.00    100 TIME STEPS, 8.0E-06 LAST STRIDE
           SEARCH     -3.36     0.00    6 SEARCH STEPS

           REFINE     -3.36             1.00 AND 1.00 RATIOS, 21 GRID POINTS
           SEARCH     -3.78     0.00    14 SEARCH STEPS

           REFINE     -3.78             0.90 AND 1.00 RATIOS, 31 GRID POINTS
           SEARCH      1.43     0.00    DIVERGING
           EVOLVE      0.43     0.00    100 TIME STEPS, 8.0E-06 LAST STRIDE
           SEARCH     -2.73     0.00    4 SEARCH STEPS

           REFINE     -2.73             0.57 AND 0.77 RATIOS, 39 GRID POINTS
           SEARCH     -3.71     0.00    16 SEARCH STEPS

           REFINE     -3.71             0.57 AND 0.67 RATIOS, 49 GRID POINTS
           SEARCH     -3.14     0.00    12 SEARCH STEPS

           REFINE     -3.14             0.32 AND 0.46 RATIOS, 59 GRID POINTS
           SEARCH     -3.65     0.00    11 SEARCH STEPS

           REFINE     -3.65             0.19 AND 0.30 RATIOS, 69 GRID POINTS
           SEARCH     -3.10     0.00    9 SEARCH STEPS

           REFINE     -3.10             0.13 AND 0.26 RATIOS, 74 GRID POINTS
           SEARCH     -2.71     0.00    8 SEARCH STEPS

           REFINE     -2.71             0.10 AND 0.27 RATIOS, 75 GRID POINTS
           SEARCH     -3.08     0.00    6 SEARCH STEPS

           REFINE     -3.08             0.10 AND 0.27 RATIOS

TWOPNT:   FINAL SOLUTION:

      X(cm)    T(K)            AREA(cm^2)      V(cm/s)         RHO(g/cm^3)     HDOT(cal/s/cm^3)
  1   0.0000   2.9800E+002     1.0000E+000     2.3975E+002     8.5513E-004     1.6681E-014
  2   0.0500   2.9800E+002     1.0000E+000     2.3975E+002     8.5513E-004     1.7245E-013
  3   0.1000   2.9800E+002     1.0000E+000     2.3975E+002     8.5513E-004     5.6636E-012
  4   0.1500   2.9800E+002     1.0000E+000     2.3975E+002     8.5513E-004     2.8460E-010
  5   0.1750   2.9800E+002     1.0000E+000     2.3974E+002     8.5514E-004     1.5655E-008
  6   0.1875   2.9800E+002     1.0000E+000     2.3974E+002     8.5516E-004     4.4428E-007
  7   0.2000   2.9803E+002     1.0000E+000     2.3973E+002     8.5520E-004     1.1090E-005
  8   0.2063   2.9811E+002     1.0000E+000     2.3973E+002     8.5519E-004     1.1433E-004
  9   0.2125   2.9846E+002     1.0000E+000     2.3983E+002     8.5482E-004     1.0925E-003
 10   0.2156   2.9905E+002     1.0000E+000     2.4011E+002     8.5384E-004     4.9507E-003
 11   0.2188   3.0060E+002     1.0000E+000     2.4098E+002     8.5077E-004     2.5208E-002
 12   0.2203   3.0231E+002     1.0000E+000     2.4204E+002     8.4702E-004     7.8580E-002
 13   0.2219   3.0542E+002     1.0000E+000     2.4407E+002     8.3997E-004     3.0639E-001
 14   0.2227   3.0789E+002     1.0000E+000     2.4576E+002     8.3420E-004     7.7095E-001
 15   0.2234   3.1135E+002     1.0000E+000     2.4817E+002     8.2612E-004     2.0271E+000
 16   0.2242   3.1616E+002     1.0000E+000     2.5157E+002     8.1495E-004     5.5329E+000
 17   0.2246   3.1926E+002     1.0000E+000     2.5378E+002     8.0784E-004     9.5877E+000
 18   0.2250   3.2293E+002     1.0000E+000     2.5643E+002     7.9948E-004     1.6359E+001
 19   0.2254   3.2728E+002     1.0000E+000     2.5959E+002     7.8975E-004     2.7579E+001
 20   0.2258   3.3241E+002     1.0000E+000     2.6334E+002     7.7851E-004     4.5839E+001
 21   0.2262   3.3843E+002     1.0000E+000     2.6776E+002     7.6566E-004     7.4831E+001
 22   0.2266   3.4545E+002     1.0000E+000     2.7294E+002     7.5115E-004     1.1945E+002
 23   0.2268   3.4938E+002     1.0000E+000     2.7584E+002     7.4324E-004     1.5010E+002
 24   0.2270   3.5360E+002     1.0000E+000     2.7897E+002     7.3490E-004     1.8709E+002
 25   0.2273   3.6299E+002     1.0000E+000     2.8594E+002     7.1699E-004     2.8151E+002
 26   0.2277   3.7365E+002     1.0000E+000     2.9386E+002     6.9765E-004     4.0865E+002
 27   0.2281   3.8560E+002     1.0000E+000     3.0277E+002     6.7713E-004     5.7052E+002
 28   0.2289   4.1333E+002     1.0000E+000     3.2344E+002     6.3385E-004     9.6905E+002
 29   0.2297   4.4541E+002     1.0000E+000     3.4734E+002     5.9024E-004     1.4386E+003
 30   0.2305   4.8101E+002     1.0000E+000     3.7379E+002     5.4847E-004     1.9112E+003
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31	0.2309	4.9979E+002	1.0000E+000	3.8771E+002	5.2879E-004	2.1355E+003
32	0.2313	5.1913E+002	1.0000E+000	4.0200E+002	5.0998E-004	2.3427E+003
33	0.2316	5.3890E+002	1.0000E+000	4.1659E+002	4.9212E-004	2.5302E+003
34	0.2320	5.5900E+002	1.0000E+000	4.3139E+002	4.7524E-004	2.6966E+003
35	0.2328	5.9988E+002	1.0000E+000	4.6137E+002	4.4436E-004	2.9634E+003
36	0.2336	6.4105E+002	1.0000E+000	4.9138E+002	4.1722E-004	3.1522E+003
37	0.2344	6.8211E+002	1.0000E+000	5.2114E+002	3.9340E-004	3.2778E+003
38	0.2352	7.2278E+002	1.0000E+000	5.5045E+002	3.7245E-004	3.3559E+003
39	0.2359	7.6292E+002	1.0000E+000	5.7921E+002	3.5396E-004	3.4008E+003
40	0.2367	8.0242E+002	1.0000E+000	6.0736E+002	3.3755E-004	3.4239E+003
41	0.2375	8.4123E+002	1.0000E+000	6.3491E+002	3.2291E-004	3.4336E+003
42	0.2383	8.7932E+002	1.0000E+000	6.6183E+002	3.0977E-004	3.4355E+003
43	0.2391	9.1666E+002	1.0000E+000	6.8814E+002	2.9792E-004	3.4334E+003
44	0.2398	9.5321E+002	1.0000E+000	7.1385E+002	2.8720E-004	3.4290E+003
45	0.2406	9.8894E+002	1.0000E+000	7.3895E+002	2.7744E-004	3.4230E+003
46	0.2422	1.0578E+003	1.0000E+000	7.8731E+002	2.6040E-004	3.4062E+003
47	0.2437	1.1231E+003	1.0000E+000	8.3315E+002	2.4607E-004	3.3632E+003
48	0.2445	1.1542E+003	1.0000E+000	8.5503E+002	2.3977E-004	3.3264E+003
49	0.2453	1.1842E+003	1.0000E+000	8.7615E+002	2.3399E-004	3.2807E+003
50	0.2461	1.2130E+003	1.0000E+000	8.9648E+002	2.2869E-004	3.2252E+003
51	0.2469	1.2406E+003	1.0000E+000	9.1600E+002	2.2382E-004	3.1593E+003
52	0.2477	1.2671E+003	1.0000E+000	9.3468E+002	2.1934E-004	3.0834E+003
53	0.2484	1.2923E+003	1.0000E+000	9.5250E+002	2.1524E-004	2.9982E+003
54	0.2492	1.3163E+003	1.0000E+000	9.6947E+002	2.1147E-004	2.9050E+003
55	0.2500	1.3391E+003	1.0000E+000	9.8557E+002	2.0802E-004	2.8054E+003
56	0.2516	1.3812E+003	1.0000E+000	1.0152E+003	2.0194E-004	2.5948E+003
57	0.2531	1.4191E+003	1.0000E+000	1.0419E+003	1.9677E-004	2.3766E+003
58	0.2547	1.4533E+003	1.0000E+000	1.0658E+003	1.9236E-004	2.1628E+003
59	0.2562	1.4840E+003	1.0000E+000	1.0871E+003	1.8858E-004	1.9614E+003
60	0.2594	1.5362E+003	1.0000E+000	1.1231E+003	1.8254E-004	1.6203E+003
61	0.2625	1.5800E+003	1.0000E+000	1.1530E+003	1.7782E-004	1.3508E+003
62	0.2688	1.6481E+003	1.0000E+000	1.1985E+003	1.7105E-004	1.0027E+003
63	0.2750	1.7022E+003	1.0000E+000	1.2342E+003	1.6611E-004	7.8707E+002
64	0.2812	1.7468E+003	1.0000E+000	1.2634E+003	1.6228E-004	6.4425E+002
65	0.2875	1.7847E+003	1.0000E+000	1.2878E+003	1.5919E-004	5.4285E+002
66	0.2938	1.8173E+003	1.0000E+000	1.3088E+003	1.5665E-004	4.6700E+002
67	0.3000	1.8458E+003	1.0000E+000	1.3269E+003	1.5450E-004	4.0828E+002
68	0.3125	1.8921E+003	1.0000E+000	1.3560E+003	1.5119E-004	3.2475E+002
69	0.3250	1.9300E+003	1.0000E+000	1.3797E+003	1.4859E-004	2.6684E+002
70	0.3500	1.9864E+003	1.0000E+000	1.4144E+003	1.4495E-004	1.9475E+002
71	0.3750	2.0299E+003	1.0000E+000	1.4409E+003	1.4228E-004	1.5004E+002
72	0.4000	2.0647E+003	1.0000E+000	1.4621E+003	1.4022E-004	1.2017E+002
73	0.4250	2.0933E+003	1.0000E+000	1.4796E+003	1.3856E-004	9.9444E+001
74	0.4500	2.1159E+003	1.0000E+000	1.4937E+003	1.3725E-004	8.5558E+001
75	0.5000	2.1159E+003	1.0000E+000	1.4937E+003	1.3725E-004	8.5558E+001

Appendix:E

a. Premix Laminar Flame Model for H_2/air Mixtures Developed by GRI-Mech Mechanism at 673K

```
KEYWORD INPUT

!
! problem type definition
!
ENRG   ! Solve Gas Energy Equation
FLUX   ! Flux Balance for Inlet Species
FREE   ! Freely Propagating Flame
MIX   ! Use Mixture-averaged Transport
!
! physical property
!
EQUI 1.0   ! Equivalence Ratio
FLRT 1.0   ! Mass Flow Rate (g/cm2-sec)
PRES 1.0   ! Pressure (atm)
QLOS 0.0   ! Heat Flux Per Unit Length (cal/cm-sec)
TINF 298.0   ! Ambient Temperature (K)
TUNBURNT 673.0   ! Unburnt Gas Temperature (K)
!
! reactor dimension definition
!
CURV 0.5   ! Adaptive Grid Control Based On Solution Curvature
GRAD 0.1   ! Adaptive Grid Control Based On Solution Gradient
NADP 10   ! Number of Adaptive Grid Points
NPTS 6   ! Number of Uniform Grid Points
NTOT 250   ! Maximum Number of Grid Points Allowed
XEND 0.5   ! Ending Axial Position (cm)
XSTR 0.0   ! Starting Axial Position (cm)
!
! species property
!
CPROD H2O   ! Complete-Combustion Products
CPROD N2   ! Complete-Combustion Products
FUEL H2 0.295   ! Fuel Fraction of Total Fuel Species (mole fraction)
MOLE   ! Print Mole Fractions
OXID N2 0.556   ! Oxidizer Fraction of Total Oxidizer Species (mole fraction)
OXID O2 0.1479   ! Oxidizer Fraction of Total Oxidizer Species (mole fraction)
PRMN 0.0   ! Minimum for Product Estimates (mole fraction)
XIMN 0.0   ! Minimum for Estimated Intermediate Fraction (mole fraction)
!
TWOPNT:  SOLVE THE PROBLEM.

          LOG10   LOG10
   TASK   NORM F  COND J   REMARK

  START     4.04          7 GRID POINTS
 SEARCH     2.94    0.00   GOING OUT OF BOUNDS
 EVOLVE   -10.40    0.00   200 TIME STEPS, 3.2E-05 LAST STRIDE
 SEARCH   -12.20    0.00   1 SEARCH STEP

 REFINE   -12.20          1.00 AND 1.00 RATIOS, 13 GRID POINTS
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SEARCH  -4.82   0.00  12 SEARCH STEPS

REFINE  -4.82        0.99 AND 1.00 RATIOS, 23 GRID POINTS
SEARCH   3.65   0.00  GOING OUT OF BOUNDS
EVOLVE  -10.04   0.00  200 TIME STEPS, 1.3E-04 LAST STRIDE
SEARCH  -11.97   0.00  1 SEARCH STEP

REFINE  -11.97        0.70 AND 0.96 RATIOS, 33 GRID POINTS
SEARCH   -2.86   0.00  23 SEARCH STEPS

REFINE   -2.86        0.59 AND 0.61 RATIOS, 43 GRID POINTS
SEARCH   -3.63   0.00  19 SEARCH STEPS

REFINE   -3.63        0.28 AND 0.37 RATIOS, 53 GRID POINTS
SEARCH   -2.63   0.00  10 SEARCH STEPS

REFINE   -2.63        0.22 AND 0.38 RATIOS, 63 GRID POINTS
SEARCH   -2.70   0.00  8 SEARCH STEPS

REFINE   -2.70        0.19 AND 0.33 RATIOS, 73 GRID POINTS
SEARCH   -2.85   0.00  8 SEARCH STEPS

REFINE   -2.85        0.19 AND 0.44 RATIOS, 79 GRID POINTS
SEARCH   -2.68   0.00  8 SEARCH STEPS

REFINE   -2.68        0.10 AND 0.43 RATIOS, 81 GRID POINTS
SEARCH   -2.52   0.00  6 SEARCH STEPS

REFINE   -2.52        0.10 AND 0.33 RATIOS

TWOPNT:  FINAL SOLUTION:
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	X(cm)	T(K)	AREA(cm^2)	V(cm/s)	RHO(g/cm^3)	HDOT(cal/s/cm^3)
1	0.0000	6.7300E+002	1.0000E+000	9.4993E+002	3.7865E-004	-4.6080E-011
2	0.0500	6.7300E+002	1.0000E+000	9.4993E+002	3.7865E-004	-5.2986E-012
3	0.0750	6.7300E+002	1.0000E+000	9.4993E+002	3.7865E-004	4.7606E-011
4	0.1000	6.7300E+002	1.0000E+000	9.4993E+002	3.7865E-004	2.4252E-009
5	0.1250	6.7300E+002	1.0000E+000	9.4993E+002	3.7865E-004	1.1492E-007
6	0.1500	6.7300E+002	1.0000E+000	9.4993E+002	3.7865E-004	5.4808E-006
7	0.1625	6.7300E+002	1.0000E+000	9.4993E+002	3.7865E-004	1.0292E-004
8	0.1750	6.7300E+002	1.0000E+000	9.4993E+002	3.7865E-004	1.4918E-003
9	0.1813	6.7301E+002	1.0000E+000	9.4993E+002	3.7865E-004	9.2156E-003
10	0.1875	6.7302E+002	1.0000E+000	9.4993E+002	3.7865E-004	4.9581E-002
11	0.1938	6.7307E+002	1.0000E+000	9.4996E+002	3.7864E-004	2.6671E-001
12	0.1969	6.7315E+002	1.0000E+000	9.5002E+002	3.7861E-004	7.3599E-001
13	0.2000	6.7333E+002	1.0000E+000	9.5016E+002	3.7856E-004	1.9907E+000
14	0.2016	6.7349E+002	1.0000E+000	9.5032E+002	3.7849E-004	3.4211E+000
15	0.2031	6.7376E+002	1.0000E+000	9.5058E+002	3.7839E-004	5.9275E+000
16	0.2047	6.7420E+002	1.0000E+000	9.5103E+002	3.7821E-004	1.0371E+001
17	0.2055	6.7451E+002	1.0000E+000	9.5136E+002	3.7808E-004	1.3858E+001
18	0.2063	6.7491E+002	1.0000E+000	9.5180E+002	3.7791E-004	1.8596E+001
19	0.2070	6.7543E+002	1.0000E+000	9.5238E+002	3.7767E-004	2.5036E+001

20	0.2078	6.7610E+002	1.0000E+000	9.5315E+002	3.7737E-004	3.3773E+001
21	0.2086	6.7696E+002	1.0000E+000	9.5416E+002	3.7697E-004	4.5578E+001
22	0.2094	6.7806E+002	1.0000E+000	9.5546E+002	3.7646E-004	6.1428E+001
23	0.2102	6.7945E+002	1.0000E+000	9.5713E+002	3.7580E-004	8.2514E+001
24	0.2109	6.8120E+002	1.0000E+000	9.5927E+002	3.7496E-004	1.1024E+002
25	0.2117	6.8340E+002	1.0000E+000	9.6197E+002	3.7391E-004	1.4618E+002
26	0.2125	6.8611E+002	1.0000E+000	9.6534E+002	3.7261E-004	1.9202E+002
27	0.2133	6.8944E+002	1.0000E+000	9.6950E+002	3.7100E-004	2.4946E+002
28	0.2141	6.9348E+002	1.0000E+000	9.7460E+002	3.6906E-004	3.2012E+002
29	0.2148	6.9835E+002	1.0000E+000	9.8076E+002	3.6674E-004	4.0545E+002
30	0.2156	7.0414E+002	1.0000E+000	9.8814E+002	3.6401E-004	5.0668E+002
31	0.2164	7.1098E+002	1.0000E+000	9.9687E+002	3.6082E-004	6.2474E+002
32	0.2172	7.1897E+002	1.0000E+000	1.0071E+003	3.5716E-004	7.6024E+002
33	0.2180	7.2820E+002	1.0000E+000	1.0189E+003	3.5301E-004	9.1336E+002
34	0.2188	7.3878E+002	1.0000E+000	1.0325E+003	3.4837E-004	1.0838E+003
35	0.2195	7.5078E+002	1.0000E+000	1.0479E+003	3.4325E-004	1.2705E+003
36	0.2203	7.6428E+002	1.0000E+000	1.0652E+003	3.3767E-004	1.4718E+003
37	0.2219	7.9591E+002	1.0000E+000	1.1058E+003	3.2529E-004	1.9015E+003
38	0.2234	8.3294E+002	1.0000E+000	1.1530E+003	3.1196E-004	2.3538E+003
39	0.2250	8.7501E+002	1.0000E+000	1.2063E+003	2.9818E-004	2.8096E+003
40	0.2258	8.9774E+002	1.0000E+000	1.2349E+003	2.9128E-004	3.0371E+003
41	0.2266	9.2168E+002	1.0000E+000	1.2649E+003	2.8437E-004	3.2618E+003
42	0.2273	9.4673E+002	1.0000E+000	1.2962E+003	2.7750E-004	3.4825E+003
43	0.2281	9.7282E+002	1.0000E+000	1.3287E+003	2.7071E-004	3.6981E+003
44	0.2289	9.9983E+002	1.0000E+000	1.3622E+003	2.6405E-004	3.9075E+003
45	0.2297	1.0277E+003	1.0000E+000	1.3967E+003	2.5753E-004	4.1095E+003
46	0.2305	1.0562E+003	1.0000E+000	1.4320E+003	2.5119E-004	4.3025E+003
47	0.2313	1.0852E+003	1.0000E+000	1.4678E+003	2.4505E-004	4.4842E+003
48	0.2320	1.1146E+003	1.0000E+000	1.5041E+003	2.3913E-004	4.6514E+003
49	0.2328	1.1442E+003	1.0000E+000	1.5407E+003	2.3346E-004	4.8006E+003
50	0.2336	1.1738E+003	1.0000E+000	1.5773E+003	2.2804E-004	4.9276E+003
51	0.2344	1.2033E+003	1.0000E+000	1.6138E+003	2.2289E-004	5.0283E+003
52	0.2352	1.2324E+003	1.0000E+000	1.6498E+003	2.1802E-004	5.0990E+003
53	0.2359	1.2610E+003	1.0000E+000	1.6853E+003	2.1342E-004	5.1368E+003
54	0.2367	1.2890E+003	1.0000E+000	1.7200E+003	2.0912E-004	5.1397E+003
55	0.2375	1.3162E+003	1.0000E+000	1.7538E+003	2.0509E-004	5.1077E+003
56	0.2383	1.3424E+003	1.0000E+000	1.7865E+003	2.0134E-004	5.0419E+003
57	0.2391	1.3677E+003	1.0000E+000	1.8179E+003	1.9786E-004	4.9449E+003
58	0.2398	1.3919E+003	1.0000E+000	1.8480E+003	1.9464E-004	4.8204E+003
59	0.2406	1.4149E+003	1.0000E+000	1.8766E+003	1.9167E-004	4.6732E+003
60	0.2422	1.4575E+003	1.0000E+000	1.9296E+003	1.8641E-004	4.3322E+003
61	0.2430	1.4773E+003	1.0000E+000	1.9542E+003	1.8406E-004	4.1450E+003
62	0.2437	1.4960E+003	1.0000E+000	1.9773E+003	1.8191E-004	3.9546E+003
63	0.2453	1.5302E+003	1.0000E+000	2.0195E+003	1.7811E-004	3.5807E+003
64	0.2469	1.5609E+003	1.0000E+000	2.0572E+003	1.7485E-004	3.2274E+003
65	0.2484	1.5885E+003	1.0000E+000	2.0908E+003	1.7203E-004	2.9073E+003
66	0.2500	1.6134E+003	1.0000E+000	2.1210E+003	1.6959E-004	2.6236E+003
67	0.2562	1.6896E+003	1.0000E+000	2.2114E+003	1.6265E-004	1.9009E+003
68	0.2625	1.7494E+003	1.0000E+000	2.2811E+003	1.5768E-004	1.4760E+003
69	0.2688	1.7987E+003	1.0000E+000	2.3379E+003	1.5385E-004	1.2086E+003
70	0.2750	1.8406E+003	1.0000E+000	2.3857E+003	1.5077E-004	1.0244E+003
71	0.2812	1.8770E+003	1.0000E+000	2.4268E+003	1.4821E-004	8.8858E+002

72	0.2875	1.9091E+003	1.0000E+000	2.4628E+003	1.4605E-004	7.8383E+002
73	0.3000	1.9616E+003	1.0000E+000	2.5210E+003	1.4268E-004	6.3518E+002
74	0.3125	2.0056E+003	1.0000E+000	2.5692E+003	1.4000E-004	5.3094E+002
75	0.3250	2.0431E+003	1.0000E+000	2.6100E+003	1.3781E-004	4.5410E+002
76	0.3500	2.1017E+003	1.0000E+000	2.6729E+003	1.3457E-004	3.5191E+002
77	0.3750	2.1489E+003	1.0000E+000	2.7232E+003	1.3209E-004	2.8410E+002
78	0.4000	2.1882E+003	1.0000E+000	2.7646E+003	1.3011E-004	2.3608E+002
79	0.4250	2.2214E+003	1.0000E+000	2.7997E+003	1.2847E-004	2.0080E+002
80	0.4500	2.2487E+003	1.0000E+000	2.8292E+003	1.2714E-004	1.7539E+002
81	0.5000	2.2487E+003	1.0000E+000	2.8292E+003	1.2714E-004	1.7539E+002

b. Premix Laminar Flame Model for H_2/air Mixtures Developed by Reduced Mechanism at 673K

```
KEYWORD INPUT

!
! problem type definition
!
ENRG   ! Solve Gas Energy Equation
FLUX   ! Flux Balance for Inlet Species
FREE   ! Freely Propagating Flame
MIX   ! Use Mixture-averaged Transport
!
! physical property
!
EQUI 1.0   ! Equivalence Ratio
FLRT 1.0   ! Mass Flow Rate (g/cm2-sec)
PRES 1.0   ! Pressure (atm)
QLOS 0.0   ! Heat Flux Per Unit Length (cal/cm-sec)
TINF 298.0   ! Ambient Temperature (K)
TUNBURNT 673.0   ! Unburnt Gas Temperature (K)
!
! reactor dimension definition
!
CURV 0.5   ! Adaptive Grid Control Based On Solution Curvature
GRAD 0.1   ! Adaptive Grid Control Based On Solution Gradient
NADP 10   ! Number of Adaptive Grid Points
NPTS 6   ! Number of Uniform Grid Points
NTOT 250   ! Maximum Number of Grid Points Allowed
XEND 0.5   ! Ending Axial Position (cm)
XSTR 0.0   ! Starting Axial Position (cm)
!
! species property
!
CPROD H2O   ! Complete-Combustion Products
CPROD N2   ! Complete-Combustion Products
FUEL H2 0.295   ! Fuel Fraction of Total Fuel Species (mole fraction)
MOLE   ! Print Mole Fractions
OXID N2 0.556   ! Oxidizer Fraction of Total Oxidizer Species (mole fraction)
OXID O2 0.1479   ! Oxidizer Fraction of Total Oxidizer Species (mole fraction)
PRMN 0.0   ! Minimum for Product Estimates (mole fraction)
XIMN 0.0   ! Minimum for Estimated Intermediate Fraction (mole fraction)


TWOPNT:  SOLVE THE PROBLEM.

LOG10  LOG10
TASK   NORM F  COND J   REMARK

START    4.05          7 GRID POINTS
SEARCH    2.84    0.00   GOING OUT OF BOUNDS
EVOLVE    1.62    0.00   100 TIME STEPS, 2.0E-06 LAST STRIDE
SEARCH   -4.24    0.00   4 SEARCH STEPS
```

```
REFINE   -4.24        1.00 AND 1.00 RATIOS, 13 GRID POINTS
SEARCH   -3.49   0.00  13 SEARCH STEPS

REFINE   -3.49        0.88 AND 1.00 RATIOS, 23 GRID POINTS
SEARCH   -2.36   0.00  17 SEARCH STEPS

REFINE   -2.36        0.90 AND 0.73 RATIOS, 32 GRID POINTS
SEARCH   -3.89   0.00  34 SEARCH STEPS

REFINE   -3.89        0.51 AND 0.67 RATIOS, 42 GRID POINTS
SEARCH   -3.91   0.00  19 SEARCH STEPS

REFINE   -3.91        0.37 AND 0.41 RATIOS, 52 GRID POINTS
SEARCH   -2.38   0.00  11 SEARCH STEPS

REFINE   -2.38        0.47 AND 0.42 RATIOS, 62 GRID POINTS
SEARCH   -2.80   0.00  10 SEARCH STEPS

REFINE   -2.80        0.40 AND 0.42 RATIOS, 72 GRID POINTS
SEARCH   -2.52   0.00  8 SEARCH STEPS

REFINE   -2.52        0.23 AND 0.42 RATIOS, 79 GRID POINTS
SEARCH   -2.67   0.00  8 SEARCH STEPS

REFINE   -2.67        0.13 AND 0.42 RATIOS, 85 GRID POINTS
SEARCH   -2.34   0.00  6 SEARCH STEPS

REFINE   -2.34        0.11 AND 0.42 RATIOS, 86 GRID POINTS
SEARCH   -2.45   0.00  6 SEARCH STEPS

REFINE   -2.45        0.10 AND 0.42 RATIOS

TWOPNT:  FINAL SOLUTION:
```

	X(cm)	T(K)	AREA(cm^2)	V(cm/s)	RHO(g/cm^3)	HDOT(cal/s/cm^3)
1	0.0000	6.7300E+002	1.0000E+000	9.7240E+002	3.7865E-004	-3.2568E-011
2	0.0500	6.7300E+002	1.0000E+000	9.7240E+002	3.7865E-004	1.0877E-011
3	0.0750	6.7300E+002	1.0000E+000	9.7240E+002	3.7865E-004	6.9031E-010
4	0.1000	6.7300E+002	1.0000E+000	9.7240E+002	3.7865E-004	2.2730E-008
5	0.1125	6.7300E+002	1.0000E+000	9.7240E+002	3.7865E-004	2.9732E-007
6	0.1250	6.7300E+002	1.0000E+000	9.7240E+002	3.7865E-004	3.1558E-006
7	0.1375	6.7300E+002	1.0000E+000	9.7240E+002	3.7865E-004	3.3337E-005
8	0.1500	6.7300E+002	1.0000E+000	9.7240E+002	3.7865E-004	3.5237E-004
9	0.1625	6.7300E+002	1.0000E+000	9.7240E+002	3.7865E-004	3.7317E-003
10	0.1750	6.7301E+002	1.0000E+000	9.7241E+002	3.7864E-004	3.9807E-002
11	0.1781	6.7302E+002	1.0000E+000	9.7241E+002	3.7864E-004	1.0343E-001
12	0.1813	6.7304E+002	1.0000E+000	9.7243E+002	3.7864E-004	2.4675E-001
13	0.1844	6.7307E+002	1.0000E+000	9.7246E+002	3.7862E-004	5.8050E-001
14	0.1859	6.7311E+002	1.0000E+000	9.7249E+002	3.7861E-004	9.1636E-001
15	0.1875	6.7316E+002	1.0000E+000	9.7255E+002	3.7859E-004	1.4592E+000
16	0.1891	6.7325E+002	1.0000E+000	9.7263E+002	3.7856E-004	2.3455E+000
17	0.1906	6.7338E+002	1.0000E+000	9.7277E+002	3.7850E-004	3.8081E+000

18	0.1922	6.7358E+002	1.0000E+000	9.7299E+002	3.7842E-004	6.2390E+000
19	0.1930	6.7372E+002	1.0000E+000	9.7315E+002	3.7836E-004	8.0403E+000
20	0.1938	6.7389E+002	1.0000E+000	9.7335E+002	3.7828E-004	1.0400E+001
21	0.1945	6.7412E+002	1.0000E+000	9.7362E+002	3.7817E-004	1.3485E+001
22	0.1953	6.7441E+002	1.0000E+000	9.7396E+002	3.7804E-004	1.7509E+001
23	0.1961	6.7478E+002	1.0000E+000	9.7440E+002	3.7787E-004	2.2734E+001
24	0.1969	6.7524E+002	1.0000E+000	9.7497E+002	3.7765E-004	2.9476E+001
25	0.1977	6.7582E+002	1.0000E+000	9.7569E+002	3.7737E-004	3.8105E+001
26	0.1984	6.7655E+002	1.0000E+000	9.7661E+002	3.7702E-004	4.9041E+001
27	0.1992	6.7747E+002	1.0000E+000	9.7777E+002	3.7657E-004	6.2746E+001
28	0.2000	6.7861E+002	1.0000E+000	9.7922E+002	3.7601E-004	7.9708E+001
29	0.2016	6.8171E+002	1.0000E+000	9.8324E+002	3.7447E-004	1.2479E+002
30	0.2031	6.8613E+002	1.0000E+000	9.8905E+002	3.7228E-004	1.8777E+002
31	0.2063	7.0029E+002	1.0000E+000	1.0078E+003	3.6534E-004	3.7384E+002
32	0.2094	7.2259E+002	1.0000E+000	1.0376E+003	3.5487E-004	6.6419E+002
33	0.2109	7.3737E+002	1.0000E+000	1.0572E+003	3.4827E-004	8.6368E+002
34	0.2125	7.5545E+002	1.0000E+000	1.0812E+003	3.4054E-004	1.1002E+003
35	0.2141	7.7705E+002	1.0000E+000	1.1099E+003	3.3175E-004	1.3701E+003
36	0.2156	8.0225E+002	1.0000E+000	1.1432E+003	3.2209E-004	1.6669E+003
37	0.2164	8.1618E+002	1.0000E+000	1.1615E+003	3.1701E-004	1.8244E+003
38	0.2172	8.3111E+002	1.0000E+000	1.1811E+003	3.1175E-004	1.9863E+003
39	0.2180	8.4704E+002	1.0000E+000	1.2019E+003	3.0635E-004	2.1512E+003
40	0.2188	8.6395E+002	1.0000E+000	1.2239E+003	3.0083E-004	2.3178E+003
41	0.2195	8.8183E+002	1.0000E+000	1.2471E+003	2.9523E-004	2.4850E+003
42	0.2203	9.0063E+002	1.0000E+000	1.2715E+003	2.8958E-004	2.6517E+003
43	0.2211	9.2033E+002	1.0000E+000	1.2969E+003	2.8390E-004	2.8172E+003
44	0.2219	9.4088E+002	1.0000E+000	1.3234E+003	2.7823E-004	2.9807E+003
45	0.2227	9.6223E+002	1.0000E+000	1.3508E+003	2.7258E-004	3.1415E+003
46	0.2234	9.8432E+002	1.0000E+000	1.3790E+003	2.6700E-004	3.2989E+003
47	0.2242	1.0071E+003	1.0000E+000	1.4081E+003	2.6149E-004	3.4520E+003
48	0.2250	1.0304E+003	1.0000E+000	1.4378E+003	2.5608E-004	3.5998E+003
49	0.2258	1.0543E+003	1.0000E+000	1.4682E+003	2.5078E-004	3.7409E+003
50	0.2266	1.0785E+003	1.0000E+000	1.4990E+003	2.4563E-004	3.8737E+003
51	0.2273	1.1031E+003	1.0000E+000	1.5302E+003	2.4062E-004	3.9959E+003
52	0.2281	1.1278E+003	1.0000E+000	1.5616E+003	2.3578E-004	4.1054E+003
53	0.2289	1.1526E+003	1.0000E+000	1.5931E+003	2.3112E-004	4.1996E+003
54	0.2297	1.1773E+003	1.0000E+000	1.6246E+003	2.2665E-004	4.2763E+003
55	0.2313	1.2263E+003	1.0000E+000	1.6869E+003	2.1827E-004	4.3718E+003
56	0.2320	1.2503E+003	1.0000E+000	1.7173E+003	2.1440E-004	4.3829E+003
57	0.2328	1.2737E+003	1.0000E+000	1.7472E+003	2.1073E-004	4.3715E+003
58	0.2336	1.2966E+003	1.0000E+000	1.7764E+003	2.0728E-004	4.3377E+003
59	0.2344	1.3188E+003	1.0000E+000	1.8047E+003	2.0402E-004	4.2826E+003
60	0.2352	1.3404E+003	1.0000E+000	1.8321E+003	2.0097E-004	4.2078E+003
61	0.2359	1.3612E+003	1.0000E+000	1.8586E+003	1.9810E-004	4.1157E+003
62	0.2367	1.3812E+003	1.0000E+000	1.8841E+003	1.9542E-004	4.0090E+003
63	0.2375	1.4004E+003	1.0000E+000	1.9085E+003	1.9292E-004	3.8907E+003
64	0.2383	1.4187E+003	1.0000E+000	1.9319E+003	1.9059E-004	3.7635E+003
65	0.2391	1.4363E+003	1.0000E+000	1.9542E+003	1.8841E-004	3.6305E+003
66	0.2398	1.4531E+003	1.0000E+000	1.9755E+003	1.8638E-004	3.4943E+003
67	0.2406	1.4691E+003	1.0000E+000	1.9957E+003	1.8449E-004	3.3573E+003
68	0.2422	1.4988E+003	1.0000E+000	2.0332E+003	1.8110E-004	3.0894E+003
69	0.2437	1.5260E+003	1.0000E+000	2.0672E+003	1.7811E-004	2.8359E+003

70	0.2453	1.5509E+003	1.0000E+000	2.0982E+003	1.7548E-004	2.6034E+003
71	0.2469	1.5736E+003	1.0000E+000	2.1265E+003	1.7315E-004	2.3947E+003
72	0.2500	1.6135E+003	1.0000E+000	2.1754E+003	1.6926E-004	2.0541E+003
73	0.2562	1.6774E+003	1.0000E+000	2.2525E+003	1.6346E-004	1.6015E+003
74	0.2625	1.7298E+003	1.0000E+000	2.3150E+003	1.5905E-004	1.3078E+003
75	0.2688	1.7742E+003	1.0000E+000	2.3674E+003	1.5553E-004	1.1050E+003
76	0.2750	1.8125E+003	1.0000E+000	2.4122E+003	1.5264E-004	9.5622E+002
77	0.2875	1.8738E+003	1.0000E+000	2.4830E+003	1.4829E-004	7.5557E+002
78	0.3000	1.9242E+003	1.0000E+000	2.5405E+003	1.4493E-004	6.2012E+002
79	0.3125	1.9667E+003	1.0000E+000	2.5885E+003	1.4224E-004	5.2270E+002
80	0.3250	2.0031E+003	1.0000E+000	2.6294E+003	1.4003E-004	4.4972E+002
81	0.3500	2.0604E+003	1.0000E+000	2.6928E+003	1.3674E-004	3.5109E+002
82	0.3750	2.1068E+003	1.0000E+000	2.7436E+003	1.3420E-004	2.8482E+002
83	0.4000	2.1455E+003	1.0000E+000	2.7858E+003	1.3217E-004	2.3755E+002
84	0.4250	2.1784E+003	1.0000E+000	2.8216E+003	1.3049E-004	2.0267E+002
85	0.4500	2.2055E+003	1.0000E+000	2.8517E+003	1.2911E-004	1.7751E+002
86	0.5000	2.2055E+003	1.0000E+000	2.8517E+003	1.2911E-004	1.7751E+002

Appendix:F

Premix Laminar Flame Model for H_2/air Mixtures Developed by GRI-Mech at 298K and different equivalence ratio (0.6, 1, 1.3)

```
KEYWORD INPUT

!
! problem type definition
!
ENRG   ! Solve Gas Energy Equation
FLUX   ! Flux Balance for Inlet Species
FREE   ! Freely Propagating Flame
MIX   ! Use Mixture-averaged Transport
!
! physical property
!
EQUI 0.6   ! Equivalence Ratio
FLRT 1.0   ! Mass Flow Rate (g/cm2-sec)
PRES 1.0   ! Pressure (atm)
QLOS 0.0   ! Heat Flux Per Unit Length (cal/cm-sec)
TINF 298.0   ! Ambient Temperature (K)
TUNBURNT 298.0   ! Unburnt Gas Temperature (K)
!
! reactor dimension definition
!
CURV 0.5   ! Adaptive Grid Control Based On Solution Curvature
GRAD 0.1   ! Adaptive Grid Control Based On Solution Gradient
NADP 10   ! Number of Adaptive Grid Points
NPTS 6   ! Number of Uniform Grid Points
NTOT 250   ! Maximum Number of Grid Points Allowed
XEND 0.5   ! Ending Axial Position (cm)
XSTR 0.0   ! Starting Axial Position (cm)
!
! species property
!
CPROD H2O   ! Complete-Combustion Products
CPROD N2   ! Complete-Combustion Products
FUEL H2 0.295   ! Fuel Fraction of Total Fuel Species (mole fraction)
MOLE   ! Print Mole Fractions
OXID N2 0.556   ! Oxidizer Fraction of Total Oxidizer Species (mole fraction)
OXID O2 0.1479   ! Oxidizer Fraction of Total Oxidizer Species (mole fraction)
PRMN 0.0   ! Minimum for Product Estimates (mole fraction)
XIMN 0.0   ! Minimum for Estimated Intermediate Fraction (mole fraction)
!
! solver control
!
!USE_ADVANCED_TECHNIQUE   ! Advanced Solution Technique (Default)
ATIM 1.0E-9   ! Absolute Tolerance for Pseudo Timestepping
ATOL 1.0E-9   ! Absolute Tolerance
DTMN 1.0E-10   ! Minimum Pseudo Time Step (sec)
DTMX 0.01   ! Maximum Pseudo Time Step (sec)
IRET 25   ! Number Time Steps Before Increasing
ISTP 0   ! Number of Initial Pseudo Time Steps
MAXTIME 100   ! Maximum Number of Pseudo Time Stepping Operations Allowed
NDPR 100   ! Output Frequency during Integration
NJAC 20   ! Number of Iterations before Updating Jacobian
RTIM 0.0001   ! Relative Tolerance for Pseudo Timestepping
RTOL 0.0001   ! Relative Tolerance
SFLR -0.001   ! Minimum Bounds on Species Fractions
SPOS 0.0   ! Positive Value to Reset Species Fractions
SSMAXITER 100   ! Maximum Number of Iterations per Steady State Search
TIM1 100.0 5.0E-7   ! Pseudo Time Steps (Fixed Temperature) (none, sec)
TIM2 200.0 1.0E-6   ! Pseudo Time Steps (Energy Equation) (none, sec)
TJAC 20   ! Number of Transient Iterations before Updating Jacobian
TPROF   ! Automatic Estimated Temperature Profile
TRMAXITER 25   ! Maximum Number of Iterations per Pseudo Time Step
WDIF   ! Windward Differencing
!
! output control and other misc. property
!
ASEN H2   ! A-factor Sensitivity
DFAC 2.0   ! Time Step Decrement Factor
EPSS 0.001   ! Threshold for Species Sensitivity
FLT_NPOINTS 50   ! Flamelet Grid Points
```

```
          GFAC 1.0   ! Gas Reaction Rate Multiplier
          HSEN H2   ! Heat of Formation Sensitivity
          PRNT 1   ! Print Level Control
          SIZE 100000000   ! Solution Data Block Size (bytes)
          UFAC 2.0   ! Time Step Increment Factor
          ! Number of Continuation 0   ! Continuation Coun

TWOPNT:  SOLVE THE PROBLEM.

                    LOG10   LOG10
             TASK   NORM F  COND J   REMARK

              START     4.07          7 GRID POINTS
             SEARCH    -4.01    0.00   24 SEARCH STEPS

             REFINE    -4.01          0.99 AND 1.00 RATIOS, 12 GRID POINTS
             SEARCH    -5.19    0.00   23 SEARCH STEPS

             REFINE    -5.19          0.98 AND 1.00 RATIOS, 20 GRID POINTS
             SEARCH    -5.13    0.00   17 SEARCH STEPS

             REFINE    -5.13          0.80 AND 1.00 RATIOS, 30 GRID POINTS
             SEARCH    -3.22    0.00   12 SEARCH STEPS

             REFINE    -3.22          0.63 AND 1.00 RATIOS, 40 GRID POINTS
             SEARCH    -3.87    0.00   11 SEARCH STEPS

             REFINE    -3.87          0.44 AND 0.53 RATIOS, 50 GRID POINTS
             SEARCH    -3.29    0.00   8 SEARCH STEPS

             REFINE    -3.29          0.23 AND 0.32 RATIOS, 60 GRID POINTS
             SEARCH    -2.96    0.00   7 SEARCH STEPS

             REFINE    -2.96          0.20 AND 0.25 RATIOS, 70 GRID POINTS
             SEARCH    -3.02    0.00   5 SEARCH STEPS

             REFINE    -3.02          0.15 AND 0.17 RATIOS, 76 GRID POINTS
             SEARCH    -2.93    0.00   4 SEARCH STEPS

             REFINE    -2.93          0.10 AND 0.17 RATIOS

TWOPNT:  FINAL SOLUTION:

      X(cm)    T(K)            AREA(cm^2)      V(cm/s)         RHO(g/cm^3)     HDOT(cal/s/cm^3)
  1   0.0000  2.9800E+002     1.0000E+000     7.2904E+001     9.5889E-004     7.5391E-010
  2   0.1000  2.9801E+002     1.0000E+000     7.2886E+001     9.5913E-004     5.3916E-009
  3   0.1500  2.9810E+002     1.0000E+000     7.2828E+001     9.5989E-004     7.2557E-008
  4   0.1750  2.9844E+002     1.0000E+000     7.2744E+001     9.6100E-004     1.3316E-006
  5   0.2000  3.0048E+002     1.0000E+000     7.2702E+001     9.6156E-004     6.0291E-005
  6   0.2063  3.0255E+002     1.0000E+000     7.2888E+001     9.5911E-004     3.1637E-004
  7   0.2125  3.0716E+002     1.0000E+000     7.3514E+001     9.5094E-004     1.9202E-003
  8   0.2156  3.1158E+002     1.0000E+000     7.4238E+001     9.4167E-004     5.6158E-003
  9   0.2188  3.1867E+002     1.0000E+000     7.5511E+001     9.2579E-004     1.7584E-002
 10   0.2219  3.3000E+002     1.0000E+000     7.7680E+001     8.9995E-004     5.8396E-002
 11   0.2234  3.3816E+002     1.0000E+000     7.9302E+001     8.8154E-004     1.1675E-001
 12   0.2250  3.4866E+002     1.0000E+000     8.1431E+001     8.5848E-004     2.4504E-001
 13   0.2258  3.5500E+002     1.0000E+000     8.2738E+001     8.4492E-004     3.7615E-001
 14   0.2266  3.6222E+002     1.0000E+000     8.4235E+001     8.2990E-004     5.9209E-001
 15   0.2273  3.7040E+002     1.0000E+000     8.5946E+001     8.1339E-004     9.6070E-001
 16   0.2281  3.7965E+002     1.0000E+000     8.7892E+001     7.9538E-004     1.6038E+000
 17   0.2289  3.9008E+002     1.0000E+000     9.0098E+001     7.7590E-004     2.7345E+000
 18   0.2297  4.0179E+002     1.0000E+000     9.2588E+001     7.5504E-004     4.7109E+000
 19   0.2305  4.1488E+002     1.0000E+000     9.5384E+001     7.3290E-004     8.1008E+000
 20   0.2313  4.2947E+002     1.0000E+000     9.8509E+001     7.0965E-004     1.3748E+001
 21   0.2320  4.4563E+002     1.0000E+000     1.0198E+002     6.8550E-004     2.2811E+001
 22   0.2328  4.6342E+002     1.0000E+000     1.0581E+002     6.6067E-004     3.6735E+001
 23   0.2336  4.8288E+002     1.0000E+000     1.1001E+002     6.3545E-004     5.7105E+001
 24   0.2344  5.0401E+002     1.0000E+000     1.1458E+002     6.1012E-004     8.5366E+001
 25   0.2352  5.2676E+002     1.0000E+000     1.1950E+002     5.8498E-004     1.2244E+002
 26   0.2359  5.5106E+002     1.0000E+000     1.2476E+002     5.6032E-004     1.6837E+002
 27   0.2363  5.6374E+002     1.0000E+000     1.2751E+002     5.4824E-004     1.9469E+002
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28	0.2367	5.7676E+002	1.0000E+000	1.3033E+002	5.3637E-004	2.2277E+002
29	0.2371	5.9010E+002	1.0000E+000	1.3322E+002	5.2473E-004	2.5232E+002
30	0.2375	6.0374E+002	1.0000E+000	1.3618E+002	5.1334E-004	2.8305E+002
31	0.2379	6.1764E+002	1.0000E+000	1.3919E+002	5.0223E-004	3.1462E+002
32	0.2383	6.3179E+002	1.0000E+000	1.4226E+002	4.9140E-004	3.4670E+002
33	0.2391	6.6072E+002	1.0000E+000	1.4853E+002	4.7065E-004	4.1069E+002
34	0.2398	6.9030E+002	1.0000E+000	1.5495E+002	4.5117E-004	4.7323E+002
35	0.2406	7.2034E+002	1.0000E+000	1.6145E+002	4.3299E-004	5.3264E+002
36	0.2414	7.5064E+002	1.0000E+000	1.6802E+002	4.1607E-004	5.8782E+002
37	0.2422	7.8106E+002	1.0000E+000	1.7461E+002	4.0037E-004	6.3816E+002
38	0.2430	8.1145E+002	1.0000E+000	1.8119E+002	3.8583E-004	6.8347E+002
39	0.2437	8.4167E+002	1.0000E+000	1.8773E+002	3.7238E-004	7.2378E+002
40	0.2445	8.7163E+002	1.0000E+000	1.9422E+002	3.5993E-004	7.5928E+002
41	0.2453	9.0122E+002	1.0000E+000	2.0063E+002	3.4843E-004	7.9023E+002
42	0.2461	9.3037E+002	1.0000E+000	2.0695E+002	3.3780E-004	8.1692E+002
43	0.2469	9.5899E+002	1.0000E+000	2.1316E+002	3.2796E-004	8.3961E+002
44	0.2484	1.0145E+003	1.0000E+000	2.2522E+002	3.1040E-004	8.7398E+002
45	0.2500	1.0673E+003	1.0000E+000	2.3672E+002	2.9532E-004	8.9372E+002
46	0.2516	1.1172E+003	1.0000E+000	2.4760E+002	2.8234E-004	8.9974E+002
47	0.2531	1.1640E+003	1.0000E+000	2.5782E+002	2.7114E-004	8.9280E+002
48	0.2547	1.2074E+003	1.0000E+000	2.6736E+002	2.6147E-004	8.7391E+002
49	0.2562	1.2476E+003	1.0000E+000	2.7620E+002	2.5310E-004	8.4452E+002
50	0.2578	1.2846E+003	1.0000E+000	2.8435E+002	2.4585E-004	8.0655E+002
51	0.2594	1.3185E+003	1.0000E+000	2.9182E+002	2.3955E-004	7.6224E+002
52	0.2609	1.3495E+003	1.0000E+000	2.9865E+002	2.3408E-004	7.1390E+002
53	0.2625	1.3777E+003	1.0000E+000	3.0488E+002	2.2930E-004	6.6369E+002
54	0.2641	1.4034E+003	1.0000E+000	3.1054E+002	2.2512E-004	6.1342E+002
55	0.2656	1.4268E+003	1.0000E+000	3.1568E+002	2.2145E-004	5.6446E+002
56	0.2688	1.4673E+003	1.0000E+000	3.2454E+002	2.1540E-004	4.7526E+002
57	0.2719	1.5013E+003	1.0000E+000	3.3195E+002	2.1059E-004	3.9887E+002
58	0.2750	1.5302E+003	1.0000E+000	3.3819E+002	2.0671E-004	3.3573E+002
59	0.2781	1.5548E+003	1.0000E+000	3.4348E+002	2.0353E-004	2.8435E+002
60	0.2812	1.5760E+003	1.0000E+000	3.4801E+002	2.0088E-004	2.4267E+002
61	0.2844	1.5944E+003	1.0000E+000	3.5191E+002	1.9865E-004	2.0873E+002
62	0.2875	1.6104E+003	1.0000E+000	3.5531E+002	1.9675E-004	1.8092E+002
63	0.2906	1.6245E+003	1.0000E+000	3.5828E+002	1.9512E-004	1.5795E+002
64	0.2938	1.6369E+003	1.0000E+000	3.6088E+002	1.9371E-004	1.3883E+002
65	0.3000	1.6575E+003	1.0000E+000	3.6517E+002	1.9144E-004	1.0924E+002
66	0.3063	1.6742E+003	1.0000E+000	3.6863E+002	1.8964E-004	8.7571E+001
67	0.3125	1.6879E+003	1.0000E+000	3.7146E+002	1.8820E-004	7.1281E+001
68	0.3188	1.6993E+003	1.0000E+000	3.7380E+002	1.8702E-004	5.8784E+001
69	0.3250	1.7088E+003	1.0000E+000	3.7574E+002	1.8605E-004	4.9069E+001
70	0.3375	1.7232E+003	1.0000E+000	3.7868E+002	1.8461E-004	3.5340E+001
71	0.3500	1.7339E+003	1.0000E+000	3.8086E+002	1.8355E-004	2.6240E+001
72	0.3750	1.7477E+003	1.0000E+000	3.8361E+002	1.8223E-004	1.5860E+001
73	0.4000	1.7566E+003	1.0000E+000	3.8541E+002	1.8138E-004	1.0259E+001
74	0.4250	1.7628E+003	1.0000E+000	3.8665E+002	1.8080E-004	7.0795E+000
75	0.4500	1.7668E+003	1.0000E+000	3.8747E+002	1.8042E-004	5.3442E+000
76	0.5000	1.7668E+003	1.0000E+000	3.8747E+002	1.8042E-004	5.3442E+000

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KEYWORD INPUT

!
! problem type definition
!
ENRG   ! Solve Gas Energy Equation
FLUX   ! Flux Balance for Inlet Species
FREE   ! Freely Propagating Flame
MIX   ! Use Mixture-averaged Transport
!
! physical property
!
EQUI 1.0   ! Equivalence Ratio
FLRT 1.0   ! Mass Flow Rate (g/cm2-sec)
PRES 1.0   ! Pressure (atm)
QLOS 0.0   ! Heat Flux Per Unit Length (cal/cm-sec)
TINF 298.0   ! Ambient Temperature (K)
TUNBURNT 298.0   ! Unburnt Gas Temperature (K)
!
! reactor dimension definition
!
CURV 0.5   ! Adaptive Grid Control Based On Solution Curvature
GRAD 0.1   ! Adaptive Grid Control Based On Solution Gradient
NADP 10   ! Number of Adaptive Grid Points
NPTS 6   ! Number of Uniform Grid Points
NTOT 250   ! Maximum Number of Grid Points Allowed
XEND 0.5   ! Ending Axial Position (cm)
XSTR 0.0   ! Starting Axial Position (cm)
!
! species property
!
CPROD H2O   ! Complete-Combustion Products
CPROD N2   ! Complete-Combustion Products
FUEL H2 0.295   ! Fuel Fraction of Total Fuel Species (mole fraction)
MOLE   ! Print Mole Fractions
OXID N2 0.556   ! Oxidizer Fraction of Total Oxidizer Species (mole fraction)
OXID O2 0.1479   ! Oxidizer Fraction of Total Oxidizer Species (mole fraction)
PRMN 0.0   ! Minimum for Product Estimates (mole fraction)
XIMN 0.0   ! Minimum for Estimated Intermediate Fraction (mole fraction)
!
! solver control
!
!USE_ADVANCED_TECHNIQUE   ! Advanced Solution Technique (Default)
ATIM 1.0E-9   ! Absolute Tolerance for Pseudo Timestepping
ATOL 1.0E-9   ! Absolute Tolerance
DTMN 1.0E-10   ! Minimum Pseudo Time Step (sec)
DTMX 0.01   ! Maximum Pseudo Time Step (sec)
IRET 25   ! Number Time Steps Before Increasing
ISTP 0   ! Number of Initial Pseudo Time Steps
MAXTIME 100   ! Maximum Number of Pseudo Time Stepping Operations Allowed
NDPR 100   ! Output Frequency during Integration
NJAC 20   ! Number of Iterations before Updating Jacobian
RTIM 0.0001   ! Relative Tolerance for Pseudo Timestepping
RTOL 0.0001   ! Relative Tolerance
SFLR -0.001   ! Minimum Bounds on Species Fractions
SPOS 0.0   ! Positive Value to Reset Species Fractions
SSMAXITER 100   ! Maximum Number of Iterations per Steady State Search
TIM1 100.0 5.0E-7   ! Pseudo Time Steps (Fixed Temperature) (none, sec)
TIM2 200.0 1.0E-6   ! Pseudo Time Steps (Energy Equation) (none, sec)
TJAC 20   ! Number of Transient Iterations before Updating Jacobian
TPROF   ! Automatic Estimated Temperature Profile
TRMAXITER 25   ! Maximum Number of Iterations per Pseudo Time Step
WDIF   ! Windward Differencing
!
! output control and other misc. property
!
ASEN H2   ! A-factor Sensitivity
DFAC 2.0   ! Time Step Decrement Factor
EPSS 0.001   ! Threshold for Species Sensitivity
FLT_NPOINTS 50   ! Flamelet Grid Points
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          GFAC 1.0   ! Gas Reaction Rate Multiplier
          HSEN H2   ! Heat of Formation Sensitivity
          PRNT 1   ! Print Level Control
          SIZE 100000000   ! Solution Data Block Size (bytes)
          UFAC 2.0   ! Time Step Increment Factor
          ! Number of Continuation 0   ! Continuation Count

TWOPNT:  SOLVE THE PROBLEM.

                    LOG10   LOG10
             TASK   NORM F  COND J   REMARK

            START     4.31           7 GRID POINTS
           SEARCH    -3.07    0.00   22 SEARCH STEPS

           REFINE    -3.07           1.00 AND 1.00 RATIOS, 13 GRID POINTS
           SEARCH    -4.67    0.00   18 SEARCH STEPS

           REFINE    -4.67           1.00 AND 1.00 RATIOS, 21 GRID POINTS
           SEARCH    -4.80    0.00   32 SEARCH STEPS

           REFINE    -4.80           0.83 AND 1.00 RATIOS, 30 GRID POINTS
           SEARCH    -4.91    0.00   18 SEARCH STEPS

           REFINE    -4.91           0.72 AND 0.65 RATIOS, 40 GRID POINTS
           SEARCH    -3.21    0.00   12 SEARCH STEPS

           REFINE    -3.21           0.46 AND 0.79 RATIOS, 50 GRID POINTS
           SEARCH    -4.19    0.00   16 SEARCH STEPS

           REFINE    -4.19           0.31 AND 0.48 RATIOS, 60 GRID POINTS
           SEARCH    -3.32    0.00   9 SEARCH STEPS

           REFINE    -3.32           0.23 AND 0.43 RATIOS, 70 GRID POINTS
           SEARCH    -3.28    0.00   9 SEARCH STEPS

           REFINE    -3.28           0.15 AND 0.27 RATIOS, 76 GRID POINTS
           SEARCH    -2.90    0.00   8 SEARCH STEPS

           REFINE    -2.90           0.10 AND 0.23 RATIOS, 77 GRID POINTS
           SEARCH    -3.15    0.00   7 SEARCH STEPS

           REFINE    -3.15           0.10 AND 0.19 RATIOS

TWOPNT:  FINAL SOLUTION:

      X(cm)    T(K)            AREA(cm^2)      V(cm/s)         RHO(g/cm^3)     HDOT(cal/s/cm^3)
  1   0.0000  2.9800E+002     1.0000E+000     2.3622E+002     8.5513E-004     6.1179E-014
  2   0.0500  2.9800E+002     1.0000E+000     2.3622E+002     8.5513E-004     6.2491E-013
  3   0.1000  2.9800E+002     1.0000E+000     2.3622E+002     8.5513E-004     1.9803E-011
  4   0.1500  2.9800E+002     1.0000E+000     2.3622E+002     8.5513E-004     8.7716E-010
  5   0.1750  2.9800E+002     1.0000E+000     2.3622E+002     8.5515E-004     4.2164E-008
  6   0.2000  2.9802E+002     1.0000E+000     2.3620E+002     8.5521E-004     3.0771E-006
  7   0.2063  2.9806E+002     1.0000E+000     2.3619E+002     8.5525E-004     4.2588E-005
  8   0.2125  2.9821E+002     1.0000E+000     2.3620E+002     8.5521E-004     4.0848E-004
  9   0.2156  2.9848E+002     1.0000E+000     2.3628E+002     8.5492E-004     1.7828E-003
 10   0.2188  2.9918E+002     1.0000E+000     2.3659E+002     8.5382E-004     7.9235E-003
 11   0.2219  3.0098E+002     1.0000E+000     2.3755E+002     8.5034E-004     3.8850E-002
 12   0.2234  3.0297E+002     1.0000E+000     2.3874E+002     8.4611E-004     1.1114E-001
 13   0.2250  3.0652E+002     1.0000E+000     2.4100E+002     8.3817E-004     3.7758E-001
 14   0.2266  3.1286E+002     1.0000E+000     2.4522E+002     8.2377E-004     1.5944E+000
 15   0.2273  3.1786E+002     1.0000E+000     2.4863E+002     8.1245E-004     4.0861E+000
 16   0.2281  3.2473E+002     1.0000E+000     2.5342E+002     7.9712E-004     1.0553E+001
 17   0.2285  3.2912E+002     1.0000E+000     2.5650E+002     7.8754E-004     1.7685E+001
 18   0.2289  3.3429E+002     1.0000E+000     2.6016E+002     7.7647E-004     2.9217E+001
 19   0.2293  3.4036E+002     1.0000E+000     2.6448E+002     7.6378E-004     4.7666E+001
 20   0.2297  3.4746E+002     1.0000E+000     2.6955E+002     7.4940E-004     7.6572E+001
 21   0.2301  3.5570E+002     1.0000E+000     2.7547E+002     7.3330E-004     1.2065E+002
 22   0.2305  3.6520E+002     1.0000E+000     2.8232E+002     7.1551E-004     1.8572E+002
 23   0.2309  3.7607E+002     1.0000E+000     2.9017E+002     6.9614E-004     2.7827E+002
 24   0.2313  3.8838E+002     1.0000E+000     2.9909E+002     6.7539E-004     4.0450E+002
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25	0.2316	4.0218E+002	1.0000E+000	3.0910E+002	6.5352E-004	5.6894E+002
26	0.2320	4.1747E+002	1.0000E+000	3.2020E+002	6.3087E-004	7.7286E+002
27	0.2324	4.3420E+002	1.0000E+000	3.3235E+002	6.0781E-004	1.0132E+003
28	0.2328	4.5230E+002	1.0000E+000	3.4548E+002	5.8470E-004	1.2825E+003
29	0.2332	4.7163E+002	1.0000E+000	3.5950E+002	5.6190E-004	1.5700E+003
30	0.2336	4.9205E+002	1.0000E+000	3.7429E+002	5.3969E-004	1.8634E+003
31	0.2344	5.3559E+002	1.0000E+000	4.0576E+002	4.9783E-004	2.4113E+003
32	0.2352	5.8140E+002	1.0000E+000	4.3871E+002	4.6045E-004	2.8775E+003
33	0.2359	6.2843E+002	1.0000E+000	4.7236E+002	4.2765E-004	3.2393E+003
34	0.2367	6.7591E+002	1.0000E+000	5.0613E+002	3.9911E-004	3.5013E+003
35	0.2375	7.2330E+002	1.0000E+000	5.3963E+002	3.7434E-004	3.6811E+003
36	0.2383	7.7023E+002	1.0000E+000	5.7261E+002	3.5278E-004	3.7990E+003
37	0.2387	7.9343E+002	1.0000E+000	5.8885E+002	3.4305E-004	3.8410E+003
38	0.2391	8.1643E+002	1.0000E+000	6.0491E+002	3.3394E-004	3.8746E+003
39	0.2395	8.3922E+002	1.0000E+000	6.2078E+002	3.2540E-004	3.9014E+003
40	0.2398	8.6177E+002	1.0000E+000	6.3646E+002	3.1738E-004	3.9227E+003
41	0.2406	9.0615E+002	1.0000E+000	6.6723E+002	3.0275E-004	3.9529E+003
42	0.2414	9.4952E+002	1.0000E+000	6.9721E+002	2.8973E-004	3.9693E+003
43	0.2422	9.9179E+002	1.0000E+000	7.2637E+002	2.7810E-004	3.9759E+003
44	0.2430	1.0329E+003	1.0000E+000	7.5470E+002	2.6766E-004	3.9741E+003
45	0.2437	1.0727E+003	1.0000E+000	7.8216E+002	2.5826E-004	3.9637E+003
46	0.2445	1.1113E+003	1.0000E+000	8.0872E+002	2.4978E-004	3.9432E+003
47	0.2453	1.1484E+003	1.0000E+000	8.3434E+002	2.4211E-004	3.9110E+003
48	0.2461	1.1841E+003	1.0000E+000	8.5899E+002	2.3516E-004	3.8651E+003
49	0.2469	1.2182E+003	1.0000E+000	8.8263E+002	2.2887E-004	3.8041E+003
50	0.2477	1.2508E+003	1.0000E+000	9.0521E+002	2.2316E-004	3.7272E+003
51	0.2484	1.2818E+003	1.0000E+000	9.2672E+002	2.1798E-004	3.6347E+003
52	0.2492	1.3112E+003	1.0000E+000	9.4714E+002	2.1328E-004	3.5273E+003
53	0.2500	1.3390E+003	1.0000E+000	9.6645E+002	2.0901E-004	3.4070E+003
54	0.2508	1.3651E+003	1.0000E+000	9.8467E+002	2.0515E-004	3.2759E+003
55	0.2516	1.3898E+003	1.0000E+000	1.0018E+003	2.0164E-004	3.1369E+003
56	0.2531	1.4346E+003	1.0000E+000	1.0329E+003	1.9557E-004	2.8482E+003
57	0.2547	1.4743E+003	1.0000E+000	1.0604E+003	1.9050E-004	2.5568E+003
58	0.2562	1.5094E+003	1.0000E+000	1.0846E+003	1.8624E-004	2.2797E+003
59	0.2578	1.5406E+003	1.0000E+000	1.1060E+003	1.8264E-004	2.0276E+003
60	0.2594	1.5684E+003	1.0000E+000	1.1250E+003	1.7956E-004	1.8050E+003
61	0.2625	1.6154E+003	1.0000E+000	1.1567E+003	1.7464E-004	1.4574E+003
62	0.2656	1.6549E+003	1.0000E+000	1.1830E+003	1.7076E-004	1.2038E+003
63	0.2688	1.6888E+003	1.0000E+000	1.2053E+003	1.6760E-004	1.0194E+003
64	0.2719	1.7184E+003	1.0000E+000	1.2246E+003	1.6495E-004	8.8278E+002
65	0.2750	1.7447E+003	1.0000E+000	1.2416E+003	1.6269E-004	7.7839E+002
66	0.2812	1.7888E+003	1.0000E+000	1.2698E+003	1.5908E-004	6.3247E+002
67	0.2875	1.8261E+003	1.0000E+000	1.2934E+003	1.5618E-004	5.3061E+002
68	0.2938	1.8581E+003	1.0000E+000	1.3136E+003	1.5378E-004	4.5515E+002
69	0.3000	1.8861E+003	1.0000E+000	1.3310E+003	1.5177E-004	3.9712E+002
70	0.3125	1.9314E+003	1.0000E+000	1.3590E+003	1.4864E-004	3.1508E+002
71	0.3250	1.9686E+003	1.0000E+000	1.3817E+003	1.4620E-004	2.5850E+002
72	0.3500	2.0237E+003	1.0000E+000	1.4149E+003	1.4277E-004	1.8834E+002
73	0.3750	2.0662E+003	1.0000E+000	1.4402E+003	1.4026E-004	1.4491E+002
74	0.4000	2.1002E+003	1.0000E+000	1.4605E+003	1.3831E-004	1.1587E+002
75	0.4250	2.1280E+003	1.0000E+000	1.4771E+003	1.3675E-004	9.5693E+001
76	0.4500	2.1498E+003	1.0000E+000	1.4905E+003	1.3552E-004	8.2128E+001
77	0.5000	2.1498E+003	1.0000E+000	1.4905E+003	1.3552E-004	8.2128E+001

```
 KEYWORD INPUT

!
! problem type definition
!
ENRG   ! Solve Gas Energy Equation
FLUX   ! Flux Balance for Inlet Species
FREE   ! Freely Propagating Flame
MIX   ! Use Mixture-averaged Transport
!
! physical property
!
EQUI 1.3   ! Equivalence Ratio
FLRT 1.0   ! Mass Flow Rate (g/cm2-sec)
PRES 1.0   ! Pressure (atm)
QLOS 0.0   ! Heat Flux Per Unit Length (cal/cm-sec)
TINF 298.0   ! Ambient Temperature (K)
TUNBURNT 298.0   ! Unburnt Gas Temperature (K)
!
! reactor dimension definition
!
CURV 0.5   ! Adaptive Grid Control Based On Solution Curvature
GRAD 0.1   ! Adaptive Grid Control Based On Solution Gradient
NADP 10   ! Number of Adaptive Grid Points
NPTS 6   ! Number of Uniform Grid Points
NTOT 250   ! Maximum Number of Grid Points Allowed
XEND 0.5   ! Ending Axial Position (cm)
XSTR 0.0   ! Starting Axial Position (cm)
!
! species property
!
CPROD H2O   ! Complete-Combustion Products
CPROD N2   ! Complete-Combustion Products
FUEL H2 0.295   ! Fuel Fraction of Total Fuel Species (mole fraction)
MOLE   ! Print Mole Fractions
OXID N2 0.556   ! Oxidizer Fraction of Total Oxidizer Species (mole fraction)
OXID O2 0.1479   ! Oxidizer Fraction of Total Oxidizer Species (mole fraction)
PRMN 0.0   ! Minimum for Product Estimates (mole fraction)
XIMN 0.0   ! Minimum for Estimated Intermediate Fraction (mole fraction)
!
! solver control
!
!USE_ADVANCED_TECHNIQUE   ! Advanced Solution Technique (Default)
ATIM 1.0E-9   ! Absolute Tolerance for Pseudo Timestepping
ATOL 1.0E-9   ! Absolute Tolerance
DTMN 1.0E-10   ! Minimum Pseudo Time Step (sec)
DTMX 0.01   ! Maximum Pseudo Time Step (sec)
IRET 25   ! Number Time Steps Before Increasing
ISTP 0   ! Number of Initial Pseudo Time Steps
MAXTIME 100   ! Maximum Number of Pseudo Time Stepping Operations Allowed
NDPR 100   ! Output Frequency during Integration
NJAC 20   ! Number of Iterations before Updating Jacobian
RTIM 0.0001   ! Relative Tolerance for Pseudo Timestepping
RTOL 0.0001   ! Relative Tolerance
SFLR -0.001   ! Minimum Bounds on Species Fractions
SPOS 0.0   ! Positive Value to Reset Species Fractions
SSMAXITER 100   ! Maximum Number of Iterations per Steady State Search
TIM1 100.0 5.0E-7   ! Pseudo Time Steps (Fixed Temperature) (none, sec)
TIM2 200.0 1.0E-6   ! Pseudo Time Steps (Energy Equation) (none, sec)
TJAC 20   ! Number of Transient Iterations before Updating Jacobian
TPROF   ! Automatic Estimated Temperature Profile
WARNING...TPROF default non-uniform 12-point grid will be superceded by a uniform grid with given
NPTS grid count of:    6
TRMAXITER 25   ! Maximum Number of Iterations per Pseudo Time Step
WDIF   ! Windward Differencing
!
! output control and other misc. property
!
ASEN H2   ! A-factor Sensitivity
DFAC 2.0   ! Time Step Decrement Factor
```

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EPSS 0.001   ! Threshold for Species Sensitivity
FLT_NPOINTS 50   ! Flamelet Grid Points
GFAC 1.0   ! Gas Reaction Rate Multiplier
HSEN H2   ! Heat of Formation Sensitivity
PRNT 1   ! Print Level Control
SIZE 100000000   ! Solution Data Block Size (bytes)
UFAC 2.0   ! Time Step Increment Factor
! Number of Continuation 0   ! Continuation Count
```

TWOPNT: SOLVE THE PROBLEM.

TASK	LOG10 NORM F	LOG10 COND J	REMARK
START	4.29		7 GRID POINTS
SEARCH	-2.80	0.00	22 SEARCH STEPS
REFINE	-2.80		1.00 AND 1.00 RATIOS, 13 GRID POINTS
SEARCH	-3.63	0.00	24 SEARCH STEPS
REFINE	-3.63		1.00 AND 1.00 RATIOS, 21 GRID POINTS
SEARCH	-4.86	0.00	26 SEARCH STEPS
REFINE	-4.86		0.85 AND 1.00 RATIOS, 30 GRID POINTS
SEARCH	-4.59	0.00	19 SEARCH STEPS
REFINE	-4.59		0.67 AND 0.79 RATIOS, 39 GRID POINTS
SEARCH	-3.13	0.00	15 SEARCH STEPS
REFINE	-3.13		0.43 AND 0.90 RATIOS, 49 GRID POINTS
SEARCH	-3.90	0.00	16 SEARCH STEPS
REFINE	-3.90		0.34 AND 0.50 RATIOS, 59 GRID POINTS
SEARCH	-3.52	0.00	10 SEARCH STEPS
REFINE	-3.52		0.21 AND 0.30 RATIOS, 69 GRID POINTS
SEARCH	-3.13	0.00	9 SEARCH STEPS
REFINE	-3.13		0.17 AND 0.29 RATIOS, 79 GRID POINTS
SEARCH	-3.03	0.00	9 SEARCH STEPS
REFINE	-3.03		0.17 AND 0.29 RATIOS, 82 GRID POINTS
SEARCH	-3.01	0.00	7 SEARCH STEPS
REFINE	-3.01		0.10 AND 0.17 RATIOS

TWOPNT: FINAL SOLUTION:

	X(cm)	T(K)	AREA(cm^2)	V(cm/s)	RHO(g/cm^3)	HDOT(cal/s/cm^3)
1	0.0000	2.9800E+002	1.0000E+000	2.9696E+002	7.9214E-004	7.4499E-015
2	0.0500	2.9800E+002	1.0000E+000	2.9696E+002	7.9214E-004	9.1124E-014
3	0.1000	2.9800E+002	1.0000E+000	2.9696E+002	7.9214E-004	3.4446E-012
4	0.1500	2.9800E+002	1.0000E+000	2.9696E+002	7.9214E-004	1.8517E-010
5	0.1750	2.9800E+002	1.0000E+000	2.9696E+002	7.9214E-004	1.0587E-008
6	0.2000	2.9800E+002	1.0000E+000	2.9696E+002	7.9215E-004	8.8709E-007
7	0.2063	2.9802E+002	1.0000E+000	2.9696E+002	7.9215E-004	1.3932E-005
8	0.2125	2.9807E+002	1.0000E+000	2.9697E+002	7.9212E-004	1.5051E-004
9	0.2156	2.9817E+002	1.0000E+000	2.9701E+002	7.9200E-004	7.2431E-004
10	0.2188	2.9845E+002	1.0000E+000	2.9717E+002	7.9157E-004	3.4723E-003
11	0.2219	2.9922E+002	1.0000E+000	2.9771E+002	7.9014E-004	1.7388E-002
12	0.2234	3.0014E+002	1.0000E+000	2.9841E+002	7.8828E-004	4.8794E-002
13	0.2250	3.0189E+002	1.0000E+000	2.9982E+002	7.8459E-004	1.5629E-001
14	0.2266	3.0520E+002	1.0000E+000	3.0260E+002	7.7738E-004	6.2138E-001
15	0.2281	3.1143E+002	1.0000E+000	3.0801E+002	7.6373E-004	3.1089E+000
16	0.2289	3.1657E+002	1.0000E+000	3.1256E+002	7.5261E-004	8.7839E+000
17	0.2293	3.1996E+002	1.0000E+000	3.1559E+002	7.4539E-004	1.5204E+001
18	0.2297	3.2405E+002	1.0000E+000	3.1927E+002	7.3679E-004	2.5913E+001
19	0.2301	3.2897E+002	1.0000E+000	3.2372E+002	7.2665E-004	4.3675E+001
20	0.2305	3.3486E+002	1.0000E+000	3.2908E+002	7.1482E-004	7.2621E+001
21	0.2309	3.4187E+002	1.0000E+000	3.3548E+002	7.0118E-004	1.1864E+002

22	0.2313	3.5014E+002	1.0000E+000	3.4307E+002	6.8568E-004	1.8956E+002
23	0.2314	3.5481E+002	1.0000E+000	3.4735E+002	6.7722E-004	2.3838E+002
24	0.2316	3.5986E+002	1.0000E+000	3.5201E+002	6.6827E-004	2.9742E+002
25	0.2318	3.6532E+002	1.0000E+000	3.5703E+002	6.5886E-004	3.6802E+002
26	0.2320	3.7119E+002	1.0000E+000	3.6245E+002	6.4901E-004	4.5141E+002
27	0.2324	3.8421E+002	1.0000E+000	3.7447E+002	6.2818E-004	6.5706E+002
28	0.2328	3.9889E+002	1.0000E+000	3.8805E+002	6.0620E-004	9.2053E+002
29	0.2332	4.1523E+002	1.0000E+000	4.0315E+002	5.8349E-004	1.2393E+003
30	0.2336	4.3313E+002	1.0000E+000	4.1969E+002	5.6049E-004	1.6034E+003
31	0.2340	4.5246E+002	1.0000E+000	4.3755E+002	5.3761E-004	1.9965E+003
32	0.2344	4.7306E+002	1.0000E+000	4.5656E+002	5.1523E-004	2.3993E+003
33	0.2352	5.1739E+002	1.0000E+000	4.9735E+002	4.7297E-004	3.1446E+003
34	0.2355	5.4054E+002	1.0000E+000	5.1857E+002	4.5362E-004	3.4797E+003
35	0.2359	5.6421E+002	1.0000E+000	5.4020E+002	4.3545E-004	3.7758E+003
36	0.2363	5.8823E+002	1.0000E+000	5.6210E+002	4.1849E-004	4.0310E+003
37	0.2367	6.1248E+002	1.0000E+000	5.8414E+002	4.0270E-004	4.2464E+003
38	0.2375	6.6132E+002	1.0000E+000	6.2831E+002	3.7439E-004	4.5651E+003
39	0.2383	7.0999E+002	1.0000E+000	6.7203E+002	3.5004E-004	4.7660E+003
40	0.2387	7.3412E+002	1.0000E+000	6.9359E+002	3.3915E-004	4.8339E+003
41	0.2391	7.5808E+002	1.0000E+000	7.1493E+002	3.2903E-004	4.8858E+003
42	0.2395	7.8184E+002	1.0000E+000	7.3603E+002	3.1960E-004	4.9248E+003
43	0.2398	8.0539E+002	1.0000E+000	7.5687E+002	3.1080E-004	4.9536E+003
44	0.2402	8.2870E+002	1.0000E+000	7.7745E+002	3.0257E-004	4.9745E+003
45	0.2406	8.5178E+002	1.0000E+000	7.9776E+002	2.9487E-004	4.9895E+003
46	0.2410	8.7460E+002	1.0000E+000	8.1781E+002	2.8764E-004	5.0002E+003
47	0.2414	8.9716E+002	1.0000E+000	8.3759E+002	2.8085E-004	5.0077E+003
48	0.2422	9.4149E+002	1.0000E+000	8.7634E+002	2.6843E-004	5.0165E+003
49	0.2430	9.8473E+002	1.0000E+000	9.1405E+002	2.5735E-004	5.0172E+003
50	0.2437	1.0268E+003	1.0000E+000	9.5068E+002	2.4744E-004	5.0116E+003
51	0.2445	1.0676E+003	1.0000E+000	9.8621E+002	2.3852E-004	4.9987E+003
52	0.2453	1.1071E+003	1.0000E+000	1.0206E+003	2.3049E-004	4.9759E+003
53	0.2461	1.1452E+003	1.0000E+000	1.0538E+003	2.2323E-004	4.9398E+003
54	0.2469	1.1818E+003	1.0000E+000	1.0857E+003	2.1667E-004	4.8868E+003
55	0.2477	1.2168E+003	1.0000E+000	1.1162E+003	2.1074E-004	4.8139E+003
56	0.2484	1.2501E+003	1.0000E+000	1.1454E+003	2.0537E-004	4.7193E+003
57	0.2492	1.2818E+003	1.0000E+000	1.1731E+003	2.0052E-004	4.6023E+003
58	0.2500	1.3117E+003	1.0000E+000	1.1994E+003	1.9613E-004	4.4640E+003
59	0.2508	1.3399E+003	1.0000E+000	1.2242E+003	1.9216E-004	4.3063E+003
60	0.2516	1.3664E+003	1.0000E+000	1.2474E+003	1.8858E-004	4.1327E+003
61	0.2523	1.3912E+003	1.0000E+000	1.2692E+003	1.8534E-004	3.9470E+003
62	0.2531	1.4144E+003	1.0000E+000	1.2895E+003	1.8242E-004	3.7534E+003
63	0.2547	1.4562E+003	1.0000E+000	1.3259E+003	1.7741E-004	3.3601E+003
64	0.2562	1.4927E+003	1.0000E+000	1.3576E+003	1.7327E-004	2.9757E+003
65	0.2578	1.5247E+003	1.0000E+000	1.3852E+003	1.6982E-004	2.6202E+003
66	0.2594	1.5528E+003	1.0000E+000	1.4093E+003	1.6692E-004	2.3045E+003
67	0.2625	1.5992E+003	1.0000E+000	1.4484E+003	1.6241E-004	1.8132E+003
68	0.2656	1.6372E+003	1.0000E+000	1.4801E+003	1.5893E-004	1.4606E+003
69	0.2688	1.6692E+003	1.0000E+000	1.5066E+003	1.5614E-004	1.2112E+003
70	0.2750	1.7201E+003	1.0000E+000	1.5479E+003	1.5197E-004	9.1641E+002
71	0.2812	1.7617E+003	1.0000E+000	1.5813E+003	1.4876E-004	7.3875E+002
72	0.2875	1.7968E+003	1.0000E+000	1.6093E+003	1.4617E-004	6.1964E+002
73	0.2938	1.8271E+003	1.0000E+000	1.6332E+003	1.4403E-004	5.3305E+002
74	0.3000	1.8536E+003	1.0000E+000	1.6540E+003	1.4222E-004	4.6677E+002
75	0.3125	1.8967E+003	1.0000E+000	1.6876E+003	1.3939E-004	3.7293E+002
76	0.3250	1.9323E+003	1.0000E+000	1.7149E+003	1.3717E-004	3.0746E+002
77	0.3500	1.9852E+003	1.0000E+000	1.7551E+003	1.3403E-004	2.2540E+002
78	0.3750	2.0261E+003	1.0000E+000	1.7859E+003	1.3172E-004	1.7387E+002
79	0.4000	2.0588E+003	1.0000E+000	1.8104E+003	1.2993E-004	1.3909E+002
80	0.4250	2.0855E+003	1.0000E+000	1.8306E+003	1.2850E-004	1.1472E+002
81	0.4500	2.1066E+003	1.0000E+000	1.8469E+003	1.2737E-004	9.8177E+001
82	0.5000	2.1066E+003	1.0000E+000	1.8469E+003	1.2737E-004	9.8177E+001

Appendix:G

a. Premix Laminar Flame Model for H_2/air Mixtures Developed by GRI-Mech/K-species Mechanism

```
          KEYWORD INPUT

     !
     ! problem type definition
     !
     ENRG   ! Solve Gas Energy Equation
     FLUX   ! Flux Balance for Inlet Species
     FREE   ! Freely Propagating Flame
     MIX   ! Use Mixture-averaged Transport
     !
     ! physical property
     !
     EQUI 1.0   ! Equivalence Ratio
     FLRT 1.0   ! Mass Flow Rate (g/cm2-sec)
     PRES 1.0   ! Pressure (atm)
     QLOS 0.0   ! Heat Flux Per Unit Length (cal/cm-sec)
     TINF 298.0   ! Ambient Temperature (K)
     TUNBURNT 673.0   ! Unburnt Gas Temperature (K)
     !
     ! reactor dimension definition
     !
     CURV 0.5   ! Adaptive Grid Control Based On Solution Curvature
     GRAD 0.1   ! Adaptive Grid Control Based On Solution Gradient
     NADP 10   ! Number of Adaptive Grid Points
     NPTS 6   ! Number of Uniform Grid Points
     NTOT 250   ! Maximum Number of Grid Points Allowed
     XEND 0.5   ! Ending Axial Position (cm)
     XSTR 0.0   ! Starting Axial Position (cm)
     !
     ! species property
     !
     CPROD H2O   ! Complete-Combustion Products
     CPROD N2   ! Complete-Combustion Products
     FUEL H2 0.295   ! Fuel Fraction of Total Fuel Species (mole fraction)
     MOLE   ! Print Mole Fractions
     OXID N2 0.556   ! Oxidizer Fraction of Total Oxidizer Species (mole fraction)
     OXID O2 0.1479   ! Oxidizer Fraction of Total Oxidizer Species (mole fraction)
     PRMN 0.0   ! Minimum for Product Estimates (mole fraction)
     XIMN 0.0   ! Minimum for Estimated Intermediate Fraction (mole fraction)
TWOPNT:  SOLVE THE PROBLEM.

            LOG10   LOG10
      TASK   NORM F  COND J   REMARK

      START     4.04          7 GRID POINTS
     SEARCH     2.93    0.00   GOING OUT OF BOUNDS
     EVOLVE     1.17    0.00   100 TIME STEPS, 2.0E-06 LAST STRIDE
     SEARCH    -3.51    0.00   3 SEARCH STEPS

     REFINE    -3.51          1.00 AND 1.00 RATIOS, 13 GRID POINTS
     SEARCH    -3.19    0.00   9 SEARCH STEPS
```

```
REFINE   -3.19        0.99 AND 1.00 RATIOS, 23 GRID POINTS
SEARCH    4.80   0.00  DIVERGING
EVOLVE    3.25   0.00  100 TIME STEPS, 2.5E-07 LAST STRIDE
SEARCH    4.36   0.00  DIVERGING
EVOLVE    2.06   0.00  100 TIME STEPS, 4.0E-06 LAST STRIDE
SEARCH   -2.72   0.00  7 SEARCH STEPS

REFINE   -2.72        0.70 AND 0.97 RATIOS, 33 GRID POINTS
SEARCH   -2.68   0.00  11 SEARCH STEPS

REFINE   -2.68        0.59 AND 0.61 RATIOS, 43 GRID POINTS
SEARCH   -2.59   0.00  10 SEARCH STEPS

REFINE   -2.59        0.28 AND 0.37 RATIOS, 53 GRID POINTS
SEARCH   -2.92   0.00  11 SEARCH STEPS

REFINE   -2.92        0.22 AND 0.38 RATIOS, 63 GRID POINTS
SEARCH   -2.81   0.00  9 SEARCH STEPS

REFINE   -2.81        0.19 AND 0.33 RATIOS, 73 GRID POINTS
SEARCH   -2.95   0.00  8 SEARCH STEPS

REFINE   -2.95        0.19 AND 0.44 RATIOS, 79 GRID POINTS
SEARCH   -2.76   0.00  9 SEARCH STEPS

REFINE   -2.76        0.10 AND 0.43 RATIOS, 81 GRID POINTS
SEARCH   -2.51   0.00  6 SEARCH STEPS

REFINE   -2.51        0.10 AND 0.43 RATIOS

TWOPNT:  FINAL SOLUTION:
```

	X(cm)	T(K)	AREA(cm^2)	V(cm/s)	RHO(g/cm^3)	HDOT(cal/s/cm^3)
1	0.0000	6.7300E+002	1.0000E+000	9.4974E+002	3.7865E-004	-4.6079E-011
2	0.0500	6.7300E+002	1.0000E+000	9.4974E+002	3.7865E-004	-5.3144E-012
3	0.0750	6.7300E+002	1.0000E+000	9.4974E+002	3.7865E-004	4.8314E-011
4	0.1000	6.7300E+002	1.0000E+000	9.4974E+002	3.7865E-004	2.4203E-009
5	0.1250	6.7300E+002	1.0000E+000	9.4974E+002	3.7865E-004	1.1471E-007
6	0.1500	6.7300E+002	1.0000E+000	9.4974E+002	3.7865E-004	5.4696E-006
7	0.1625	6.7300E+002	1.0000E+000	9.4974E+002	3.7865E-004	1.0269E-004
8	0.1750	6.7300E+002	1.0000E+000	9.4974E+002	3.7865E-004	1.4910E-003
9	0.1813	6.7301E+002	1.0000E+000	9.4974E+002	3.7865E-004	9.1937E-003
10	0.1875	6.7302E+002	1.0000E+000	9.4974E+002	3.7865E-004	4.9447E-002
11	0.1938	6.7307E+002	1.0000E+000	9.4977E+002	3.7864E-004	2.6594E-001
12	0.1969	6.7315E+002	1.0000E+000	9.4982E+002	3.7861E-004	7.3129E-001
13	0.2000	6.7333E+002	1.0000E+000	9.4997E+002	3.7856E-004	1.9451E+000
14	0.2016	6.7349E+002	1.0000E+000	9.5012E+002	3.7849E-004	3.4089E+000
15	0.2031	6.7376E+002	1.0000E+000	9.5039E+002	3.7839E-004	5.9070E+000
16	0.2047	6.7419E+002	1.0000E+000	9.5083E+002	3.7821E-004	1.0333E+001
17	0.2055	6.7450E+002	1.0000E+000	9.5116E+002	3.7808E-004	1.3807E+001
18	0.2063	6.7490E+002	1.0000E+000	9.5160E+002	3.7791E-004	1.8527E+001

19	0.2070	6.7542E+002	1.0000E+000	9.5218E+002	3.7768E-004	2.4942E+001
20	0.2078	6.7609E+002	1.0000E+000	9.5295E+002	3.7737E-004	3.3643E+001
21	0.2086	6.7695E+002	1.0000E+000	9.5395E+002	3.7698E-004	4.5401E+001
22	0.2094	6.7804E+002	1.0000E+000	9.5525E+002	3.7646E-004	6.1189E+001
23	0.2102	6.7943E+002	1.0000E+000	9.5692E+002	3.7581E-004	8.2195E+001
24	0.2109	6.8118E+002	1.0000E+000	9.5905E+002	3.7497E-004	1.0982E+002
25	0.2117	6.8336E+002	1.0000E+000	9.6174E+002	3.7392E-004	1.4563E+002
26	0.2125	6.8607E+002	1.0000E+000	9.6509E+002	3.7262E-004	1.9131E+002
27	0.2133	6.8939E+002	1.0000E+000	9.6925E+002	3.7103E-004	2.4857E+002
28	0.2141	6.9342E+002	1.0000E+000	9.7433E+002	3.6909E-004	3.1902E+002
29	0.2148	6.9827E+002	1.0000E+000	9.8047E+002	3.6678E-004	4.0412E+002
30	0.2156	7.0405E+002	1.0000E+000	9.8782E+002	3.6405E-004	5.0509E+002
31	0.2164	7.1087E+002	1.0000E+000	9.9652E+002	3.6087E-004	6.2289E+002
32	0.2172	7.1883E+002	1.0000E+000	1.0067E+003	3.5722E-004	7.5811E+002
33	0.2180	7.2804E+002	1.0000E+000	1.0185E+003	3.5308E-004	9.1097E+002
34	0.2188	7.3859E+002	1.0000E+000	1.0320E+003	3.4845E-004	1.0811E+003
35	0.2195	7.5056E+002	1.0000E+000	1.0474E+003	3.4334E-004	1.2676E+003
36	0.2203	7.6403E+002	1.0000E+000	1.0647E+003	3.3777E-004	1.4688E+003
37	0.2219	7.9559E+002	1.0000E+000	1.1051E+003	3.2540E-004	1.8983E+003
38	0.2234	8.3257E+002	1.0000E+000	1.1523E+003	3.1209E-004	2.3505E+003
39	0.2250	8.7459E+002	1.0000E+000	1.2055E+003	2.9831E-004	2.8065E+003
40	0.2258	8.9730E+002	1.0000E+000	1.2341E+003	2.9141E-004	3.0341E+003
41	0.2266	9.2121E+002	1.0000E+000	1.2641E+003	2.8449E-004	3.2589E+003
42	0.2273	9.4626E+002	1.0000E+000	1.2953E+003	2.7762E-004	3.4797E+003
43	0.2281	9.7234E+002	1.0000E+000	1.3278E+003	2.7083E-004	3.6954E+003
44	0.2289	9.9935E+002	1.0000E+000	1.3614E+003	2.6416E-004	3.9048E+003
45	0.2297	1.0272E+003	1.0000E+000	1.3958E+003	2.5763E-004	4.1068E+003
46	0.2305	1.0557E+003	1.0000E+000	1.4311E+003	2.5129E-004	4.2998E+003
47	0.2313	1.0847E+003	1.0000E+000	1.4670E+003	2.4514E-004	4.4815E+003
48	0.2320	1.1142E+003	1.0000E+000	1.5033E+003	2.3922E-004	4.6488E+003
49	0.2328	1.1438E+003	1.0000E+000	1.5399E+003	2.3353E-004	4.7981E+003
50	0.2336	1.1734E+003	1.0000E+000	1.5765E+003	2.2811E-004	4.9253E+003
51	0.2344	1.2029E+003	1.0000E+000	1.6130E+003	2.2295E-004	5.0263E+003
52	0.2352	1.2321E+003	1.0000E+000	1.6491E+003	2.1807E-004	5.0973E+003
53	0.2359	1.2608E+003	1.0000E+000	1.6846E+003	2.1347E-004	5.1354E+003
54	0.2367	1.2888E+003	1.0000E+000	1.7194E+003	2.0916E-004	5.1387E+003
55	0.2375	1.3160E+003	1.0000E+000	1.7531E+003	2.0513E-004	5.1071E+003
56	0.2383	1.3422E+003	1.0000E+000	1.7858E+003	2.0137E-004	5.0416E+003
57	0.2391	1.3675E+003	1.0000E+000	1.8173E+003	1.9789E-004	4.9449E+003
58	0.2398	1.3917E+003	1.0000E+000	1.8474E+003	1.9466E-004	4.8208E+003
59	0.2406	1.4148E+003	1.0000E+000	1.8761E+003	1.9169E-004	4.6737E+003
60	0.2422	1.4574E+003	1.0000E+000	1.9291E+003	1.8642E-004	4.3331E+003
61	0.2430	1.4772E+003	1.0000E+000	1.9537E+003	1.8407E-004	4.1461E+003
62	0.2437	1.4959E+003	1.0000E+000	1.9768E+003	1.8192E-004	3.9557E+003
63	0.2453	1.5302E+003	1.0000E+000	2.0190E+003	1.7811E-004	3.5818E+003
64	0.2469	1.5609E+003	1.0000E+000	2.0567E+003	1.7485E-004	3.2285E+003
65	0.2484	1.5885E+003	1.0000E+000	2.0904E+003	1.7203E-004	2.9082E+003
66	0.2500	1.6134E+003	1.0000E+000	2.1206E+003	1.6959E-004	2.6245E+003
67	0.2562	1.6897E+003	1.0000E+000	2.2110E+003	1.6265E-004	1.9014E+003
68	0.2625	1.7495E+003	1.0000E+000	2.2808E+003	1.5767E-004	1.4763E+003
69	0.2688	1.7988E+003	1.0000E+000	2.3375E+003	1.5384E-004	1.2087E+003
70	0.2750	1.8407E+003	1.0000E+000	2.3853E+003	1.5076E-004	1.0245E+003

71	0.2812	1.8771E+003	1.0000E+000	2.4265E+003	1.4821E-004	8.8866E+002
72	0.2875	1.9091E+003	1.0000E+000	2.4624E+003	1.4604E-004	7.8389E+002
73	0.3000	1.9617E+003	1.0000E+000	2.5206E+003	1.4267E-004	6.3521E+002
74	0.3125	2.0057E+003	1.0000E+000	2.5688E+003	1.3999E-004	5.3095E+002
75	0.3250	2.0432E+003	1.0000E+000	2.6096E+003	1.3780E-004	4.5411E+002
76	0.3500	2.1017E+003	1.0000E+000	2.6725E+003	1.3456E-004	3.5190E+002
77	0.3750	2.1490E+003	1.0000E+000	2.7227E+003	1.3208E-004	2.8409E+002
78	0.4000	2.1883E+003	1.0000E+000	2.7641E+003	1.3010E-004	2.3606E+002
79	0.4250	2.2215E+003	1.0000E+000	2.7992E+003	1.2847E-004	2.0079E+002
80	0.4500	2.2487E+003	1.0000E+000	2.8286E+003	1.2713E-004	1.7539E+002
81	0.5000	2.2487E+003	1.0000E+000	2.8286E+003	1.2713E-004	1.7539E+002

b. Premix Laminar Flame Model for H_2/air Mixtures Developed by Reduced/K-species Mechanism

```
KEYWORD INPUT

!
! problem type definition
!
ENRG   ! Solve Gas Energy Equation
FLUX   ! Flux Balance for Inlet Species
FREE   ! Freely Propagating Flame
MIX   ! Use Mixture-averaged Transport
!
! physical property
!
EQUI 1.0   ! Equivalence Ratio
FLRT 1.0   ! Mass Flow Rate (g/cm2-sec)
PRES 1.0   ! Pressure (atm)
QLOS 0.0   ! Heat Flux Per Unit Length (cal/cm-sec)
TINF 298.0   ! Ambient Temperature (K)
TUNBURNT 673.0   ! Unburnt Gas Temperature (K)
!
! reactor dimension definition
!
CURV 0.5   ! Adaptive Grid Control Based On Solution Curvature
GRAD 0.1   ! Adaptive Grid Control Based On Solution Gradient
NADP 10   ! Number of Adaptive Grid Points
NPTS 6   ! Number of Uniform Grid Points
NTOT 250   ! Maximum Number of Grid Points Allowed
XEND 0.5   ! Ending Axial Position (cm)
XSTR 0.0   ! Starting Axial Position (cm)
!
! species property
!
CPROD H2O   ! Complete-Combustion Products
CPROD N2   ! Complete-Combustion Products
FUEL H2 0.294   ! Fuel Fraction of Total Fuel Species (mole fraction)
MOLE   ! Print Mole Fractions
OXID N2 0.556   ! Oxidizer Fraction of Total Oxidizer Species (mole fraction)
OXID O2 0.1479   ! Oxidizer Fraction of Total Oxidizer Species (mole fraction)
PRMN 0.0   ! Minimum for Product Estimates (mole fraction)
XIMN 0.0   ! Minimum for Estimated Intermediate Fraction (mole fraction)


        LOG10   LOG10
  TASK   NORM F  COND J   REMARK

  START     4.05          7 GRID POINTS
 SEARCH     2.85    0.00   GOING OUT OF BOUNDS
 EVOLVE     1.59    0.00   100 TIME STEPS, 2.0E-06 LAST STRIDE
 SEARCH    -4.24    0.00   4 SEARCH STEPS

 REFINE    -4.24          1.00 AND 1.00 RATIOS, 13 GRID POINTS
 SEARCH    -3.02    0.00   12 SEARCH STEPS
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REFINE -3.02 0.89 AND 1.00 RATIOS, 23 GRID POINTS
SEARCH -2.64 0.00 17 SEARCH STEPS

REFINE -2.64 0.90 AND 0.73 RATIOS, 32 GRID POINTS
SEARCH -2.15 0.00 16 SEARCH STEPS

REFINE -2.15 0.51 AND 0.67 RATIOS, 42 GRID POINTS
SEARCH -3.24 0.00 14 SEARCH STEPS

REFINE -3.24 0.89 AND 0.98 RATIOS, 52 GRID POINTS
SEARCH -4.51 0.00 21 SEARCH STEPS

REFINE -4.51 0.49 AND 0.42 RATIOS, 62 GRID POINTS
SEARCH -2.69 0.00 9 SEARCH STEPS

REFINE -2.69 0.39 AND 0.42 RATIOS, 72 GRID POINTS
SEARCH -3.51 0.00 12 SEARCH STEPS

REFINE -3.51 0.23 AND 0.42 RATIOS, 81 GRID POINTS
SEARCH -2.71 0.00 9 SEARCH STEPS

REFINE -2.71 0.13 AND 0.42 RATIOS, 87 GRID POINTS
SEARCH -3.80 0.00 10 SEARCH STEPS

REFINE -3.80 0.10 AND 0.42 RATIOS

TWOPNT: FINAL SOLUTION:

	X(cm)	T(K)	AREA(cm^2)	V(cm/s)	RHO(g/cm^3)	HDOT(cal/s/cm^3)
1	0.0000	6.7300E+002	1.0000E+000	9.6770E+002	3.7865E-004	-3.2677E-011
2	0.0500	6.7300E+002	1.0000E+000	9.6770E+002	3.7865E-004	9.6453E-012
3	0.0750	6.7300E+002	1.0000E+000	9.6770E+002	3.7865E-004	6.4479E-010
4	0.1000	6.7300E+002	1.0000E+000	9.6770E+002	3.7865E-004	2.0890E-008
5	0.1125	6.7300E+002	1.0000E+000	9.6770E+002	3.7865E-004	2.7299E-007
6	0.1250	6.7300E+002	1.0000E+000	9.6770E+002	3.7865E-004	2.8939E-006
7	0.1375	6.7300E+002	1.0000E+000	9.6770E+002	3.7865E-004	3.0532E-005
8	0.1500	6.7300E+002	1.0000E+000	9.6770E+002	3.7865E-004	3.2232E-004
9	0.1625	6.7300E+002	1.0000E+000	9.6770E+002	3.7865E-004	3.4091E-003
10	0.1750	6.7301E+002	1.0000E+000	9.6770E+002	3.7864E-004	3.6303E-002
11	0.1781	6.7302E+002	1.0000E+000	9.6771E+002	3.7864E-004	9.4227E-002
12	0.1813	6.7303E+002	1.0000E+000	9.6772E+002	3.7864E-004	2.2441E-001
13	0.1844	6.7307E+002	1.0000E+000	9.6775E+002	3.7863E-004	5.2664E-001
14	0.1859	6.7310E+002	1.0000E+000	9.6778E+002	3.7862E-004	8.2999E-001
15	0.1875	6.7315E+002	1.0000E+000	9.6783E+002	3.7860E-004	1.3189E+000
16	0.1891	6.7322E+002	1.0000E+000	9.6790E+002	3.7857E-004	2.1149E+000
17	0.1906	6.7334E+002	1.0000E+000	9.6803E+002	3.7852E-004	3.4244E+000
18	0.1922	6.7352E+002	1.0000E+000	9.6823E+002	3.7844E-004	5.5956E+000
19	0.1930	6.7365E+002	1.0000E+000	9.6837E+002	3.7839E-004	7.2030E+000
20	0.1938	6.7381E+002	1.0000E+000	9.6855E+002	3.7831E-004	9.3076E+000
21	0.1945	6.7402E+002	1.0000E+000	9.6879E+002	3.7822E-004	1.2061E+001
22	0.1953	6.7428E+002	1.0000E+000	9.6910E+002	3.7810E-004	1.5654E+001

23	0.1961	6.7462E+002	1.0000E+000	9.6950E+002	3.7794E-004	2.0328E+001
24	0.1969	6.7504E+002	1.0000E+000	9.7001E+002	3.7774E-004	2.6371E+001
25	0.1977	6.7557E+002	1.0000E+000	9.7066E+002	3.7749E-004	3.4130E+001
26	0.1984	6.7623E+002	1.0000E+000	9.7149E+002	3.7717E-004	4.4000E+001
27	0.1992	6.7707E+002	1.0000E+000	9.7253E+002	3.7676E-004	5.6421E+001
28	0.2000	6.7810E+002	1.0000E+000	9.7385E+002	3.7625E-004	7.1864E+001
29	0.2016	6.8093E+002	1.0000E+000	9.7749E+002	3.7486E-004	1.1322E+002
30	0.2031	6.8495E+002	1.0000E+000	9.8273E+002	3.7286E-004	1.7153E+002
31	0.2063	6.9776E+002	1.0000E+000	9.9960E+002	3.6656E-004	3.4607E+002
32	0.2078	7.0682E+002	1.0000E+000	1.0115E+003	3.6224E-004	4.7604E+002
33	0.2094	7.1846E+002	1.0000E+000	1.0269E+003	3.5681E-004	6.4058E+002
34	0.2109	7.3311E+002	1.0000E+000	1.0463E+003	3.5020E-004	8.4191E+002
35	0.2125	7.5109E+002	1.0000E+000	1.0701E+003	3.4241E-004	1.0823E+003
36	0.2141	7.7266E+002	1.0000E+000	1.0986E+003	3.3353E-004	1.3547E+003
37	0.2156	7.9788E+002	1.0000E+000	1.1318E+003	3.2376E-004	1.6546E+003
38	0.2164	8.1184E+002	1.0000E+000	1.1500E+003	3.1861E-004	1.8136E+003
39	0.2172	8.2681E+002	1.0000E+000	1.1696E+003	3.1329E-004	1.9770E+003
40	0.2180	8.4279E+002	1.0000E+000	1.1904E+003	3.0781E-004	2.1431E+003
41	0.2188	8.5977E+002	1.0000E+000	1.2124E+003	3.0222E-004	2.3111E+003
42	0.2195	8.7771E+002	1.0000E+000	1.2357E+003	2.9654E-004	2.4792E+003
43	0.2203	8.9660E+002	1.0000E+000	1.2600E+003	2.9080E-004	2.6471E+003
44	0.2211	9.1640E+002	1.0000E+000	1.2855E+003	2.8505E-004	2.8129E+003
45	0.2219	9.3705E+002	1.0000E+000	1.3119E+003	2.7930E-004	2.9769E+003
46	0.2227	9.5852E+002	1.0000E+000	1.3393E+003	2.7358E-004	3.1380E+003
47	0.2234	9.8073E+002	1.0000E+000	1.3676E+003	2.6792E-004	3.2956E+003
48	0.2242	1.0036E+003	1.0000E+000	1.3967E+003	2.6234E-004	3.4489E+003
49	0.2250	1.0271E+003	1.0000E+000	1.4265E+003	2.5686E-004	3.5969E+003
50	0.2258	1.0511E+003	1.0000E+000	1.4569E+003	2.5150E-004	3.7383E+003
51	0.2266	1.0755E+003	1.0000E+000	1.4878E+003	2.4628E-004	3.8714E+003
52	0.2273	1.1002E+003	1.0000E+000	1.5191E+003	2.4121E-004	3.9941E+003
53	0.2281	1.1251E+003	1.0000E+000	1.5505E+003	2.3631E-004	4.1041E+003
54	0.2289	1.1501E+003	1.0000E+000	1.5821E+003	2.3160E-004	4.1991E+003
55	0.2297	1.1751E+003	1.0000E+000	1.6137E+003	2.2707E-004	4.2764E+003
56	0.2305	1.1999E+003	1.0000E+000	1.6450E+003	2.2274E-004	4.3340E+003
57	0.2313	1.2244E+003	1.0000E+000	1.6760E+003	2.1862E-004	4.3701E+003
58	0.2320	1.2485E+003	1.0000E+000	1.7066E+003	2.1471E-004	4.3835E+003
59	0.2328	1.2721E+003	1.0000E+000	1.7365E+003	2.1101E-004	4.3738E+003
60	0.2336	1.2951E+003	1.0000E+000	1.7657E+003	2.0752E-004	4.3413E+003
61	0.2344	1.3175E+003	1.0000E+000	1.7941E+003	2.0424E-004	4.2872E+003
62	0.2352	1.3391E+003	1.0000E+000	1.8215E+003	2.0116E-004	4.2132E+003
63	0.2359	1.3600E+003	1.0000E+000	1.8480E+003	1.9827E-004	4.1218E+003
64	0.2367	1.3801E+003	1.0000E+000	1.8735E+003	1.9558E-004	4.0157E+003
65	0.2375	1.3994E+003	1.0000E+000	1.8979E+003	1.9306E-004	3.8978E+003
66	0.2383	1.4178E+003	1.0000E+000	1.9213E+003	1.9072E-004	3.7711E+003
67	0.2391	1.4355E+003	1.0000E+000	1.9435E+003	1.8853E-004	3.6386E+003
68	0.2406	1.4682E+003	1.0000E+000	1.9847E+003	1.8462E-004	3.3674E+003
69	0.2422	1.4981E+003	1.0000E+000	2.0222E+003	1.8119E-004	3.0984E+003
70	0.2437	1.5255E+003	1.0000E+000	2.0564E+003	1.7819E-004	2.8435E+003
71	0.2453	1.5505E+003	1.0000E+000	2.0874E+003	1.7553E-004	2.6096E+003
72	0.2469	1.5734E+003	1.0000E+000	2.1157E+003	1.7319E-004	2.3995E+003
73	0.2500	1.6135E+003	1.0000E+000	2.1647E+003	1.6927E-004	2.0568E+003
74	0.2562	1.6776E+003	1.0000E+000	2.2418E+003	1.6345E-004	1.6018E+003

75	0.2625	1.7303E+003	1.0000E+000	2.3043E+003	1.5902E-004	1.3071E+003
76	0.2688	1.7748E+003	1.0000E+000	2.3566E+003	1.5549E-004	1.1038E+003
77	0.2750	1.8132E+003	1.0000E+000	2.4013E+003	1.5259E-004	9.5484E+002
78	0.2875	1.8747E+003	1.0000E+000	2.4719E+003	1.4823E-004	7.5408E+002
79	0.3000	1.9252E+003	1.0000E+000	2.5292E+003	1.4487E-004	6.1865E+002
80	0.3125	1.9678E+003	1.0000E+000	2.5771E+003	1.4218E-004	5.2130E+002
81	0.3250	2.0043E+003	1.0000E+000	2.6178E+003	1.3997E-004	4.4841E+002
82	0.3500	2.0616E+003	1.0000E+000	2.6809E+003	1.3667E-004	3.4993E+002
83	0.3750	2.1081E+003	1.0000E+000	2.7316E+003	1.3414E-004	2.8380E+002
84	0.4000	2.1468E+003	1.0000E+000	2.7736E+003	1.3211E-004	2.3664E+002
85	0.4250	2.1797E+003	1.0000E+000	2.8092E+003	1.3043E-004	2.0187E+002
86	0.4500	2.2067E+003	1.0000E+000	2.8392E+003	1.2906E-004	1.7680E+002
87	0.5000	2.2067E+003	1.0000E+000	2.8392E+003	1.2906E-004	1.7680E+002

Appendix:H

Premix Laminar Flame Model for H_2/air Mixtures with addition of KO_2 Mole Fraction at Different Equivalence Ratios (0.9, 1, 1.1)

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KEYWORD INPUT

!
! problem type definition
!
ENRG   ! Solve Gas Energy Equation
FLUX   ! Flux Balance for Inlet Species
FREE   ! Freely Propagating Flame
MIX   ! Use Mixture-averaged Transport
!
! physical property
!
EQUI 0.9   ! Equivalence Ratio
FLRT 1.0   ! Mass Flow Rate (g/cm2-sec)
PRES 1.0   ! Pressure (atm)
QLOS 0.0   ! Heat Flux Per Unit Length (cal/cm-sec)
TINF 298.0   ! Ambient Temperature (K)
TUNBURNT 673.0   ! Unburnt Gas Temperature (K)
!
! reactor dimension definition
!
CURV 0.5   ! Adaptive Grid Control Based On Solution Curvature
GRAD 0.1   ! Adaptive Grid Control Based On Solution Gradient
NADP 10   ! Number of Adaptive Grid Points
NPTS 6   ! Number of Uniform Grid Points
NTOT 250   ! Maximum Number of Grid Points Allowed
XEND 0.5   ! Ending Axial Position (cm)
XSTR 0.0   ! Starting Axial Position (cm)
!
! species property
!
ADD KO2 1.47E-5   ! Added Species Fraction of Total Reactant Species (mole fraction)
CPROD H2O   ! Complete-Combustion Products
CPROD N2   ! Complete-Combustion Products
FUEL H2 2.0   ! Fuel Fraction of Total Fuel Species (mole fraction)
MOLE   ! Print Mole Fractions
OXID N2 3.76   ! Oxidizer Fraction of Total Oxidizer Species (mole fraction)
OXID O2 1.0   ! Oxidizer Fraction of Total Oxidizer Species (mole fraction)
PRMN 0.0   ! Minimum for Product Estimates (mole fraction)
XIMN 0.0   ! Minimum for Estimated Intermediate Fraction (mole fraction)
!
! solver control
!
!USE_ADVANCED_TECHNIQUE   ! Advanced Solution Technique (Default)
ATIM 1.0E-9   ! Absolute Tolerance for Pseudo Timestepping
ATOL 1.0E-9   ! Absolute Tolerance
DTMN 1.0E-10   ! Minimum Pseudo Time Step (sec)
DTMX 0.01   ! Maximum Pseudo Time Step (sec)
IRET 25   ! Number Time Steps Before Increasing
ISTP 0   ! Number of Initial Pseudo Time Steps
MAXTIME 100   ! Maximum Number of Pseudo Time Stepping Operations Allowed
NDPR 100   ! Output Frequency during Integration
NJAC 20   ! Number of Iterations before Updating Jacobian
RTIM 0.0001   ! Relative Tolerance for Pseudo Timestepping
RTOL 0.0001   ! Relative Tolerance
SFLR -0.001   ! Minimum Bounds on Species Fractions
SPOS 0.0   ! Positive Value to Reset Species Fractions
SSMAXITER 100   ! Maximum Number of Iterations per Steady State Search
TIM1 100.0 1.0E-6   ! Pseudo Time Steps (Fixed Temperature) (none, sec)
TIM2 100.0 1.0E-6   ! Pseudo Time Steps (Energy Equation) (none, sec)
TJAC 20   ! Number of Transient Iterations before Updating Jacobian
TPROF   ! Automatic Estimated Temperature Profile
TRMAXITER 25   ! Maximum Number of Iterations per Pseudo Time Step
WDIF   ! Windward Differencing
!
! output control and other misc. property
!
DFAC 2.0   ! Time Step Decrement Factor
EPSS 0.001   ! Threshold for Species Sensitivity
FLT_NPOINTS 50   ! Flamelet Grid Points
```

```
         GFAC 1.0   ! Gas Reaction Rate Multiplier
         PRNT 1   ! Print Level Control
         SIZE 100000000   ! Solution Data Block Size (bytes)
         UFAC 2.0   ! Time Step Increment Factor
         ! Number of Continuation 0   ! Continuation Count

 FIRST SOLUTION ESTIMATE IS EQUILIBRIUM

 INFO...using default f(Tequilibrium) fixed temperature:   1584.61813457450

 TWOPNT:  DOUBLE PRECISION (TWO POINT BOUNDARY VALUE PROBLEM) SOLVER,
          VERSION 3.30 OF APRIL 1998 BY DR. JOSEPH F. GRCAR.

 TWOPNT:  INITIAL GUESS:

       X(cm)   T(K)            AREA(cm^2)      V(cm/s)         RHO(g/cm^3)     HDOT(cal/s/cm^3)


======
THIS IS THE FIRST CALL TO AREA
======

   1   0.0000  6.7300E+002     1.0000E+000     2.5700E+003     3.8911E-004    -1.5888E-005
   2   0.1000  6.7300E+002     1.0000E+000     2.5700E+003     3.8911E-004    -1.5888E-005
   3   0.2000  1.0625E+003     1.0000E+000     3.9362E+003     2.5405E-004     9.7424E+004
   4   0.2500  1.5846E+003     1.0000E+000     5.6444E+003     1.7717E-004     1.5878E+005
   5   0.3000  2.1067E+003     1.0000E+000     7.2259E+003     1.3839E-004     9.1688E+004
   6   0.4000  2.4962E+003     1.0000E+000     8.3315E+003     1.2003E-004     3.7476E-002
   7   0.5000  2.4962E+003     1.0000E+000     8.3315E+003     1.2003E-004     3.7476E-002

       X(cm)   MOLE FRACTIONS:
               H2              H               O               O2              OH              H2O             HO2
   1   0.0000  2.7439E-001     0.0000E+000     0.0000E+000     1.5244E-001     0.0000E+000     0.0000E+000     0.0000E+000
   2   0.1000  2.7439E-001     0.0000E+000     0.0000E+000     1.5244E-001     0.0000E+000     0.0000E+000     0.0000E+000
   3   0.2000  2.1854E-001     6.0202E-004     4.0070E-004     1.2359E-001     2.8025E-003     6.2594E-002     8.0228E-007
```

4	0.2500	1.4367E-001	1.4090E-003	9.3782E-004	8.4926E-002	6.5592E-003	1.4650E-001	1.8777E-006
5	0.3000	6.8812E-002	2.2160E-003	1.4749E-003	4.6260E-002	1.0316E-002	2.3041E-001	2.9532E-006
6	0.4000	1.2964E-002	2.8180E-003	1.8756E-003	1.7416E-002	1.3118E-002	2.9300E-001	3.7554E-006
7	0.5000	1.2964E-002	2.8180E-003	1.8756E-003	1.7416E-002	1.3118E-002	2.9300E-001	3.7554E-006

	X(cm)	MOLE FRACTIONS:						
		H2O2	C	CH	CH2	CH2(S)	CH3	CH4
1	0.0000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
2	0.1000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
3	0.2000	5.8131E-008	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
4	0.2500	1.3605E-007	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
5	0.3000	2.1398E-007	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
6	0.4000	2.7211E-007	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
7	0.5000	2.7211E-007	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000

	X(cm)	MOLE FRACTIONS:						
		CO	CO2	HCO	CH2O	CH2OH	CH3O	CH3OH
1	0.0000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
2	0.1000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
3	0.2000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
4	0.2500	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
5	0.3000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
6	0.4000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
7	0.5000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000

	X(cm)	MOLE FRACTIONS:						
		C2H	C2H2	C2H3	C2H4	C2H5	C2H6	HCCO
1	0.0000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
2	0.1000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
3	0.2000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
4	0.2500	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
5	0.3000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
6	0.4000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
7	0.5000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000

	X(cm)	MOLE FRACTIONS:						
		CH2CO	HCCOH	N	NH	NH2	NH3	NNH
1	0.0000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
2	0.1000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
3	0.2000	0.0000E+000	0.0000E+000	4.8939E-008	7.4441E-009	2.0882E-009	2.7465E-009	1.2122E-009
4	0.2500	0.0000E+000	0.0000E+000	1.1454E-007	1.7423E-008	4.8874E-009	6.4282E-009	2.8372E-009
5	0.3000	0.0000E+000	0.0000E+000	1.8014E-007	2.7402E-008	7.6867E-009	1.0110E-008	4.4622E-009
6	0.4000	0.0000E+000	0.0000E+000	2.2908E-007	3.4846E-008	9.7749E-009	1.2856E-008	5.6744E-009
7	0.5000	0.0000E+000	0.0000E+000	2.2908E-007	3.4846E-008	9.7749E-009	1.2856E-008	5.6744E-009

	X(cm)	MOLE FRACTIONS:						
		NO	NO2	N2O	HNO	CN	HCN	H2CN
1	0.0000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
2	0.1000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
3	0.2000	1.2835E-003	3.3145E-007	6.5282E-008	4.7933E-008	0.0000E+000	0.0000E+000	0.0000E+000
4	0.2500	3.0040E-003	7.7575E-007	1.5279E-007	1.1219E-007	0.0000E+000	0.0000E+000	0.0000E+000
5	0.3000	4.7246E-003	1.2201E-006	2.4030E-007	1.7644E-007	0.0000E+000	0.0000E+000	0.0000E+000
6	0.4000	6.0081E-003	1.5515E-006	3.0558E-007	2.2437E-007	0.0000E+000	0.0000E+000	0.0000E+000
7	0.5000	6.0081E-003	1.5515E-006	3.0558E-007	2.2437E-007	0.0000E+000	0.0000E+000	0.0000E+000

	X(cm)	MOLE FRACTIONS:						
		HCNN	HCNO	HOCN	HNCO	NCO	N2	AR
1	0.0000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	5.7316E-001	0.0000E+000
2	0.1000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	5.7316E-001	0.0000E+000
3	0.2000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	5.9017E-001	0.0000E+000
4	0.2500	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	6.1297E-001	0.0000E+000
5	0.3000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	6.3577E-001	0.0000E+000
6	0.4000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	6.5278E-001	0.0000E+000
7	0.5000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	6.5278E-001	0.0000E+000

	X(cm)	MOLE FRACTIONS:						
		C3H7	C3H8	CH2CHO	CH3CHO	K	KO	HKO
1	0.0000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
2	0.1000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
3	0.2000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	1.4458E-006	2.4226E-008	2.1219E-006
4	0.2500	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	3.3838E-006	5.6702E-008	4.9664E-006
5	0.3000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	5.3218E-006	8.9177E-008	7.8108E-006
6	0.4000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	6.7676E-006	1.1340E-007	9.9328E-006
7	0.5000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	6.7676E-006	1.1340E-007	9.9328E-006

	X(cm)	MOLE FRACTIONS:						
		KO2	HK	K2O	K2O2	K2CO3	K2H2O2	KHCO3
1	0.0000	1.4700E-005	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
2	0.1000	1.4700E-005	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
3	0.2000	1.1560E-005	1.0492E-009	2.0844E-015	3.4611E-017	0.0000E+000	2.4565E-015	0.0000E+000

3	0.2000	2.0922E-045	8.8631E-052	3.4861E-009	1.0016E-009	1.6387E-011	3.8893E-011	3.9605E-009
4	0.2500	1.2053E-043	1.4429E-048	6.7346E-008	1.8156E-008	1.5980E-010	6.2116E-011	4.9674E-008
5	0.3000	6.1016E-043	6.6327E-047	6.6453E-008	2.5432E-008	6.3773E-010	2.1623E-010	6.3115E-008
6	0.4000	4.0229E-042	2.7847E-045	2.3947E-007	2.7897E-008	1.7154E-009	7.1540E-010	5.4376E-008
7	0.5000	4.0229E-042	2.7847E-045	2.3947E-007	2.7897E-008	1.7154E-009	7.1540E-010	5.4376E-008

	X(cm)	MOLE FRACTIONS:						
		NO	NO2	N2O	HNO	CN	HCN	H2CN
1	0.0000	4.9447E-012	5.8058E-013	7.3267E-014	6.0638E-015	2.9296E-044	6.7986E-037	3.9163E-039
2	0.1000	1.2320E-009	1.6330E-010	2.2752E-011	1.4924E-012	7.3569E-042	2.0214E-034	1.1746E-036
3	0.2000	2.9947E-007	1.3242E-010	6.1730E-009	1.9383E-010	1.5981E-036	5.2012E-032	2.7067E-034
4	0.2500	6.1066E-006	7.3860E-010	5.2376E-008	1.8824E-009	1.6864E-032	4.0284E-030	1.7886E-033
5	0.3000	1.3329E-005	1.3148E-009	8.1043E-008	2.8106E-009	5.2583E-030	2.6715E-028	1.1446E-032
6	0.4000	4.7890E-005	6.0787E-009	1.3598E-007	5.1008E-009	1.0105E-028	3.0959E-027	3.3358E-032
7	0.5000	4.7890E-005	6.0787E-009	1.3598E-007	5.1008E-009	1.0105E-028	3.0959E-027	3.3358E-032

	X(cm)	MOLE FRACTIONS:						
		HCNN	HCNO	HOCN	HNCO	NCO	N2	AR
1	0.0000	5.0566E-043	4.6804E-042	9.4878E-041	9.2731E-036	2.6465E-038	5.7317E-001	0.0000E+000
2	0.1000	9.9716E-041	1.4483E-039	2.9352E-038	2.8689E-033	8.1509E-036	5.7393E-001	0.0000E+000
3	0.2000	1.1420E-035	3.9813E-037	8.1512E-036	7.7364E-031	6.4143E-033	5.9745E-001	0.0000E+000
4	0.2500	1.3369E-034	1.9706E-035	1.0702E-032	4.9267E-029	2.7608E-030	6.1313E-001	0.0000E+000
5	0.3000	5.4631E-035	1.1941E-034	1.6004E-030	9.1350E-028	2.1946E-028	6.1920E-001	0.0000E+000
6	0.4000	1.8826E-034	8.2551E-033	3.6538E-029	7.2439E-027	2.1626E-027	6.2581E-001	0.0000E+000
7	0.5000	1.8826E-034	8.2551E-033	3.6538E-029	7.2439E-027	2.1626E-027	6.2581E-001	0.0000E+000

	X(cm)	MOLE FRACTIONS:						
		C3H7	C3H8	CH2CHO	CH3CHO	K	KO	HKO
1	0.0000	1.5423E-077	6.1306E-076	6.4951E-052	7.7444E-053	5.0229E-015	1.2865E-015	6.3375E-010
2	0.1000	6.4668E-075	2.5811E-073	2.2508E-049	2.6951E-050	2.0247E-012	4.3811E-013	3.0921E-007
3	0.2000	8.5933E-072	9.2361E-071	1.0534E-046	2.8136E-048	5.1661E-009	1.8152E-009	1.5244E-005
4	0.2500	2.6570E-072	5.0105E-072	6.0324E-046	3.2331E-048	5.2151E-009	3.2153E-009	1.5707E-005
5	0.3000	1.0381E-073	3.6030E-074	2.9705E-046	2.5336E-048	2.4368E-007	1.0377E-007	1.5519E-005
6	0.4000	1.2098E-073	2.8606E-075	4.0129E-046	5.6707E-048	3.4717E-006	3.6695E-007	1.2184E-005
7	0.5000	1.2098E-073	2.8606E-075	4.0129E-046	5.6707E-048	3.4717E-006	3.6695E-007	1.2184E-005

	X(cm)	MOLE FRACTIONS:						
		KO2	HK	K2O	K2O2	K2CO3	K2H2O2	KHCO3
1	0.0000	1.4678E-005	8.6097E-014	2.9070E-017	3.5717E-018	3.5667E-041	9.6937E-012	1.8466E-020
2	0.1000	3.2431E-006	2.2187E-011	1.5822E-014	1.9750E-015	2.0114E-038	5.3693E-009	1.0114E-017
3	0.2000	2.3671E-008	1.2288E-008	6.6433E-013	8.7788E-013	6.0959E-033	7.0963E-009	1.0525E-017
4	0.2500	3.4739E-009	4.8075E-009	2.2252E-014	6.6535E-014	2.0324E-032	5.5870E-012	8.3383E-019
5	0.3000	1.7140E-009	1.3563E-008	1.0485E-014	8.5318E-015	4.3317E-032	1.4965E-013	2.7755E-021
6	0.4000	5.4628E-010	2.5607E-008	1.6196E-014	1.6967E-015	7.0932E-032	1.7301E-014	7.0765E-023
7	0.5000	5.4628E-010	2.5607E-008	1.6196E-014	1.6967E-015	7.0932E-032	1.7301E-014	7.0765E-023

	X(cm)	MOLE FRACTIONS:	
		KCO3	KO3
1	0.0000	1.2947E-022	2.0682E-008
2	0.1000	7.0841E-020	1.1159E-005
3	0.2000	8.1875E-020	1.9129E-008
4	0.2500	8.9901E-018	8.5330E-014
5	0.3000	3.9897E-018	6.3749E-016
6	0.4000	1.4692E-018	1.0076E-016
7	0.5000	1.4692E-018	1.0076E-016

TWOPNT: SUCCESS. PROBLEM SOLVED.

PREMIX: FINISHED FIXED TEMPERATURE CASE,ADDING THE ENERGY EQUATION.

TWOPNT: DOUBLE PRECISION (TWO POINT BOUNDARY VALUE PROBLEM) SOLVER,
VERSION 3.30 OF APRIL 1998 BY DR. JOSEPH F. GRCAR.

TWOPNT: INITIAL GUESS:

	X(cm)	T(K)	AREA(cm^2)	V(cm/s)	RHO(g/cm^3)	HDOT(cal/s/cm^3)
1	0.0000	6.7300E+002	1.0000E+000	2.5699E+003	3.8911E-004	1.7199E-001
2	0.1000	6.7300E+002	1.0000E+000	2.5665E+003	3.8963E-004	1.1621E+001
3	0.2000	1.0625E+003	1.0000E+000	3.8913E+003	2.5698E-004	2.1527E+003
4	0.2500	1.5846E+003	1.0000E+000	5.6558E+003	1.7681E-004	2.9156E+003
5	0.3000	2.1067E+003	1.0000E+000	7.4460E+003	1.3430E-004	9.1604E+002
6	0.4000	2.4962E+003	1.0000E+000	8.7293E+003	1.1456E-004	5.2660E+002
7	0.5000	2.4962E+003	1.0000E+000	8.7293E+003	1.1456E-004	5.2660E+002

	X(cm)	MOLE FRACTIONS:						
		H2	H	O	O2	OH	H2O	HO2
1	0.0000	2.7437E-001	3.9744E-007	1.7780E-009	1.5244E-001	1.9382E-008	3.6925E-006	5.7568E-007
2	0.1000	2.7296E-001	1.7815E-005	2.8445E-007	1.5219E-001	3.1575E-006	7.3507E-004	1.4112E-004
3	0.2000	1.8732E-001	9.7031E-003	1.2734E-003	1.1295E-001	9.5428E-004	9.0202E-002	1.2935E-004
4	0.2500	6.1313E-002	5.0655E-002	1.2293E-002	5.1634E-002	1.0877E-002	2.0003E-001	3.8006E-005

5	0.3000	1.7140E-009	1.3563E-008	1.0485E-014	8.5318E-015	4.3317E-032	1.4965E-013	2.7755E-021
6	0.4000	5.4628E-010	2.5607E-008	1.6196E-014	1.6967E-015	7.0932E-032	1.7301E-014	7.0765E-023
7	0.5000	5.4628E-010	2.5607E-008	1.6196E-014	1.6967E-015	7.0932E-032	1.7301E-014	7.0765E-023

	X(cm)	MOLE FRACTIONS: KCO3	KO3
1	0.0000	1.2947E-022	2.0682E-008
2	0.1000	7.0841E-020	1.1159E-005
3	0.2000	8.1875E-020	1.9129E-008
4	0.2500	8.9901E-018	8.5330E-014
5	0.3000	3.9897E-018	6.3749E-016
6	0.4000	1.4692E-018	1.0076E-016
7	0.5000	1.4692E-018	1.0076E-016

TWOPNT: SOLVE THE PROBLEM.

TASK	LOG10 NORM F	LOG10 COND J	REMARK
START	3.92		7 GRID POINTS
SEARCH	4.62	0.00	DIVERGING
EVOLVE	-4.91	0.00	100 TIME STEPS, 8.0E-06 LAST STRIDE
SEARCH	-6.23	0.00	1 SEARCH STEP
REFINE	-6.23		1.00 AND 1.00 RATIOS, 13 GRID POINTS
SEARCH	2.96	0.00	DIVERGING
EVOLVE	-2.77	0.00	100 TIME STEPS, 8.0E-06 LAST STRIDE
SEARCH	-3.76	0.00	1 SEARCH STEP
REFINE	-3.76		1.00 AND 1.00 RATIOS, 23 GRID POINTS
SEARCH	3.36	0.00	GOING OUT OF BOUNDS
EVOLVE	-1.14	0.00	100 TIME STEPS, 8.0E-06 LAST STRIDE
SEARCH	-2.95	0.00	2 SEARCH STEPS
REFINE	-2.95		0.96 AND 1.00 RATIOS, 33 GRID POINTS
SEARCH	2.26	0.00	DIVERGING
EVOLVE	-2.17	0.00	100 TIME STEPS, 8.0E-06 LAST STRIDE
SEARCH	-4.53	0.00	2 SEARCH STEPS
REFINE	-4.53		0.96 AND 1.00 RATIOS, 43 GRID POINTS
SEARCH	-5.41	0.00	16 SEARCH STEPS
REFINE	-5.41		0.79 AND 1.00 RATIOS, 53 GRID POINTS
SEARCH	-4.56	0.00	14 SEARCH STEPS
REFINE	-4.56		0.49 AND 0.92 RATIOS, 63 GRID POINTS
SEARCH	-3.77	0.00	10 SEARCH STEPS
REFINE	-3.77		0.28 AND 0.92 RATIOS, 73 GRID POINTS
SEARCH	-2.94	0.00	7 SEARCH STEPS
REFINE	-2.94		0.30 AND 0.92 RATIOS, 83 GRID POINTS
SEARCH	-2.00	0.00	5 SEARCH STEPS
REFINE	-2.00		0.30 AND 0.82 RATIOS, 93 GRID POINTS
SEARCH	-2.79	0.00	12 SEARCH STEPS
REFINE	-2.79		0.15 AND 0.83 RATIOS, 103 GRID POINTS
SEARCH	-3.01	0.00	9 SEARCH STEPS
REFINE	-3.01		0.15 AND 0.83 RATIOS, 113 GRID POINTS
SEARCH	-3.00	0.00	13 SEARCH STEPS
REFINE	-3.00		0.15 AND 0.83 RATIOS, 123 GRID POINTS
SEARCH	-2.96	0.00	6 SEARCH STEPS
REFINE	-2.96		0.10 AND 0.80 RATIOS, 125 GRID POINTS
SEARCH	-3.67	0.00	4 SEARCH STEPS
REFINE	-3.67		0.10 AND 0.75 RATIOS, 127 GRID POINTS
SEARCH	-5.42	0.00	4 SEARCH STEPS
REFINE	-5.42		0.10 AND 0.61 RATIOS, 129 GRID POINTS
SEARCH	-4.44	0.00	3 SEARCH STEPS
REFINE	-4.44		0.10 AND 0.45 RATIOS

TWOPNT: FINAL SOLUTION:

X(cm)	T(K)	AREA(cm^2)	V(cm/s)	RHO(g/cm^3)	HDOT(cal/s/cm^3)

81	0.2414	1.3537E+003	1.0000E+000	1.6134E+003	2.0616E-004	4.7327E+003
82	0.2422	1.3801E+003	1.0000E+000	1.6428E+003	2.0247E-004	4.6478E+003
83	0.2430	1.4054E+003	1.0000E+000	1.6711E+003	1.9904E-004	4.5372E+003
84	0.2437	1.4296E+003	1.0000E+000	1.6982E+003	1.9587E-004	4.4052E+003
85	0.2445	1.4528E+003	1.0000E+000	1.7240E+003	1.9294E-004	4.2563E+003
86	0.2453	1.4747E+003	1.0000E+000	1.7485E+003	1.9023E-004	4.0952E+003
87	0.2461	1.4956E+003	1.0000E+000	1.7718E+003	1.8773E-004	3.9266E+003
88	0.2469	1.5154E+003	1.0000E+000	1.7938E+003	1.8542E-004	3.7544E+003
89	0.2477	1.5342E+003	1.0000E+000	1.8147E+003	1.8329E-004	3.5822E+003
90	0.2484	1.5520E+003	1.0000E+000	1.8344E+003	1.8132E-004	3.4130E+003
91	0.2500	1.5846E+003	1.0000E+000	1.8704E+003	1.7783E-004	3.0939E+003
92	0.2516	1.6142E+003	1.0000E+000	1.9028E+003	1.7481E-004	2.8043E+003
93	0.2531	1.6410E+003	1.0000E+000	1.9320E+003	1.7216E-004	2.5484E+003
94	0.2562	1.6876E+003	1.0000E+000	1.9821E+003	1.6781E-004	2.1439E+003
95	0.2594	1.7279E+003	1.0000E+000	2.0249E+003	1.6426E-004	1.8410E+003
96	0.2625	1.7634E+003	1.0000E+000	2.0623E+003	1.6128E-004	1.6126E+003
97	0.2656	1.7952E+003	1.0000E+000	2.0955E+003	1.5873E-004	1.4367E+003
98	0.2688	1.8239E+003	1.0000E+000	2.1252E+003	1.5651E-004	1.2975E+003
99	0.2750	1.8734E+003	1.0000E+000	2.1756E+003	1.5288E-004	1.0943E+003
100	0.2812	1.9164E+003	1.0000E+000	2.2191E+003	1.4989E-004	9.4832E+002
101	0.2875	1.9546E+003	1.0000E+000	2.2573E+003	1.4735E-004	8.3843E+002
102	0.2938	1.9889E+003	1.0000E+000	2.2913E+003	1.4516E-004	7.5275E+002
103	0.3000	2.0201E+003	1.0000E+000	2.3221E+003	1.4324E-004	6.8386E+002
104	0.3063	2.0487E+003	1.0000E+000	2.3502E+003	1.4153E-004	6.2686E+002
105	0.3125	2.0751E+003	1.0000E+000	2.3759E+003	1.3999E-004	5.7839E+002
106	0.3188	2.0996E+003	1.0000E+000	2.3997E+003	1.3861E-004	5.3613E+002
107	0.3250	2.1223E+003	1.0000E+000	2.4217E+003	1.3735E-004	4.9851E+002
108	0.3313	2.1435E+003	1.0000E+000	2.4421E+003	1.3620E-004	4.6449E+002
109	0.3375	2.1632E+003	1.0000E+000	2.4610E+003	1.3515E-004	4.3337E+002
110	0.3438	2.1815E+003	1.0000E+000	2.4786E+003	1.3420E-004	4.0474E+002
111	0.3500	2.1986E+003	1.0000E+000	2.4949E+003	1.3332E-004	3.7836E+002
112	0.3625	2.2288E+003	1.0000E+000	2.5235E+003	1.3181E-004	3.3189E+002
113	0.3750	2.2553E+003	1.0000E+000	2.5485E+003	1.3051E-004	2.9193E+002
114	0.3875	2.2786E+003	1.0000E+000	2.5704E+003	1.2940E-004	2.5751E+002
115	0.4000	2.2993E+003	1.0000E+000	2.5898E+003	1.2843E-004	2.2788E+002
116	0.4125	2.3176E+003	1.0000E+000	2.6068E+003	1.2759E-004	2.0235E+002
117	0.4250	2.3340E+003	1.0000E+000	2.6220E+003	1.2685E-004	1.8031E+002
118	0.4375	2.3487E+003	1.0000E+000	2.6356E+003	1.2620E-004	1.6118E+002
119	0.4437	2.3556E+003	1.0000E+000	2.6420E+003	1.2589E-004	1.5247E+002
120	0.4500	2.3621E+003	1.0000E+000	2.6481E+003	1.2561E-004	1.4439E+002
121	0.4625	2.3739E+003	1.0000E+000	2.6591E+003	1.2509E-004	1.3007E+002
122	0.4688	2.3795E+003	1.0000E+000	2.6644E+003	1.2484E-004	1.2357E+002
123	0.4750	2.3848E+003	1.0000E+000	2.6694E+003	1.2460E-004	1.1758E+002
124	0.4812	2.3898E+003	1.0000E+000	2.6743E+003	1.2438E-004	1.1214E+002
125	0.4875	2.3944E+003	1.0000E+000	2.6789E+003	1.2416E-004	1.0729E+002
126	0.4906	2.3965E+003	1.0000E+000	2.6810E+003	1.2406E-004	1.0504E+002
127	0.4938	2.3982E+003	1.0000E+000	2.6828E+003	1.2398E-004	1.0313E+002
128	0.4969	2.3993E+003	1.0000E+000	2.6840E+003	1.2393E-004	1.0173E+002
129	0.5000	2.3993E+003	1.0000E+000	2.6840E+003	1.2393E-004	1.0173E+002

	X(cm)	MOLE FRACTIONS:						
		H2	H	O	O2	OH	H2O	HO2
1	0.0000	2.7439E-001	1.2625E-011	3.5235E-015	1.5244E-001	1.0881E-012	8.3074E-011	6.4028E-011
2	0.0500	2.7439E-001	1.0461E-010	9.6607E-014	1.5244E-001	3.0363E-011	2.8172E-009	2.6610E-009
3	0.0750	2.7439E-001	1.0981E-010	1.0171E-013	1.5244E-001	3.0767E-011	4.2020E-009	4.0224E-009
4	0.1000	2.7439E-001	1.1052E-010	1.0243E-013	1.5244E-001	3.0840E-011	5.5908E-009	5.3947E-009
5	0.1250	2.7439E-001	1.1098E-010	1.0289E-013	1.5244E-001	3.0905E-011	6.9942E-009	6.8212E-009
6	0.1500	2.7439E-001	1.2061E-010	1.1198E-013	1.5244E-001	3.0988E-011	8.6047E-009	9.2883E-009
7	0.1625	2.7438E-001	3.0123E-010	2.8134E-013	1.5244E-001	3.1380E-011	1.0743E-008	1.7919E-008
8	0.1750	2.7438E-001	2.9678E-009	2.7844E-012	1.5244E-001	3.7279E-011	2.4665E-008	9.5139E-008
9	0.1875	2.7435E-001	4.2895E-008	4.0498E-011	1.5244E-001	1.7286E-010	1.4623E-007	7.6898E-007
10	0.1938	2.7431E-001	2.7176E-007	2.5959E-010	1.5245E-001	1.8230E-009	5.7002E-007	2.6606E-006
11	0.2000	2.7421E-001	1.4731E-006	1.4972E-009	1.5246E-001	2.4168E-008	2.6516E-006	9.9159E-006
12	0.2031	2.7409E-001	4.0171E-006	4.3673E-009	1.5248E-001	1.1315E-007	6.4740E-006	1.8968E-005
13	0.2047	2.7400E-001	6.7522E-006	7.7787E-009	1.5249E-001	2.5815E-007	1.0828E-005	2.6577E-005
14	0.2063	2.7387E-001	1.1246E-005	1.4146E-008	1.5250E-001	5.8823E-007	1.8887E-005	3.7815E-005
15	0.2078	2.7369E-001	1.8621E-005	2.6338E-008	1.5251E-001	1.3152E-006	3.3465E-005	5.3710E-005
16	0.2086	2.7357E-001	2.4067E-005	3.6632E-008	1.5252E-001	1.9708E-006	4.4882E-005	6.3643E-005
17	0.2094	2.7343E-001	3.1093E-005	5.1688E-008	1.5253E-001	2.9491E-006	6.0668E-005	7.5277E-005
18	0.2102	2.7327E-001	4.0139E-005	7.4093E-008	1.5254E-001	4.3859E-006	8.2313E-005	8.8666E-005
19	0.2109	2.7307E-001	5.1766E-005	1.0826E-007	1.5255E-001	6.4599E-006	1.1171E-004	1.0376E-004
20	0.2113	2.7296E-001	5.8813E-005	1.3273E-007	1.5255E-001	7.8184E-006	1.3019E-004	1.1187E-004
21	0.2117	2.7283E-001	6.6814E-005	1.6455E-007	1.5256E-001	9.4484E-006	1.5190E-004	1.2038E-004
22	0.2121	2.7270E-001	7.5893E-005	2.0680E-007	1.5256E-001	1.1394E-005	1.7735E-004	1.2923E-004
23	0.2125	2.7255E-001	8.6189E-005	2.6412E-007	1.5256E-001	1.3703E-005	2.0709E-004	1.3837E-004
24	0.2129	2.7239E-001	9.7856E-005	3.4361E-007	1.5257E-001	1.6429E-005	2.4176E-004	1.4773E-004
25	0.2133	2.7221E-001	1.1107E-004	4.5588E-007	1.5257E-001	1.9630E-005	2.8207E-004	1.5723E-004
26	0.2137	2.7202E-001	1.2602E-004	6.1645E-007	1.5257E-001	2.3368E-005	3.2882E-004	1.6677E-004
27	0.2141	2.7181E-001	1.4294E-004	8.4699E-007	1.5257E-001	2.7707E-005	3.8288E-004	1.7624E-004
28	0.2145	2.7158E-001	1.6205E-004	1.1760E-006	1.5257E-001	3.2716E-005	4.4522E-004	1.8554E-004

29	0.2148	2.7133E-001	1.8365E-004	1.6381E-006	1.5257E-001	3.8460E-005	5.1691E-004	1.9455E-004
30	0.2152	2.7106E-001	2.0801E-004	2.2711E-006	1.5256E-001	4.5009E-005	5.9913E-004	2.0314E-004
31	0.2156	2.7077E-001	2.3549E-004	3.1115E-006	1.5256E-001	5.2428E-005	6.9316E-004	2.1119E-004
32	0.2164	2.7010E-001	3.0086E-004	5.5066E-006	1.5254E-001	7.0077E-005	9.2087E-004	2.2531E-004
33	0.2172	2.6933E-001	3.8307E-004	8.8993E-006	1.5250E-001	9.1607E-005	1.2064E-003	2.3644E-004
34	0.2180	2.6843E-001	4.8605E-004	1.3340E-005	1.5245E-001	1.1729E-004	1.5600E-003	2.4423E-004
35	0.2188	2.6739E-001	6.1449E-004	1.8945E-005	1.5238E-001	1.4727E-004	1.9927E-003	2.4863E-004
36	0.2195	2.6620E-001	7.7390E-004	2.5962E-005	1.5229E-001	1.8153E-004	2.5166E-003	2.4988E-004
37	0.2203	2.6483E-001	9.7062E-004	3.4776E-005	1.5216E-001	2.1993E-004	3.1444E-003	2.4838E-004
38	0.2211	2.6326E-001	1.2119E-003	4.5928E-005	1.5200E-001	2.6220E-004	3.8901E-003	2.4466E-004
39	0.2219	2.6148E-001	1.5059E-003	6.0158E-005	1.5180E-001	3.0800E-004	4.7684E-003	2.3921E-004
40	0.2227	2.5946E-001	1.8615E-003	7.8464E-005	1.5155E-001	3.5687E-004	5.7956E-003	2.3249E-004
41	0.2234	2.5719E-001	2.2884E-003	1.0219E-004	1.5124E-001	4.0833E-004	6.9897E-003	2.2488E-004
42	0.2250	2.5182E-001	3.3838E-003	1.7111E-004	1.5041E-001	5.1711E-004	9.9329E-003	2.0797E-004
43	0.2266	2.4526E-001	4.8675E-003	2.8117E-004	1.4932E-001	6.3364E-004	1.3623E-002	1.9051E-004
44	0.2273	2.4147E-001	5.7851E-003	3.5946E-004	1.4867E-001	6.9651E-004	1.5785E-002	1.8191E-004
45	0.2277	2.3944E-001	6.2931E-003	4.0665E-004	1.4830E-001	7.2957E-004	1.6965E-002	1.7767E-004
46	0.2281	2.3730E-001	6.8356E-003	4.6021E-004	1.4790E-001	7.6393E-004	1.8220E-002	1.7347E-004
47	0.2285	2.3506E-001	7.4136E-003	5.2079E-004	1.4747E-001	7.9979E-004	1.9555E-002	1.6932E-004
48	0.2289	2.3272E-001	8.0280E-003	5.8906E-004	1.4700E-001	8.3739E-004	2.0974E-002	1.6524E-004
49	0.2291	2.3150E-001	8.3493E-003	6.2633E-004	1.4675E-001	8.5697E-004	2.1717E-002	1.6322E-004
50	0.2293	2.3026E-001	8.6802E-003	6.6586E-004	1.4649E-001	8.7712E-004	2.2485E-002	1.6123E-004
51	0.2295	2.2900E-001	9.0207E-003	7.0774E-004	1.4622E-001	8.9792E-004	2.3277E-002	1.5925E-004
52	0.2297	2.2770E-001	9.3709E-003	7.5206E-004	1.4593E-001	9.1943E-004	2.4094E-002	1.5729E-004
53	0.2299	2.2637E-001	9.7309E-003	7.9889E-004	1.4563E-001	9.4172E-004	2.4938E-002	1.5536E-004
54	0.2301	2.2502E-001	1.0101E-002	8.4833E-004	1.4532E-001	9.6489E-004	2.5809E-002	1.5344E-004
55	0.2303	2.2364E-001	1.0481E-002	9.0044E-004	1.4500E-001	9.8904E-004	2.6707E-002	1.5155E-004
56	0.2305	2.2223E-001	1.0871E-002	9.5531E-004	1.4466E-001	1.0143E-003	2.7634E-002	1.4968E-004
57	0.2307	2.2079E-001	1.1271E-002	1.0130E-003	1.4431E-001	1.0407E-003	2.8591E-002	1.4783E-004
58	0.2309	2.1932E-001	1.1681E-002	1.0736E-003	1.4394E-001	1.0684E-003	2.9577E-002	1.4601E-004
59	0.2311	2.1783E-001	1.2101E-002	1.1371E-003	1.4355E-001	1.0975E-003	3.0593E-002	1.4421E-004
60	0.2313	2.1630E-001	1.2531E-002	1.2037E-003	1.4315E-001	1.1282E-003	3.1642E-002	1.4244E-004
61	0.2314	2.1474E-001	1.2971E-002	1.2733E-003	1.4273E-001	1.1606E-003	3.2722E-002	1.4070E-004
62	0.2316	2.1316E-001	1.3421E-002	1.3461E-003	1.4229E-001	1.1947E-003	3.3835E-002	1.3898E-004
63	0.2318	2.1155E-001	1.3881E-002	1.4222E-003	1.4183E-001	1.2306E-003	3.4982E-002	1.3728E-004
64	0.2320	2.0990E-001	1.4351E-002	1.5014E-003	1.4135E-001	1.2685E-003	3.6162E-002	1.3561E-004
65	0.2322	2.0823E-001	1.4831E-002	1.5841E-003	1.4086E-001	1.3084E-003	3.7378E-002	1.3397E-004
66	0.2324	2.0654E-001	1.5320E-002	1.6701E-003	1.4034E-001	1.3504E-003	3.8629E-002	1.3235E-004
67	0.2326	2.0481E-001	1.5818E-002	1.7596E-003	1.3980E-001	1.3946E-003	3.9916E-002	1.3076E-004
68	0.2328	2.0306E-001	1.6326E-002	1.8525E-003	1.3924E-001	1.4410E-003	4.1239E-002	1.2919E-004
69	0.2330	2.0128E-001	1.6843E-002	1.9490E-003	1.3865E-001	1.4897E-003	4.2600E-002	1.2764E-004
70	0.2332	1.9947E-001	1.7368E-002	2.0492E-003	1.3805E-001	1.5408E-003	4.3998E-002	1.2612E-004
71	0.2336	1.9577E-001	1.8444E-002	2.2603E-003	1.3676E-001	1.6503E-003	4.6908E-002	1.2315E-004
72	0.2344	1.8809E-001	2.0690E-002	2.7251E-003	1.3390E-001	1.8997E-003	5.3168E-002	1.1745E-004
73	0.2352	1.8008E-001	2.3037E-002	3.2431E-003	1.3069E-001	2.1903E-003	5.9967E-002	1.1205E-004
74	0.2359	1.7179E-001	2.5458E-002	3.8114E-003	1.2714E-001	2.5240E-003	6.7271E-002	1.0688E-004
75	0.2367	1.6330E-001	2.7923E-002	4.4252E-003	1.2325E-001	2.9011E-003	7.5028E-002	1.0192E-004
76	0.2375	1.5470E-001	3.0398E-002	5.0776E-003	1.1907E-001	3.3199E-003	8.3163E-002	9.7099E-005
77	0.2383	1.4607E-001	3.2848E-002	5.7599E-003	1.1464E-001	3.7774E-003	9.1587E-002	9.2399E-005
78	0.2391	1.3750E-001	3.5238E-002	6.4625E-003	1.1002E-001	4.2688E-003	1.0020E-001	8.7799E-005
79	0.2398	1.2909E-001	3.7535E-002	7.1751E-003	1.0527E-001	4.7882E-003	1.0888E-001	8.3292E-005
80	0.2406	1.2092E-001	3.9710E-002	7.8873E-003	1.0047E-001	5.3290E-003	1.1754E-001	7.8883E-005
81	0.2414	1.1307E-001	4.1735E-002	8.5890E-003	9.5673E-002	5.8845E-003	1.2605E-001	7.4586E-005
82	0.2422	1.0561E-001	4.3590E-002	9.2714E-003	9.0957E-002	6.4478E-003	1.3433E-001	7.0423E-005
83	0.2430	9.8578E-002	4.5261E-002	9.9265E-003	8.6375E-002	7.0126E-003	1.4229E-001	6.6416E-005
84	0.2437	9.2023E-002	4.6737E-002	1.0548E-002	8.1975E-002	7.5734E-003	1.4986E-001	6.2589E-005
85	0.2445	8.5967E-002	4.8016E-002	1.1130E-002	7.7798E-002	8.1254E-003	1.5699E-001	5.8963E-005
86	0.2453	8.0420E-002	4.9098E-002	1.1670E-002	7.3872E-002	8.6646E-003	1.6364E-001	5.5553E-005
87	0.2461	7.5380E-002	4.9988E-002	1.2166E-002	7.0218E-002	9.1879E-003	1.6980E-001	5.2373E-005
88	0.2469	7.0835E-002	5.0695E-002	1.2616E-002	6.6847E-002	9.6929E-003	1.7545E-001	4.9428E-005
89	0.2477	6.6766E-002	5.1232E-002	1.3021E-002	6.3764E-002	1.0178E-002	1.8060E-001	4.6720E-005
90	0.2484	6.3147E-002	5.1610E-002	1.3381E-002	6.0968E-002	1.0642E-002	1.8525E-001	4.4247E-005
91	0.2500	5.7166E-002	5.1937E-002	1.3969E-002	5.6223E-002	1.1502E-002	1.9316E-001	3.9988E-005
92	0.2516	5.2539E-002	5.1820E-002	1.4410E-002	5.2380E-002	1.2280E-002	1.9956E-001	3.6472E-005
93	0.2531	4.9009E-002	5.1367E-002	1.4723E-002	4.9314E-002	1.2979E-002	2.0469E-001	3.3595E-005
94	0.2562	4.4525E-002	4.9742E-002	1.5015E-002	4.5135E-002	1.4142E-002	2.1188E-001	2.9406E-005
95	0.2594	4.1953E-002	4.7699E-002	1.5033E-002	4.2401E-002	1.5084E-002	2.1680E-001	2.6434E-005
96	0.2625	4.0458E-002	4.5536E-002	1.4875E-002	4.0563E-002	1.5849E-002	2.2035E-001	2.4233E-005
97	0.2656	3.9543E-002	4.3409E-002	1.4617E-002	3.9265E-002	1.6477E-002	2.2309E-001	2.2523E-005
98	0.2688	3.8923E-002	4.1391E-002	1.4306E-002	3.8293E-002	1.6998E-002	2.2534E-001	2.1134E-005
99	0.2750	3.8090E-002	3.7773E-002	1.3623E-002	3.6930E-002	1.7783E-002	2.2899E-001	1.9001E-005
100	0.2812	3.7372E-002	3.4639E-002	1.2943E-002	3.5861E-002	1.8371E-002	2.3215E-001	1.7302E-005
101	0.2875	3.6667E-002	3.1908E-002	1.2294E-002	3.4953E-002	1.8819E-002	2.3502E-001	1.5888E-005
102	0.2938	3.5949E-002	2.9504E-002	1.1682E-002	3.4148E-002	1.9160E-002	2.3769E-001	1.4679E-005
103	0.3000	3.5220E-002	2.7369E-002	1.1109E-002	3.3418E-002	1.9418E-002	2.4019E-001	1.3627E-005
104	0.3063	3.4483E-002	2.5458E-002	1.0572E-002	3.2747E-002	1.9607E-002	2.4255E-001	1.2702E-005
105	0.3125	3.3744E-002	2.3737E-002	1.0069E-002	3.2124E-002	1.9740E-002	2.4480E-001	1.1882E-005
106	0.3188	3.3009E-002	2.2182E-002	9.5989E-003	3.1543E-002	1.9827E-002	2.4692E-001	1.1151E-005
107	0.3250	3.2281E-002	2.0772E-002	9.1592E-003	3.1000E-002	1.9873E-002	2.4895E-001	1.0498E-005
108	0.3313	3.1565E-002	1.9490E-002	8.7485E-003	3.0489E-002	1.9887E-002	2.5088E-001	9.9136E-006

109	0.3375	3.0864E-002	1.8324E-002	8.3655E-003	3.0010E-002	1.9873E-002	2.5271E-001	9.3898E-006
110	0.3438	3.0180E-002	1.7263E-002	8.0089E-003	2.9559E-002	1.9835E-002	2.5444E-001	8.9205E-006
111	0.3500	2.9517E-002	1.6297E-002	7.6776E-003	2.9136E-002	1.9778E-002	2.5609E-001	8.5009E-006
112	0.3625	2.8262E-002	1.4628E-002	7.0904E-003	2.8382E-002	1.9619E-002	2.5908E-001	7.7997E-006
113	0.3750	2.7086E-002	1.3216E-002	6.5772E-003	2.7711E-002	1.9420E-002	2.6179E-001	7.2291E-006
114	0.3875	2.5990E-002	1.2015E-002	6.1281E-003	2.7111E-002	1.9195E-002	2.6425E-001	6.7637E-006
115	0.4000	2.4973E-002	1.0987E-002	5.7340E-003	2.6575E-002	1.8955E-002	2.6647E-001	6.3827E-006
116	0.4125	2.4031E-002	1.0103E-002	5.3870E-003	2.6094E-002	1.8709E-002	2.6848E-001	6.0696E-006
117	0.4250	2.3160E-002	9.3373E-003	5.0803E-003	2.5661E-002	1.8461E-002	2.7032E-001	5.8111E-006
118	0.4375	2.2354E-002	8.6697E-003	4.8076E-003	2.5269E-002	1.8216E-002	2.7199E-001	5.5963E-006
119	0.4437	2.1974E-002	8.3663E-003	4.6815E-003	2.5083E-002	1.8096E-002	2.7277E-001	5.5016E-006
120	0.4500	2.1612E-002	8.0847E-003	4.5635E-003	2.4907E-002	1.7978E-002	2.7352E-001	5.4158E-006
121	0.4625	2.0949E-002	7.5849E-003	4.3513E-003	2.4581E-002	1.7754E-002	2.7490E-001	5.2685E-006
122	0.4688	2.0646E-002	7.3615E-003	4.2544E-003	2.4424E-002	1.7648E-002	2.7554E-001	5.2039E-006
123	0.4750	2.0372E-002	7.1600E-003	4.1656E-003	2.4271E-002	1.7550E-002	2.7614E-001	5.1459E-006
124	0.4812	2.0133E-002	6.9835E-003	4.0861E-003	2.4123E-002	1.7462E-002	2.7669E-001	5.0947E-006
125	0.4875	1.9942E-002	6.8383E-003	4.0185E-003	2.3979E-002	1.7391E-002	2.7717E-001	5.0509E-006
126	0.4906	1.9870E-002	6.7819E-003	3.9909E-003	2.3912E-002	1.7363E-002	2.7738E-001	5.0328E-006
127	0.4938	1.9818E-002	6.7400E-003	3.9697E-003	2.3853E-002	1.7344E-002	2.7754E-001	5.0184E-006
128	0.4969	1.9790E-002	6.7166E-003	3.9570E-003	2.3814E-002	1.7333E-002	2.7764E-001	5.0095E-006
129	0.5000	1.9790E-002	6.7166E-003	3.9570E-003	2.3814E-002	1.7333E-002	2.7764E-001	5.0095E-006

	X(cm)	MOLE FRACTIONS:						
		H2O2	C	CH	CH2	CH2(S)	CH3	CH4
1	0.0000	2.5814E-015	5.0000E-070	1.8927E-061	9.0200E-053	1.0772E-053	2.9489E-043	3.8231E-043
2	0.0500	1.0795E-013	1.4651E-068	4.8776E-060	3.3938E-051	4.0529E-052	1.1328E-041	1.4728E-041
3	0.0750	1.8913E-013	3.1119E-067	9.8696E-059	6.5422E-050	7.8125E-051	2.1550E-040	1.9472E-040
4	0.1000	3.0126E-013	6.9256E-066	2.2154E-057	1.4591E-048	1.7426E-049	4.7954E-039	3.3835E-039
5	0.1250	4.8195E-013	-4.3624E-063	4.7568E-056	3.1324E-047	3.9122E-048	1.0743E-037	5.8202E-038
6	0.1500	1.4916E-012	-1.9449E-058	-2.0682E-053	-8.4783E-045	8.6875E-047	2.4075E-036	9.5789E-037
7	0.1625	8.2185E-012	-3.1415E-054	-2.4378E-049	-2.2139E-041	-1.6852E-045	2.2025E-035	6.1945E-036
8	0.1750	8.1448E-011	-3.3832E-050	-3.6174E-045	-3.5608E-038	-4.0139E-042	2.3939E-034	5.1142E-035
9	0.1875	8.8081E-010	-3.6129E-046	-5.1559E-041	-5.7253E-035	-6.7640E-039	2.6469E-033	4.1523E-034
10	0.1938	4.0164E-009	-1.2040E-042	-1.6285E-037	-3.4564E-032	-1.2257E-035	1.3154E-032	1.4416E-033
11	0.2000	2.0729E-008	-4.4935E-043	-1.0623E-038	-5.2262E-034	-6.1248E-038	1.1932E-032	3.5436E-033
12	0.2031	4.8700E-008	1.0460E-042	-2.4994E-037	-3.6640E-033	2.1931E-037	1.1672E-032	7.3829E-033
13	0.2047	7.8177E-008	9.1356E-042	-1.4136E-037	1.5250E-033	-1.0362E-037	1.0775E-032	1.2305E-032
14	0.2063	1.3052E-007	-1.3044E-040	1.4299E-037	-3.8134E-033	5.7375E-038	9.7013E-033	2.2629E-032
15	0.2078	2.1987E-007	3.6623E-041	5.8631E-038	-1.7252E-034	7.7546E-038	8.4940E-033	4.4545E-032
16	0.2086	2.8480E-007	4.1926E-040	-1.4113E-037	1.5096E-033	1.7977E-037	7.8549E-033	6.4870E-032
17	0.2094	3.7012E-007	-1.5515E-040	2.2157E-036	3.8451E-033	1.8964E-037	7.1844E-033	9.6887E-032
18	0.2102	4.8045E-007	-1.8131E-039	-1.1186E-035	-2.1806E-032	3.9069E-036	6.5364E-033	1.4738E-031
19	0.2109	6.2044E-007	1.0488E-037	2.6756E-035	4.8366E-032	-4.5546E-036	5.7245E-033	2.2710E-031
20	0.2113	7.0304E-007	8.0753E-038	1.5697E-035	2.3416E-032	5.7818E-036	4.2990E-033	2.8432E-031
21	0.2117	7.9581E-007	1.8255E-037	-3.5189E-035	8.3428E-032	4.8036E-036	2.6207E-033	3.5818E-031
22	0.2121	8.9946E-007	-2.3243E-037	-2.0253E-034	-1.1348E-031	-1.1077E-035	4.7223E-034	4.5350E-031
23	0.2125	1.0146E-006	-3.0412E-037	-1.3388E-034	-3.9610E-031	-2.9851E-035	-2.1653E-033	5.7654E-031
24	0.2129	1.1418E-006	-2.1758E-037	3.6976E-034	3.8180E-031	-1.3705E-035	-5.7624E-033	7.3516E-031
25	0.2133	1.2815E-006	-2.0244E-036	-8.1950E-034	2.5692E-032	-9.5040E-035	-2.6742E-033	9.4061E-031
26	0.2137	1.4339E-006	2.2728E-036	-2.1131E-033	-1.8627E-030	-1.4884E-034	7.2822E-033	1.2065E-030
27	0.2141	1.5991E-006	-4.4032E-036	-1.3153E-033	-6.7971E-031	-8.2834E-035	-1.7228E-033	1.5498E-030
28	0.2145	1.7772E-006	-2.6809E-036	-5.6474E-034	-2.4768E-031	-3.1088E-035	-4.0298E-033	1.9925E-030
29	0.2148	1.9679E-006	-1.3160E-036	-2.3363E-034	-9.0017E-032	-1.1415E-035	-3.5408E-033	2.5634E-030
30	0.2152	2.1709E-006	-6.0857E-037	-9.5441E-035	-3.2350E-032	-3.9233E-036	-1.7749E-033	3.2993E-030
31	0.2156	2.3856E-006	-1.8853E-037	-4.3238E-035	-1.0523E-032	-9.4258E-037	7.6106E-034	4.2473E-030
32	0.2164	2.8485E-006	-9.0645E-038	-9.7010E-036	-1.7911E-033	2.0730E-036	7.2149E-033	6.9619E-030
33	0.2172	3.3451E-006	-1.5899E-038	-1.3783E-036	-2.5675E-034	6.6669E-036	1.7227E-032	1.1227E-029
34	0.2180	3.8678E-006	6.9617E-039	4.8986E-037	6.4994E-035	1.6255E-035	3.3073E-032	1.7912E-029
35	0.2188	4.4094E-006	4.2221E-038	2.3476E-036	2.8036E-034	3.8342E-035	6.0422E-032	2.8367E-029
36	0.2195	4.9624E-006	1.5291E-037	6.7871E-036	6.4004E-034	8.8256E-035	1.0844E-031	4.4663E-029
37	0.2203	5.5191E-006	5.2390E-037	1.8610E-035	1.4049E-033	2.0118E-034	1.9393E-031	6.9974E-029
38	0.2211	6.0707E-006	1.7548E-036	5.0162E-035	3.0449E-033	4.5599E-034	3.4784E-031	1.0912E-028
39	0.2219	6.6055E-006	5.7625E-036	1.3320E-034	6.5375E-033	1.0291E-033	6.2735E-031	1.6937E-028
40	0.2227	7.1090E-006	1.8585E-035	3.4868E-034	1.3917E-032	2.3122E-033	1.1391E-030	2.6158E-028
41	0.2234	7.5629E-006	5.9848E-035	9.0459E-034	2.9476E-032	5.1700E-033	2.0839E-030	4.0177E-028
42	0.2250	8.2574E-006	4.8515E-034	5.0915E-033	1.1435E-031	2.3114E-032	6.4076E-030	8.9466E-028
43	0.2266	8.6054E-006	3.2713E-033	2.4450E-032	3.9031E-031	9.1621E-032	1.8493E-029	1.8546E-027
44	0.2273	8.6396E-006	8.3013E-033	5.2425E-032	7.1185E-031	1.7991E-031	3.1697E-029	2.6503E-027
45	0.2277	8.6162E-006	1.3224E-032	7.6779E-032	9.6351E-031	2.5263E-031	4.1765E-029	3.1751E-027
46	0.2281	8.5635E-006	2.0949E-032	1.1217E-031	1.3038E-030	3.5497E-031	5.5161E-029	3.8100E-027
47	0.2285	8.4826E-006	3.2996E-032	1.6325E-031	1.7608E-030	4.9799E-031	7.2886E-029	4.5744E-027
48	0.2289	8.3752E-006	5.1562E-032	2.3623E-031	2.3690E-030	6.9620E-031	9.6191E-029	5.4905E-027
49	0.2291	8.3124E-006	6.4415E-032	2.8386E-031	2.7458E-030	8.2234E-031	1.1052E-028	6.0148E-027
50	0.2293	8.2436E-006	8.0331E-032	3.4068E-031	3.1805E-030	9.7072E-031	1.2697E-028	6.5891E-027
51	0.2295	8.1690E-006	1.0001E-031	4.0835E-031	3.6808E-030	1.1449E-030	1.4583E-028	7.2173E-027
52	0.2297	8.0892E-006	1.2427E-031	4.8875E-031	4.2555E-030	1.3489E-030	1.6741E-028	7.9036E-027
53	0.2299	8.0046E-006	1.5413E-031	5.8404E-031	4.9141E-030	1.5874E-030	1.9205E-028	8.6522E-027
54	0.2301	7.9156E-006	1.9077E-031	6.9670E-031	5.6673E-030	1.8655E-030	2.2014E-028	9.4674E-027
55	0.2303	7.8227E-006	2.3561E-031	8.2956E-031	6.5265E-030	2.1889E-030	2.5209E-028	1.0354E-026
56	0.2305	7.7264E-006	2.9032E-031	9.8584E-031	7.5044E-030	2.5643E-030	2.8837E-028	1.1316E-026

57	0.2307	7.6273E-006	3.5692E-031	1.1692E-030	8.6151E-030	2.9990E-030	3.2947E-028	1.2359E-026
58	0.2309	7.5260E-006	4.3775E-031	1.3838E-030	9.8735E-030	3.5010E-030	3.7596E-028	1.3486E-026
59	0.2311	7.4229E-006	5.3558E-031	1.6342E-030	1.1296E-029	4.0796E-030	4.2841E-028	1.4704E-026
60	0.2313	7.3187E-006	6.5366E-031	1.9258E-030	1.2901E-029	4.7446E-030	4.8749E-028	1.6017E-026
61	0.2314	7.2138E-006	7.9580E-031	2.2644E-030	1.4707E-029	5.5073E-030	5.5389E-028	1.7430E-026
62	0.2316	7.1089E-006	9.6643E-031	2.6567E-030	1.6735E-029	6.3799E-030	6.2836E-028	1.8948E-026
63	0.2318	7.0045E-006	1.1707E-030	3.1100E-030	1.9008E-029	7.3761E-030	7.1174E-028	2.0574E-026
64	0.2320	6.9011E-006	1.4146E-030	3.6325E-030	2.1550E-029	8.5105E-030	8.0488E-028	2.2314E-026
65	0.2322	6.7991E-006	1.7052E-030	4.2333E-030	2.4387E-029	9.7996E-030	9.0873E-028	2.4173E-026
66	0.2324	6.6991E-006	2.0503E-030	4.9227E-030	2.7548E-029	1.1261E-029	1.0243E-027	2.6153E-026
67	0.2326	6.6015E-006	2.4595E-030	5.7119E-030	3.1063E-029	1.2915E-029	1.1527E-027	2.8259E-026
68	0.2328	6.5067E-006	2.9436E-030	6.6134E-030	3.4964E-029	1.4781E-029	1.2950E-027	3.0495E-026
69	0.2330	6.4151E-006	3.5153E-030	7.6413E-030	3.9287E-029	1.6884E-029	1.4526E-027	3.2863E-026
70	0.2332	6.3270E-006	4.1903E-030	8.8117E-030	4.4072E-029	1.9250E-029	1.6267E-027	3.5367E-026
71	0.2336	6.1625E-006	5.9070E-030	1.1638E-029	5.5151E-029	2.4865E-029	2.0289E-027	4.0784E-026
72	0.2344	5.8829E-006	1.1297E-029	1.9668E-029	8.4111E-029	4.0309E-029	3.0741E-027	5.3202E-026
73	0.2352	5.6691E-006	2.0697E-029	3.1951E-029	1.2405E-028	6.2910E-029	4.4998E-027	6.7462E-026
74	0.2359	5.5174E-006	3.6564E-029	5.0254E-029	1.7818E-028	9.5208E-029	6.3981E-027	8.3304E-026
75	0.2367	5.4166E-006	6.2613E-029	7.6935E-029	2.5059E-028	1.4046E-028	8.8685E-027	1.0035E-025
76	0.2375	5.3500E-006	1.0430E-028	1.1507E-028	3.4632E-028	2.0273E-028	1.2016E-026	1.1811E-025
77	0.2383	5.2982E-006	1.6939E-028	1.6855E-028	4.7135E-028	2.8697E-028	1.5942E-026	1.3607E-025
78	0.2391	5.2424E-006	2.6853E-028	2.4209E-028	6.3258E-028	3.9887E-028	2.0744E-026	1.5369E-025
79	0.2398	5.1673E-006	4.1566E-028	3.4116E-028	8.3743E-028	5.4470E-028	2.6499E-026	1.7048E-025
80	0.2406	5.0632E-006	6.2816E-028	4.7172E-028	1.0934E-027	7.3086E-028	3.3265E-026	1.8604E-025
81	0.2414	4.9265E-006	9.2649E-028	6.3983E-028	1.4077E-027	9.6333E-028	4.1066E-026	2.0003E-025
82	0.2422	4.7595E-006	1.3332E-027	8.5111E-028	1.7859E-027	1.2470E-027	4.9892E-026	2.1226E-025
83	0.2430	4.5684E-006	1.8713E-027	1.1102E-027	2.2324E-027	1.5851E-027	5.9695E-026	2.2261E-025
84	0.2437	4.3614E-006	2.5621E-027	1.4203E-027	2.7489E-027	1.9787E-027	7.0391E-026	2.3105E-025
85	0.2445	4.1470E-006	3.4232E-027	1.7826E-027	3.3352E-027	2.4265E-027	8.1867E-026	2.3765E-025
86	0.2453	3.9324E-006	4.4660E-027	2.1966E-027	3.9887E-027	2.9253E-027	9.3990E-026	2.4249E-025
87	0.2461	3.7232E-006	5.6940E-027	2.6596E-027	4.7049E-027	3.4695E-027	1.0661E-025	2.4571E-025
88	0.2469	3.5233E-006	7.1021E-027	3.1673E-027	5.4779E-027	4.0524E-027	1.1958E-025	2.4748E-025
89	0.2477	3.3349E-006	8.6757E-027	3.7140E-027	6.3005E-027	4.6661E-027	1.3275E-025	2.4796E-025
90	0.2484	3.1591E-006	1.0389E-026	4.2921E-027	7.1641E-027	5.3018E-027	1.4596E-025	2.4730E-025
91	0.2500	2.8465E-006	1.4118E-026	5.5114E-027	8.9793E-027	6.6019E-027	1.7194E-025	2.4297E-025
92	0.2516	2.5778E-006	1.7957E-026	6.7353E-027	1.0804E-026	7.8479E-027	1.9587E-025	2.3555E-025
93	0.2531	2.3476E-006	2.1636E-026	7.9120E-027	1.2582E-026	8.9932E-027	2.1722E-025	2.2594E-025
94	0.2562	1.9816E-006	2.7729E-026	9.9975E-027	1.5885E-026	1.0896E-026	2.5197E-025	2.0334E-025
95	0.2594	1.7012E-006	3.1605E-026	1.1542E-026	1.8527E-026	1.2117E-026	2.7392E-025	1.7897E-025
96	0.2625	1.4831E-006	3.3520E-026	1.2599E-026	2.0545E-026	1.2785E-026	2.8589E-025	1.5575E-025
97	0.2656	1.3107E-006	3.4039E-026	1.3281E-026	2.2043E-026	1.3051E-026	2.9082E-025	1.3524E-025
98	0.2688	1.1727E-006	3.3685E-026	1.3693E-026	2.3127E-026	1.3045E-026	2.9101E-025	1.1783E-025
99	0.2750	9.7105E-007	3.1755E-026	1.4050E-026	2.4472E-026	1.2601E-026	2.8395E-025	9.1889E-026
100	0.2812	8.2889E-007	2.9122E-026	1.3970E-026	2.4859E-026	1.1752E-026	2.6888E-025	7.2892E-026
101	0.2875	7.2461E-007	2.6470E-026	1.3701E-026	2.4657E-026	1.0753E-026	2.5027E-025	5.8891E-026
102	0.2938	6.4547E-007	2.4078E-026	1.3381E-026	2.4105E-026	9.7288E-027	2.3057E-025	4.8430E-026
103	0.3000	5.8372E-007	2.2026E-026	1.3076E-026	2.3355E-026	8.7423E-027	2.1104E-025	4.0471E-026
104	0.3063	5.3444E-007	2.0316E-026	1.2817E-026	2.2501E-026	7.8221E-027	1.9233E-025	3.4303E-026
105	0.3125	4.9439E-007	1.8921E-026	1.2613E-026	2.1609E-026	6.9812E-027	1.7480E-025	2.9440E-026
106	0.3188	4.6135E-007	1.7803E-026	1.2461E-026	2.0722E-026	6.2237E-027	1.5859E-025	2.5547E-026
107	0.3250	4.3377E-007	1.6927E-026	1.2353E-026	1.9865E-026	5.5484E-027	1.4379E-025	2.2388E-026
108	0.3313	4.1051E-007	1.6258E-026	1.2278E-026	1.9056E-026	4.9514E-027	1.3039E-025	1.9796E-026
109	0.3375	3.9075E-007	1.5769E-026	1.2225E-026	1.8302E-026	4.4270E-027	1.1833E-025	1.7646E-026
110	0.3438	3.7386E-007	1.5435E-026	1.2181E-026	1.7607E-026	3.9685E-027	1.0754E-025	1.5847E-026
111	0.3500	3.5938E-007	1.5230E-026	1.2135E-026	1.6967E-026	3.5693E-027	9.7935E-026	1.4330E-026
112	0.3625	3.3643E-007	1.5091E-026	1.1980E-026	1.5815E-026	2.9216E-027	8.1885E-026	1.1960E-026
113	0.3750	3.1890E-007	1.5281E-026	1.1768E-026	1.4829E-026	2.4279E-027	6.9166E-026	1.0177E-026
114	0.3875	3.0540E-007	1.5713E-026	1.1488E-026	1.3971E-026	2.0499E-027	5.9103E-026	8.8185E-027
115	0.4000	2.9496E-007	1.6312E-026	1.1144E-026	1.3208E-026	1.7579E-027	5.1108E-026	7.7636E-027
116	0.4125	2.8691E-007	1.7013E-026	1.0748E-026	1.2515E-026	1.5296E-027	4.4713E-026	6.9315E-027
117	0.4250	2.8074E-007	1.7766E-026	1.0317E-026	1.1878E-026	1.3486E-027	3.9555E-026	6.2655E-027
118	0.4375	2.7605E-007	1.8539E-026	9.8675E-027	1.1289E-026	1.2033E-027	3.5359E-026	5.7255E-027
119	0.4437	2.7415E-007	1.8942E-026	9.6447E-027	1.1014E-026	1.1412E-027	3.3547E-026	5.4916E-027
120	0.4500	2.7253E-007	1.9342E-026	9.4255E-027	1.0753E-026	1.0857E-027	3.1926E-026	5.2833E-027
121	0.4625	2.7007E-007	2.0112E-026	9.0069E-027	1.0276E-026	9.9244E-028	2.9191E-026	4.9338E-027
122	0.4688	2.6915E-007	2.0520E-026	8.8187E-027	1.0068E-026	9.5358E-028	2.8038E-026	4.7856E-027
123	0.4750	2.6841E-007	2.0945E-026	8.6548E-027	9.8898E-027	9.2075E-028	2.7056E-026	4.6604E-027
124	0.4812	2.6786E-007	2.1384E-026	8.5236E-027	9.7493E-027	8.9449E-028	2.6257E-026	4.5591E-027
125	0.4875	2.6748E-007	2.1793E-026	8.4318E-027	9.6513E-027	8.7560E-028	2.5666E-026	4.4829E-027
126	0.4906	2.6734E-007	2.1899E-026	8.4010E-027	9.6138E-027	8.6971E-028	2.5463E-026	4.4524E-027
127	0.4938	2.6725E-007	2.2012E-026	8.3726E-027	9.5847E-027	8.6420E-028	2.5295E-026	4.4293E-027
128	0.4969	2.6720E-007	2.1809E-026	8.3337E-027	9.5370E-027	8.6143E-028	2.5207E-026	4.4105E-027
129	0.5000	2.6720E-007	2.1706E-026	8.3338E-027	9.5370E-027	8.6144E-028	2.5207E-026	4.4105E-027

	X(cm)	MOLE FRACTIONS: CO	CO2	HCO	CH2O	CH2OH	CH3O	CH3OH
1	0.0000	-1.2866E-051	1.9752E-049	-3.5971E-052	-1.0834E-042	-1.0272E-053	1.4792E-048	8.7687E-046
2	0.0500	-5.3949E-050	1.0230E-047	-1.7829E-050	-5.4107E-041	-5.2063E-052	7.4975E-047	4.4662E-044
3	0.0750	-1.1083E-048	3.7735E-046	-3.6334E-049	-1.0733E-039	-1.0876E-050	2.1313E-045	8.6780E-043
4	0.1000	-2.8780E-047	1.7482E-044	-9.2791E-048	-2.7279E-038	-2.7955E-049	6.3636E-044	2.1890E-041

5	0.1250	-7.4994E-046	1.5034E-042	-2.3910E-046	-7.0029E-037	-7.2378E-048	1.9233E-042	5.5726E-040
6	0.1500	-3.4681E-045	-5.4886E-042	-6.2084E-045	-1.7966E-035	-2.0338E-046	8.2868E-041	1.4142E-038
7	0.1625	3.8516E-041	-8.8193E-041	9.8996E-043	-1.8608E-034	-5.4538E-045	3.1345E-039	1.4301E-037
8	0.1750	5.7309E-038	-9.8950E-040	5.3710E-039	-2.4176E-033	-7.1376E-043	1.5727E-037	1.7518E-036
9	0.1875	7.1016E-035	1.3471E-037	2.6392E-035	-3.2010E-032	-1.4693E-040	7.5368E-036	1.6985E-035
10	0.1938	5.8502E-033	-4.1451E-037	4.8573E-032	-1.7461E-031	-2.8582E-038	9.7102E-035	-2.0155E-035
11	0.2000	2.5365E-032	-2.6265E-036	3.1201E-032	-1.9217E-031	-2.6896E-038	2.3204E-034	4.2318E-034
12	0.2031	6.5385E-033	-7.4823E-036	6.7793E-034	-2.2290E-031	-8.9782E-038	3.7318E-034	7.8673E-034
13	0.2047	-2.6196E-033	-1.2641E-035	-1.1904E-034	-2.2388E-031	-1.4101E-037	4.7970E-034	1.0235E-033
14	0.2063	3.6278E-033	-2.0079E-035	-2.1526E-034	-2.3775E-031	-2.4244E-037	6.0131E-034	1.3186E-033
15	0.2078	7.4372E-032	-2.3512E-035	1.5316E-035	-2.6037E-031	-4.4553E-037	7.2670E-034	1.6777E-033
16	0.2086	6.2364E-031	-7.1581E-036	8.6107E-035	-2.8425E-031	-6.2874E-037	7.7792E-034	1.8867E-033
17	0.2094	4.1570E-030	7.0672E-035	-1.3588E-034	-3.2698E-031	-9.4124E-037	8.0987E-034	2.1292E-033
18	0.2102	2.6920E-029	3.6628E-034	-1.9067E-033	-4.0314E-031	-1.3537E-036	8.0095E-034	2.4252E-033
19	0.2109	1.6977E-028	1.4327E-033	-4.8475E-032	-4.9830E-031	-2.2796E-036	6.9821E-034	2.8174E-033
20	0.2113	5.1149E-028	2.8539E-033	-9.7377E-033	-5.6073E-031	-2.9752E-036	6.3357E-034	3.0833E-033
21	0.2117	1.4203E-027	5.8057E-033	-1.6202E-033	-6.6180E-031	-4.0175E-036	5.1552E-034	3.4217E-033
22	0.2121	3.8406E-027	1.2030E-032	-5.4337E-034	-7.8230E-031	-4.9362E-036	3.6836E-034	3.8678E-033
23	0.2125	1.0175E-026	2.5379E-032	-2.6236E-034	-8.7617E-031	-4.9481E-036	2.3152E-034	4.4811E-033
24	0.2129	2.6370E-026	5.4584E-032	1.0257E-035	-8.1547E-031	-4.8068E-036	2.0056E-034	5.2753E-033
25	0.2133	6.6603E-026	1.2001E-031	5.7224E-033	-5.8181E-031	-2.0406E-036	1.1474E-034	6.3450E-033
26	0.2137	1.6321E-025	2.7078E-031	2.7236E-032	2.3094E-031	2.1048E-035	3.2313E-035	7.7837E-033
27	0.2141	3.8612E-025	6.2987E-031	8.1284E-032	2.1062E-030	3.5213E-035	2.0735E-034	9.8055E-033
28	0.2145	8.7712E-025	1.5181E-030	2.1954E-031	4.9539E-030	8.1169E-035	4.8798E-034	1.2608E-032
29	0.2148	1.9034E-024	3.8080E-030	5.3493E-031	8.9797E-030	1.6230E-034	9.6943E-034	1.6484E-032
30	0.2152	3.9285E-024	9.9676E-030	1.2264E-030	1.4575E-029	2.9371E-034	1.7314E-033	2.1827E-032
31	0.2156	7.6912E-024	3.4179E-029	2.6769E-030	2.2321E-029	4.9291E-034	2.8643E-033	2.9164E-032
32	0.2164	2.3685E-023	2.2917E-028	1.0105E-029	4.5969E-029	1.3416E-033	6.5848E-033	5.1580E-032
33	0.2172	6.0772E-023	1.1059E-027	3.2117E-029	8.7603E-029	3.2593E-033	1.3015E-032	9.0297E-032
34	0.2180	1.3679E-022	6.8890E-027	8.9804E-029	1.6181E-028	7.5672E-033	2.4292E-032	1.5616E-031
35	0.2188	2.8305E-022	1.4035E-026	2.3045E-028	2.9373E-028	1.7270E-032	4.4081E-032	2.6707E-031
36	0.2195	5.5657E-022	8.0684E-026	5.5943E-028	5.2833E-028	3.8814E-032	7.8356E-032	4.5237E-031
37	0.2203	1.0606E-021	1.7944E-025	1.3078E-027	9.4530E-028	8.6404E-032	1.3777E-031	7.5981E-031
38	0.2211	1.9790E-021	3.8005E-025	2.9717E-027	1.6848E-027	1.9026E-031	2.3999E-031	1.2655E-030
39	0.2219	3.6355E-021	8.3780E-025	6.5933E-027	2.9907E-027	4.1409E-031	4.1411E-031	2.0887E-030
40	0.2227	6.5912E-021	1.9296E-024	1.4314E-026	5.2810E-027	8.8916E-031	7.0675E-031	3.4139E-030
41	0.2234	1.1807E-020	4.6442E-024	3.0503E-026	9.2594E-027	1.8842E-030	1.1896E-030	5.5188E-030
42	0.2250	3.3802E-020	2.9857E-023	1.1839E-025	2.5690E-026	7.2909E-030	3.0211E-030	1.3269E-029
43	0.2266	8.8533E-020	2.0490E-022	4.0220E-025	6.3884E-026	2.4100E-029	6.7520E-030	2.8387E-029
44	0.2273	1.4480E-019	5.4289E-022	7.3824E-025	9.9884E-026	4.2708E-029	9.9239E-030	4.0561E-029
45	0.2277	1.8662E-019	8.8786E-022	1.0046E-024	1.2539E-025	5.6843E-029	1.2050E-029	4.8489E-029
46	0.2281	2.4144E-019	1.4587E-021	1.3689E-024	1.5779E-025	7.5621E-029	1.4649E-029	5.8021E-029
47	0.2285	3.1295E-019	2.4091E-021	1.8643E-024	1.9866E-025	1.0033E-028	1.7798E-029	6.9408E-029
48	0.2289	4.0585E-019	4.0049E-021	2.5333E-024	2.4979E-025	1.3251E-028	2.1577E-029	8.2913E-029
49	0.2291	4.6255E-019	5.1817E-021	2.9530E-024	2.8000E-025	1.5206E-028	2.3738E-029	9.0563E-029
50	0.2293	5.2742E-019	6.7290E-021	3.4420E-024	3.1384E-025	1.7436E-028	2.6105E-029	9.8894E-029
51	0.2295	6.0155E-019	8.7785E-021	4.0109E-024	3.5167E-025	1.9974E-028	2.8691E-029	1.0795E-028
52	0.2297	6.8617E-019	1.1518E-020	4.6716E-024	3.9386E-025	2.2852E-028	3.1511E-029	1.1776E-028
53	0.2299	7.8261E-019	1.5221E-020	5.4375E-024	4.4084E-025	2.6109E-028	3.4578E-029	1.2839E-028
54	0.2301	8.9239E-019	2.0290E-020	6.3237E-024	4.9303E-025	2.9785E-028	3.7905E-029	1.3986E-028
55	0.2303	1.0172E-018	2.7335E-020	7.3475E-024	5.5089E-025	3.3923E-028	4.1506E-029	1.5222E-028
56	0.2305	1.1588E-018	3.7295E-020	8.5280E-024	6.1491E-025	3.8569E-028	4.5392E-029	1.6551E-028
57	0.2307	1.3193E-018	5.1637E-020	9.8866E-024	6.8560E-025	4.3770E-028	4.9578E-029	1.7977E-028
58	0.2309	1.5009E-018	7.2688E-020	1.1447E-023	7.6349E-025	4.9579E-028	5.4076E-029	1.9503E-028
59	0.2311	1.7061E-018	1.0416E-019	1.3236E-023	8.4915E-025	5.6049E-028	5.8897E-029	2.1132E-028
60	0.2313	1.9376E-018	1.5199E-019	1.5284E-023	9.4316E-025	6.3238E-028	6.4054E-029	2.2868E-028
61	0.2314	2.1983E-018	2.2541E-019	1.7622E-023	1.0462E-024	7.1205E-028	6.9557E-029	2.4713E-028
62	0.2316	2.4915E-018	3.3835E-019	2.0289E-023	1.1588E-024	8.0012E-028	7.5419E-029	2.6669E-028
63	0.2318	2.8209E-018	5.1019E-019	2.3324E-023	1.2817E-024	8.9725E-028	8.1650E-029	2.8740E-028
64	0.2320	3.1904E-018	7.6511E-019	2.6773E-023	1.4157E-024	1.0041E-027	8.8261E-029	3.0926E-028
65	0.2322	3.6045E-018	1.1289E-018	3.0686E-023	1.5614E-024	1.1214E-027	9.5263E-029	3.3229E-028
66	0.2324	4.0682E-018	1.6256E-018	3.5122E-023	1.7198E-024	1.2500E-027	1.0267E-028	3.5649E-028
67	0.2326	4.5870E-018	2.2777E-018	4.0143E-023	1.8915E-024	1.3905E-027	1.1048E-028	3.8188E-028
68	0.2328	5.1670E-018	3.1125E-018	4.5821E-023	2.0775E-024	1.5437E-027	1.1871E-028	4.0844E-028
69	0.2330	5.8151E-018	4.1712E-018	5.2235E-023	2.2788E-024	1.7106E-027	1.2737E-028	4.3617E-028
70	0.2332	6.5386E-018	5.5151E-018	5.9476E-023	2.4961E-024	1.8920E-027	1.3647E-028	4.6506E-028
71	0.2336	8.2371E-018	9.3614E-018	7.6747E-023	2.9821E-024	2.3007E-027	1.5594E-028	5.2623E-028
72	0.2344	1.2799E-017	2.5226E-017	1.2453E-022	4.1676E-024	3.3117E-027	1.9951E-028	6.6054E-028
73	0.2352	1.9410E-017	6.3265E-017	1.9610E-022	5.6670E-024	4.6027E-027	2.4851E-028	8.0664E-028
74	0.2359	2.8936E-017	1.4829E-016	3.0204E-022	7.5537E-024	6.2276E-027	3.0361E-028	9.6253E-028
75	0.2367	4.2581E-017	3.2544E-016	4.5716E-022	9.9243E-024	8.2543E-027	3.6595E-028	1.1273E-027
76	0.2375	6.2005E-017	6.6885E-016	6.8185E-022	1.2902E-023	1.0767E-026	4.3703E-028	1.3010E-027
77	0.2383	8.9464E-017	1.2870E-015	1.0038E-021	1.6639E-023	1.3865E-026	5.1860E-028	1.4844E-027
78	0.2391	1.2795E-016	2.3183E-015	1.4594E-021	2.1314E-023	1.7660E-026	6.1252E-028	1.6782E-027
79	0.2398	1.8134E-016	3.9122E-015	2.0955E-021	2.7131E-023	2.2272E-026	7.2055E-028	1.8828E-027
80	0.2406	2.5446E-016	6.1989E-015	2.9695E-021	3.4305E-023	2.7814E-026	8.4413E-028	2.0980E-027
81	0.2414	3.5315E-016	9.2621E-015	4.1492E-021	4.3053E-023	3.4387E-026	9.8424E-028	2.3226E-027
82	0.2422	4.8415E-016	1.3129E-014	5.7113E-021	5.3579E-023	4.2062E-026	1.1412E-027	2.5545E-027
83	0.2430	6.5503E-016	1.7784E-014	7.7384E-021	6.6054E-023	5.0876E-026	1.3146E-027	2.7910E-027
84	0.2437	8.7403E-016	2.3185E-014	1.0316E-020	8.0615E-023	6.0825E-026	1.5034E-027	3.0290E-027

33	0.2172	-2.5046E-061	-1.7142E-053	-5.2962E-057	-1.8446E-054	-7.8255E-057	-2.2363E-055	-2.7454E-055
34	0.2180	-6.1937E-061	-3.0536E-053	-1.1964E-056	-3.3199E-054	-1.4258E-056	-4.1227E-055	-6.7993E-055
35	0.2188	-1.5096E-060	-5.3911E-053	-2.6676E-056	-5.9288E-054	-2.5685E-056	-7.5009E-055	-1.6634E-054
36	0.2195	-3.6451E-060	-9.4622E-053	-5.8860E-056	-1.0539E-053	-4.5910E-056	-1.3509E-054	-4.0482E-054
37	0.2203	-8.7509E-060	-1.6537E-052	-1.2868E-055	-1.8682E-053	-8.1576E-056	-2.4111E-054	-9.8677E-054
38	0.2211	-2.0939E-059	-2.8799E-052	-2.7890E-055	-3.3054E-053	-1.4424E-055	-4.2646E-054	-2.4265E-053
39	0.2219	-5.0025E-059	-4.9994E-052	-5.9972E-055	-5.8405E-053	-2.5392E-055	-7.4721E-054	-6.0687E-053
40	0.2227	-1.1949E-058	-8.6527E-052	-1.2815E-054	-1.0309E-052	-4.4508E-055	-1.2959E-053	-1.5572E-052
41	0.2234	-2.8702E-058	-1.4930E-051	-2.7373E-054	-1.8179E-052	-7.7662E-055	-2.2226E-053	-4.1372E-052
42	0.2250	-1.5116E-057	-4.0823E-051	-1.0980E-053	-5.1733E-052	-2.1500E-054	-5.9134E-053	-2.3511E-051
43	0.2266	-7.4027E-057	-1.0352E-050	-4.0604E-053	-1.3751E-051	-5.4865E-054	-1.3892E-052	-1.3208E-050
44	0.2273	-1.6817E-056	-1.6832E-050	-8.1820E-053	-2.3099E-051	-8.9687E-054	-2.0993E-052	-3.4396E-050
45	0.2277	-2.5778E-056	-2.1755E-050	-1.1898E-052	-3.0409E-051	-1.1626E-053	-2.5930E-052	-5.6692E-050
46	0.2281	-3.9873E-056	-2.8352E-050	-1.7508E-052	-4.0386E-051	-1.5192E-053	-3.2163E-052	-9.3177E-050
47	0.2285	-6.2132E-056	-3.7175E-050	-2.5999E-052	-5.3966E-051	-1.9958E-053	-3.9996E-052	-1.5280E-049
48	0.2289	-9.7285E-056	-4.8957E-050	-3.8849E-052	-7.2406E-051	-2.6304E-053	-4.9784E-052	-2.4960E-049
49	0.2291	-1.2224E-055	-5.6322E-050	-4.7724E-052	-8.4083E-051	-3.0259E-053	-5.5570E-052	-3.2011E-049
50	0.2293	-1.5391E-055	-6.4904E-050	-5.8765E-052	-9.7799E-051	-3.4858E-053	-6.2063E-052	-4.1027E-049
51	0.2295	-1.9414E-055	-7.4896E-050	-7.2493E-052	-1.1390E-050	-4.0197E-053	-6.9338E-052	-5.2541E-049
52	0.2297	-2.4529E-055	-8.6525E-050	-8.9554E-052	-1.3278E-050	-4.6388E-053	-7.7477E-052	-6.7214E-049
53	0.2299	-3.1039E-055	-1.0005E-049	-1.1074E-051	-1.5489E-050	-5.3558E-053	-8.6567E-052	-8.5873E-049
54	0.2301	-3.9327E-055	-1.1577E-049	-1.3701E-051	-1.8078E-050	-6.1852E-053	-9.6703E-052	-1.0954E-048
55	0.2303	-4.9888E-055	-1.3404E-049	-1.6957E-051	-2.1106E-050	-7.1433E-053	-1.0798E-051	-1.3950E-048
56	0.2305	-6.3350E-055	-1.5525E-049	-2.0984E-051	-2.4643E-050	-8.2487E-053	-1.2052E-051	-1.7731E-048
57	0.2307	-8.0521E-055	-1.7987E-049	-2.5960E-051	-2.8771E-050	-9.5224E-053	-1.3442E-051	-2.2490E-048
58	0.2309	-1.0243E-054	-2.0842E-049	-3.2096E-051	-3.3585E-050	-1.0988E-052	-1.4981E-051	-2.8465E-048
59	0.2311	-1.3040E-054	-2.4151E-049	-3.9652E-051	-3.9191E-050	-1.2672E-052	-1.6681E-051	-3.5945E-048
60	0.2313	-1.6611E-054	-2.7984E-049	-4.8937E-051	-4.5715E-050	-1.4604E-052	-1.8555E-051	-4.5284E-048
61	0.2314	-2.1171E-054	-3.2422E-049	-6.0325E-051	-5.3296E-050	-1.6818E-052	-2.0618E-051	-5.6912E-048
62	0.2316	-2.6995E-054	-3.7557E-049	-7.4267E-051	-6.2098E-050	-1.9351E-052	-2.2883E-051	-7.1350E-048
63	0.2318	-3.4432E-054	-4.3494E-049	-9.1298E-051	-7.2303E-050	-2.2245E-052	-2.5366E-051	-8.9232E-048
64	0.2320	-4.3930E-054	-5.0354E-049	-1.1206E-050	-8.4122E-050	-2.5545E-052	-2.8081E-051	-1.1132E-047
65	0.2322	-5.6054E-054	-5.8275E-049	-1.3732E-050	-9.7793E-050	-2.9303E-052	-3.1044E-051	-1.3855E-047
66	0.2324	-7.1530E-054	-6.7415E-049	-1.6799E-050	-1.1359E-049	-3.3576E-052	-3.4271E-051	-1.7204E-047
67	0.2326	-9.1280E-054	-7.7954E-049	-2.0514E-050	-1.3181E-049	-3.8425E-052	-3.7777E-051	-2.1313E-047
68	0.2328	-1.1649E-053	-9.0098E-049	-2.5005E-050	-1.5280E-049	-4.3918E-052	-4.1578E-051	-2.6349E-047
69	0.2330	-1.4870E-053	-1.0408E-048	-3.0424E-050	-1.7694E-049	-5.0129E-052	-4.5689E-051	-3.2509E-047
70	0.2332	-1.9000E-053	-1.2017E-048	-3.6953E-050	-2.0469E-049	-5.7138E-052	-5.0124E-051	-4.0040E-047
71	0.2336	-3.0881E-053	-1.5956E-048	-5.3988E-050	-2.7240E-049	-7.3779E-052	-6.0010E-051	-6.0106E-047
72	0.2344	-7.8266E-053	-2.7337E-048	-1.0904E-049	-4.6615E-049	-1.1869E-051	-8.3811E-051	-1.2812E-046
73	0.2352	-1.9161E-052	-4.5437E-048	-2.0809E-049	-7.6639E-049	-1.8287E-051	-1.1271E-050	-2.6002E-046
74	0.2359	-4.5568E-052	-7.4063E-048	-3.8074E-049	-1.2228E-048	-2.7262E-051	-1.4686E-050	-5.0852E-046
75	0.2367	-1.0559E-051	-1.1913E-047	-6.7320E-049	-1.9035E-048	-3.9555E-051	-1.8643E-050	-9.6670E-046
76	0.2375	-2.3876E-051	-1.8985E-047	-1.1559E-048	-2.8995E-048	-5.6066E-051	-2.3161E-050	-1.7964E-045
77	0.2383	-5.2734E-051	-3.0062E-047	-1.9338E-048	-4.3302E-048	-7.7846E-051	-2.8268E-050	-3.2739E-045
78	0.2391	-1.1383E-050	-4.7385E-047	-3.1585E-048	-6.3486E-048	-1.0610E-050	-3.3994E-050	-5.8618E-045
79	0.2398	-2.4021E-050	-7.4438E-047	-5.0435E-048	-9.1459E-048	-1.4218E-050	-4.0366E-050	-1.0313E-044
80	0.2406	-4.9551E-050	-1.1658E-046	-7.8784E-048	-1.2954E-047	-1.8753E-050	-4.7401E-050	-1.7816E-044
81	0.2414	-9.9861E-050	-1.8190E-046	-1.2042E-047	-1.8048E-047	-2.4369E-050	-5.5093E-050	-3.0181E-044
82	0.2422	-1.9643E-049	-2.8245E-046	-1.8010E-047	-2.4736E-047	-3.1215E-050	-6.3405E-050	-5.0065E-044
83	0.2430	-3.7666E-049	-4.3565E-046	-2.6358E-047	-3.3359E-047	-3.9428E-050	-7.2267E-050	-8.1216E-044
84	0.2437	-7.0318E-049	-6.6609E-046	-3.7754E-047	-4.4275E-047	-4.9127E-050	-8.1581E-050	-1.2872E-043
85	0.2445	-1.2768E-048	-1.0075E-045	-5.2945E-047	-5.7846E-047	-6.0404E-050	-9.1221E-050	-1.9925E-043
86	0.2453	-2.2531E-048	-1.5049E-045	-7.2739E-047	-7.4424E-047	-7.3316E-050	-1.0105E-049	-3.0121E-043
87	0.2461	-3.8634E-048	-2.2167E-045	-9.7983E-047	-9.4344E-047	-8.7890E-050	-1.1092E-049	-4.4492E-043
88	0.2469	-6.4394E-048	-3.2174E-045	-1.2955E-046	-1.1791E-046	-1.0412E-049	-1.2070E-049	-6.4267E-043
89	0.2477	-1.0443E-047	-4.6001E-045	-1.6831E-046	-1.4538E-046	-1.2198E-049	-1.3025E-049	-9.0879E-043
90	0.2484	-1.6515E-047	-6.4811E-045	-2.1513E-046	-1.7697E-046	-1.4138E-049	-1.3944E-049	-1.2599E-042
91	0.2500	-3.7828E-047	-1.2175E-044	-3.3508E-046	-2.5276E-046	-1.8425E-049	-1.5625E-049	-2.2830E-042
92	0.2516	-7.7662E-047	-2.1163E-044	-4.8680E-046	-3.4149E-046	-2.2889E-049	-1.6925E-049	-3.8161E-042
93	0.2531	-1.4635E-046	-3.4629E-044	-6.6996E-046	-4.4125E-046	-2.7374E-049	-1.7827E-049	-5.9805E-042
94	0.2562	-4.1892E-046	-7.9558E-044	-1.1230E-045	-6.6722E-046	-3.6069E-049	-1.8653E-049	-1.2650E-041
95	0.2594	-9.4523E-046	-1.5170E-043	-1.6143E-045	-8.8835E-046	-4.2583E-049	-1.8085E-049	-2.2411E-041
96	0.2625	-1.8172E-045	-2.5517E-043	-2.0975E-045	-1.0866E-045	-4.6811E-049	-1.6726E-049	-3.5225E-041
97	0.2656	-3.1101E-045	-3.9164E-043	-2.5407E-045	-1.2537E-045	-4.9076E-049	-1.5061E-049	-5.0812E-041
98	0.2688	-4.8748E-045	-5.6052E-043	-2.9263E-045	-1.3875E-045	-4.9816E-049	-1.3370E-049	-6.8733E-041
99	0.2750	-9.9184E-045	-9.8999E-043	-3.5264E-045	-1.5699E-045	-4.8578E-049	-1.0457E-049	-1.1005E-040
100	0.2812	-1.6811E-044	-1.5032E-042	-3.8472E-045	-1.6359E-045	-4.4505E-049	-7.9935E-050	-1.5414E-040
101	0.2875	-2.5265E-044	-2.0678E-042	-3.9496E-045	-1.6192E-045	-3.9300E-049	-6.0581E-050	-1.9787E-040
102	0.2938	-3.4881E-044	-2.6545E-042	-3.9007E-045	-1.5517E-045	-3.3979E-049	-4.5894E-050	-2.3917E-040
103	0.3000	-4.5235E-044	-3.2396E-042	-3.7548E-045	-1.4566E-045	-2.9027E-049	-3.4880E-050	-2.7680E-040
104	0.3063	-5.5937E-044	-3.8058E-042	-3.5519E-045	-1.3490E-045	-2.4636E-049	-2.6642E-050	-3.1017E-040
105	0.3125	-6.6659E-044	-4.3419E-042	-3.3206E-045	-1.2386E-045	-2.0849E-049	-2.0473E-050	-3.3913E-040
106	0.3188	-7.7144E-044	-4.8410E-042	-3.0801E-045	-1.1312E-045	-1.7636E-049	-1.5839E-050	-3.6386E-040
107	0.3250	-8.7204E-044	-5.3004E-042	-2.8430E-045	-1.0302E-045	-1.4938E-049	-1.2346E-050	-3.8468E-040
108	0.3313	-9.6711E-044	-5.7195E-042	-2.6168E-045	-9.3718E-046	-1.2687E-049	-9.7008E-051	-4.0205E-040
109	0.3375	-1.0559E-043	-6.0994E-042	-2.4058E-045	-8.5283E-046	-1.0815E-049	-7.6885E-051	-4.1639E-040
110	0.3438	-1.1378E-043	-6.4417E-042	-2.2119E-045	-7.7703E-046	-9.2594E-050	-6.1498E-051	-4.2814E-040
111	0.3500	-1.2122E-043	-6.7463E-042	-2.0352E-045	-7.0930E-046	-7.9669E-050	-4.9666E-051	-4.3755E-040
112	0.3625	-1.3313E-043	-7.2182E-042	-1.7286E-045	-5.9507E-046	-5.9997E-050	-3.3477E-051	-4.4883E-040

61	0.2314	-1.9491E-046	-3.7509E-053	3.4870E-009	8.1678E-010	7.2023E-012	5.6286E-012	4.0670E-009
62	0.2316	-2.3712E-046	-4.8197E-053	3.7660E-009	8.7918E-010	7.7574E-012	6.0155E-012	4.3008E-009
63	0.2318	-2.8801E-046	-6.1947E-053	4.0631E-009	9.4555E-010	8.3495E-012	6.4245E-012	4.5455E-009
64	0.2320	-3.4922E-046	-7.9632E-053	4.3788E-009	1.0161E-009	8.9801E-012	6.8560E-012	4.8013E-009
65	0.2322	-4.2272E-046	-1.0237E-052	4.7140E-009	1.0908E-009	9.6511E-012	7.3107E-012	5.0686E-009
66	0.2324	-5.1083E-046	-1.3160E-052	5.0694E-009	1.1701E-009	1.0364E-011	7.7892E-012	5.3475E-009
67	0.2326	-6.1628E-046	-1.6914E-052	5.4455E-009	1.2540E-009	1.1121E-011	8.2921E-012	5.6384E-009
68	0.2328	-7.4228E-046	-2.1737E-052	5.8430E-009	1.3426E-009	1.1923E-011	8.8198E-012	5.9414E-009
69	0.2330	-8.9261E-046	-2.7929E-052	6.2627E-009	1.4363E-009	1.2771E-011	9.3727E-012	6.2568E-009
70	0.2332	-1.0717E-045	-3.5877E-052	6.7051E-009	1.5351E-009	1.3669E-011	9.9511E-012	6.5848E-009
71	0.2336	-1.5317E-045	-5.8523E-052	7.6596E-009	1.7486E-009	1.5613E-011	1.1186E-011	7.2792E-009
72	0.2344	-2.9719E-045	-1.4435E-051	9.8488E-009	2.2409E-009	2.0113E-011	1.3953E-011	8.8253E-009
73	0.2352	-5.4855E-045	-3.4085E-051	1.2404E-008	2.8228E-009	2.5434E-011	1.7072E-011	1.0580E-008
74	0.2359	-9.7921E-045	-7.7891E-051	1.5325E-008	3.4976E-009	3.1587E-011	2.0496E-011	1.2540E-008
75	0.2367	-1.7044E-044	-1.7274E-050	1.8598E-008	4.2652E-009	3.8533E-011	2.4158E-011	1.4694E-008
76	0.2375	-2.9065E-044	-3.7208E-050	2.2191E-008	5.1211E-009	4.6183E-011	2.7967E-011	1.7020E-008
77	0.2383	-4.8694E-044	-7.7876E-050	2.6058E-008	6.0573E-009	5.4399E-011	3.1816E-011	1.9491E-008
78	0.2391	-8.0259E-044	-1.5837E-049	3.0140E-008	7.0621E-009	6.3009E-011	3.5596E-011	2.2074E-008
79	0.2398	-1.3020E-043	-3.1286E-049	3.4367E-008	8.1209E-009	7.1816E-011	3.9196E-011	2.4729E-008
80	0.2406	-2.0780E-043	-6.0009E-049	3.8663E-008	9.2171E-009	8.0621E-011	4.2521E-011	2.7415E-008
81	0.2414	-3.2605E-043	-1.1171E-048	4.2950E-008	1.0333E-008	8.9237E-011	4.5497E-011	3.0090E-008
82	0.2422	-5.0242E-043	-2.0171E-048	4.7149E-008	1.1452E-008	9.7508E-011	4.8073E-011	3.2714E-008
83	0.2430	-7.5969E-043	-3.5328E-048	5.1187E-008	1.2556E-008	1.0532E-010	5.0229E-011	3.5252E-008
84	0.2437	-1.1264E-042	-6.0020E-048	5.4997E-008	1.3630E-008	1.1259E-010	5.1967E-011	3.7672E-008
85	0.2445	-1.6374E-042	-9.8963E-048	5.8522E-008	1.4662E-008	1.1931E-010	5.3316E-011	3.9948E-008
86	0.2453	-2.3337E-042	-1.5850E-047	6.1717E-008	1.5640E-008	1.2548E-010	5.4320E-011	4.2063E-008
87	0.2461	-3.2623E-042	-2.4689E-047	6.4550E-008	1.6556E-008	1.3114E-010	5.5036E-011	4.4002E-008
88	0.2469	-4.4766E-042	-3.7456E-047	6.6997E-008	1.7404E-008	1.3636E-010	5.5528E-011	4.5759E-008
89	0.2477	-6.0359E-042	-5.5447E-047	6.9050E-008	1.8180E-008	1.4122E-010	5.5860E-011	4.7331E-008
90	0.2484	-8.0067E-042	-8.0284E-047	7.0708E-008	1.8883E-008	1.4580E-010	5.6096E-011	4.8721E-008
91	0.2500	-1.3417E-041	-1.5716E-046	7.2860E-008	2.0063E-008	1.5442E-010	5.6454E-011	5.0965E-008
92	0.2516	-2.0925E-041	-2.8072E-046	7.3752E-008	2.0981E-008	1.6285E-010	5.6994E-011	5.2608E-008
93	0.2531	-3.0861E-041	-4.6728E-046	7.3607E-008	2.1662E-008	1.7142E-010	5.7931E-011	5.3738E-008
94	0.2562	-5.9112E-041	-1.0971E-045	7.0914E-008	2.2400E-008	1.8973E-010	6.1407E-011	5.4736E-008
95	0.2594	-9.6358E-041	-2.1197E-045	6.6812E-008	2.2606E-008	2.0945E-010	6.6731E-011	5.4745E-008
96	0.2625	-1.4097E-040	-3.5923E-045	6.2268E-008	2.2465E-008	2.2995E-010	7.3528E-011	5.4171E-008
97	0.2656	-1.9086E-040	-5.5385E-045	5.7834E-008	2.2112E-008	2.5048E-010	8.1339E-011	5.3272E-008
98	0.2688	-2.4384E-040	-7.9519E-045	5.3774E-008	2.1637E-008	2.7042E-010	8.9742E-011	5.2202E-008
99	0.2750	-3.5371E-040	-1.4113E-044	4.7067E-008	2.0517E-008	3.0694E-010	1.0724E-010	4.9851E-008
100	0.2812	-4.5451E-040	-2.1624E-044	4.2001E-008	1.9347E-008	3.3946E-010	1.2479E-010	4.7472E-008
101	0.2875	-5.4025E-040	-3.0120E-044	3.8278E-008	1.8200E-008	3.6807E-010	1.4199E-010	4.5156E-008
102	0.2938	-6.0930E-040	-3.9299E-044	3.5620E-008	1.7106E-008	3.9313E-010	1.5870E-010	4.2934E-008
103	0.3000	-6.6225E-040	-4.8928E-044	3.3808E-008	1.6078E-008	4.1506E-010	1.7488E-010	4.0816E-008
104	0.3063	-7.0084E-040	-5.8837E-044	3.2679E-008	1.5119E-008	4.3429E-010	1.9057E-010	3.8804E-008
105	0.3125	-7.2725E-040	-6.8911E-044	3.2108E-008	1.4232E-008	4.5122E-010	2.0581E-010	3.6899E-008
106	0.3188	-7.4372E-040	-7.9071E-044	3.1994E-008	1.3415E-008	4.6619E-010	2.2065E-010	3.5099E-008
107	0.3250	-7.5228E-040	-8.9267E-044	3.2256E-008	1.2668E-008	4.7956E-010	2.3515E-010	3.3402E-008
108	0.3313	-7.5469E-040	-9.9464E-044	3.2824E-008	1.1988E-008	4.9163E-010	2.4938E-010	3.1805E-008
109	0.3375	-7.5238E-040	-1.0963E-043	3.3638E-008	1.1372E-008	5.0269E-010	2.6340E-010	3.0307E-008
110	0.3438	-7.4647E-040	-1.1974E-043	3.4646E-008	1.0818E-008	5.1301E-010	2.7729E-010	2.8906E-008
111	0.3500	-7.3772E-040	-1.2971E-043	3.5796E-008	1.0322E-008	5.2276E-010	2.9107E-010	2.7597E-008
112	0.3625	-7.1234E-040	-1.4831E-043	3.8321E-008	9.4954E-009	5.4097E-010	3.1824E-010	2.5259E-008
113	0.3750	-6.8291E-040	-1.6630E-043	4.1035E-008	8.8366E-009	5.5912E-010	3.4596E-010	2.3206E-008
114	0.3875	-6.5128E-040	-1.8352E-043	4.3795E-008	8.3188E-009	5.7813E-010	3.7477E-010	2.1404E-008
115	0.4000	-6.1846E-040	-1.9973E-043	4.6499E-008	7.9167E-009	5.9853E-010	4.0505E-010	1.9820E-008
116	0.4125	-5.8517E-040	-2.1471E-043	4.9081E-008	7.6083E-009	6.2060E-010	4.3704E-010	1.8426E-008
117	0.4250	-5.5200E-040	-2.2828E-043	5.1505E-008	7.3753E-009	6.4443E-010	4.7091E-010	1.7194E-008
118	0.4375	-5.1948E-040	-2.4043E-043	5.3764E-008	7.2026E-009	6.7007E-010	5.0678E-010	1.6103E-008
119	0.4437	-5.0366E-040	-2.4615E-043	5.4849E-008	7.1351E-009	6.8366E-010	5.2556E-010	1.5601E-008
120	0.4500	-4.8823E-040	-2.5144E-043	5.5890E-008	7.0800E-009	6.9773E-010	5.4487E-010	1.5132E-008
121	0.4625	-4.5867E-040	-2.6046E-043	5.7823E-008	7.0023E-009	7.2689E-010	5.8467E-010	1.4293E-008
122	0.4688	-4.4465E-040	-2.6453E-043	5.8762E-008	6.9786E-009	7.4223E-010	6.0525E-010	1.3915E-008
123	0.4750	-4.3148E-040	-2.6815E-043	5.9685E-008	6.9667E-009	7.5813E-010	6.2627E-010	1.3574E-008
124	0.4812	-4.1936E-040	-2.7108E-043	6.0602E-008	6.9678E-009	7.7454E-010	6.4746E-010	1.3275E-008
125	0.4875	-4.0912E-040	-2.7291E-043	6.1512E-008	6.9837E-009	7.9111E-010	6.6818E-010	1.3031E-008
126	0.4906	-4.0498E-040	-2.7243E-043	6.1945E-008	6.9970E-009	7.9894E-010	6.7768E-010	1.2937E-008
127	0.4938	-4.0168E-040	-2.7231E-043	6.2326E-008	7.0121E-009	8.0573E-010	6.8573E-010	1.2868E-008
128	0.4969	-3.9984E-040	-2.6981E-043	6.2584E-008	7.0243E-009	8.1021E-010	6.9098E-010	1.2830E-008
129	0.5000	-3.9984E-040	-2.6981E-043	6.2584E-008	7.0243E-009	8.1021E-010	6.9098E-010	1.2830E-008

	X(cm)	MOLE FRACTIONS: NO	NO2	N2O	HNO	CN	HCN	H2CN
1	0.0000	3.6159E-026	1.9338E-028	3.2012E-022	4.3042E-028	1.2682E-064	1.1223E-050	1.6347E-052
2	0.0500	1.5268E-024	9.1967E-027	1.6780E-020	1.7958E-026	5.3959E-063	5.6345E-049	8.2760E-051
3	0.0750	2.3579E-023	1.7066E-025	2.5500E-020	3.4495E-025	1.0661E-061	1.0984E-047	2.0838E-049
4	0.1000	4.9184E-022	4.0873E-024	3.4360E-020	8.2868E-024	2.6952E-060	2.7702E-046	6.1303E-048
5	0.1250	1.0371E-020	9.9081E-023	4.3484E-020	1.9685E-022	6.8890E-059	7.0658E-045	1.8125E-046
6	0.1500	2.1563E-019	2.4028E-021	5.6762E-020	4.4876E-021	1.7622E-057	1.8021E-043	5.3599E-045
7	0.1625	1.7942E-018	2.3637E-020	9.6405E-020	3.8814E-020	1.8492E-056	1.8569E-042	6.3435E-044
8	0.1750	1.8556E-017	2.9173E-019	4.8834E-019	3.8963E-019	3.0535E-055	2.4102E-041	8.9962E-043

89	0.2477	3.5747E-006	4.7599E-010	4.5171E-008	1.3566E-009	1.7519E-028	3.2357E-026	1.9143E-029
90	0.2484	3.8988E-006	5.1489E-010	4.8193E-008	1.4439E-009	2.5162E-028	4.2822E-026	2.3020E-029
91	0.2500	4.5624E-006	5.9443E-010	5.3754E-008	1.6121E-009	4.8526E-028	7.2246E-026	3.2565E-029
92	0.2516	5.2337E-006	6.7471E-010	5.8684E-008	1.7699E-009	8.6078E-028	1.1522E-025	4.4270E-029
93	0.2531	5.9035E-006	7.5460E-010	6.2972E-008	1.9159E-009	1.4298E-027	1.7601E-025	5.8363E-029
94	0.2562	7.2157E-006	9.1052E-010	6.9668E-008	2.1705E-009	3.3531E-027	3.6682E-025	9.3678E-029
95	0.2594	8.4703E-006	1.0579E-009	7.4686E-008	2.3815E-009	6.5911E-027	6.5984E-025	1.3401E-028
96	0.2625	9.6555E-006	1.1950E-009	7.8461E-008	2.5547E-009	1.1487E-026	1.0760E-024	1.7810E-028
97	0.2656	1.0768E-005	1.3220E-009	8.1350E-008	2.6963E-009	1.8321E-026	1.6314E-024	2.2463E-028
98	0.2688	1.1808E-005	1.4396E-009	8.3627E-008	2.8121E-009	2.7302E-026	2.3383E-024	2.7252E-028
99	0.2750	1.3668E-005	1.6488E-009	8.6939E-008	2.9826E-009	5.2191E-026	4.2475E-024	3.7090E-028
100	0.2812	1.5332E-005	1.8375E-009	8.9568E-008	3.1004E-009	8.5751E-026	6.6777E-024	4.5427E-028
101	0.2875	1.6839E-005	2.0123E-009	9.1854E-008	3.1812E-009	1.2736E-025	9.5657E-024	5.2169E-028
102	0.2938	1.8219E-005	2.1785E-009	9.3973E-008	3.2351E-009	1.7587E-025	1.2825E-023	5.7325E-028
103	0.3000	1.9500E-005	2.3399E-009	9.6021E-008	3.2694E-009	2.2988E-025	1.6362E-023	6.1002E-028
104	0.3063	2.0701E-005	2.4997E-009	9.8052E-008	3.2890E-009	2.8795E-025	2.0091E-023	6.3374E-028
105	0.3125	2.1842E-005	2.6606E-009	1.0010E-007	3.2981E-009	3.4873E-025	2.3935E-023	6.4648E-028
106	0.3188	2.2936E-005	2.8244E-009	1.0219E-007	3.2997E-009	4.1103E-025	2.7831E-023	6.5035E-028
107	0.3250	2.3995E-005	2.9929E-009	1.0434E-007	3.2964E-009	4.7384E-025	3.1730E-023	6.4733E-028
108	0.3313	2.5028E-005	3.1675E-009	1.0655E-007	3.2901E-009	5.3637E-025	3.5594E-023	6.3917E-028
109	0.3375	2.6044E-005	3.3490E-009	1.0884E-007	3.2824E-009	5.9800E-025	3.9398E-023	6.2737E-028
110	0.3438	2.7048E-005	3.5382E-009	1.1121E-007	3.2748E-009	6.5826E-025	4.3119E-023	6.1312E-028
111	0.3500	2.8047E-005	3.7355E-009	1.1365E-007	3.2683E-009	7.1664E-025	4.6736E-023	5.9734E-028
112	0.3625	3.0037E-005	4.1544E-009	1.1872E-007	3.2632E-009	8.2472E-025	5.3522E-023	5.6404E-028
113	0.3750	3.2037E-005	4.6088E-009	1.2405E-007	3.2668E-009	9.2529E-025	5.9925E-023	5.3053E-028
114	0.3875	3.4058E-005	5.0986E-009	1.2962E-007	3.2806E-009	1.0192E-024	6.6023E-023	4.9905E-028
115	0.4000	3.6102E-005	5.6223E-009	1.3538E-007	3.3049E-009	1.1072E-024	7.1873E-023	4.7047E-028
116	0.4125	3.8169E-005	6.1780E-009	1.4129E-007	3.3391E-009	1.1899E-024	7.7521E-023	4.4491E-028
117	0.4250	4.0259E-005	6.7633E-009	1.4729E-007	3.3822E-009	1.2678E-024	8.2997E-023	4.2223E-028
118	0.4375	4.2367E-005	7.3757E-009	1.5336E-007	3.4330E-009	1.3416E-024	8.8337E-023	4.0214E-028
119	0.4437	4.3427E-005	7.6914E-009	1.5640E-007	3.4607E-009	1.3776E-024	9.0982E-023	3.9290E-028
120	0.4500	4.4490E-005	8.0121E-009	1.5944E-007	3.4904E-009	1.4128E-024	9.3602E-023	3.8443E-028
121	0.4625	4.6631E-005	8.6632E-009	1.6539E-007	3.5554E-009	1.4805E-024	9.8735E-023	3.6980E-028
122	0.4688	4.7704E-005	8.9923E-009	1.6832E-007	3.5902E-009	1.5142E-024	1.0129E-022	3.6352E-028
123	0.4750	4.8777E-005	9.3200E-009	1.7115E-007	3.6271E-009	1.5478E-024	1.0382E-022	3.5833E-028
124	0.4812	4.9845E-005	9.6407E-009	1.7385E-007	3.6663E-009	1.5813E-024	1.0629E-022	3.5456E-028
125	0.4875	5.0885E-005	9.9438E-009	1.7633E-007	3.7075E-009	1.6130E-024	1.0861E-022	3.5277E-028
126	0.4906	5.1368E-005	1.0080E-008	1.7743E-007	3.7280E-009	1.6263E-024	1.0963E-022	3.5391E-028
127	0.4938	5.1788E-005	1.0194E-008	1.7836E-007	3.7465E-009	1.6369E-024	1.1046E-022	3.5360E-028
128	0.4969	5.2072E-005	1.0269E-008	1.7898E-007	3.7594E-009	1.6399E-024	1.1095E-022	3.5711E-028
129	0.5000	5.2072E-005	1.0269E-008	1.7898E-007	3.7594E-009	1.6399E-024	1.1095E-022	3.5711E-028

	X(cm)	MOLE FRACTIONS:						
		HCNN	HCNO	HOCN	HNCO	NCO	N2	AR
1	0.0000	6.9104E-063	-1.0508E-055	1.0971E-055	2.5648E-049	2.0646E-055	5.7316E-001	0.0000E+000
2	0.0500	2.3215E-061	-5.4861E-054	5.7278E-054	1.3390E-047	1.0733E-053	5.7316E-001	0.0000E+000
3	0.0750	4.6975E-060	-1.1151E-052	1.1642E-052	2.7215E-046	6.2473E-052	5.7316E-001	0.0000E+000
4	0.1000	1.0509E-058	-2.9320E-051	3.0612E-051	7.1560E-045	3.2710E-050	5.7316E-001	0.0000E+000
5	0.1250	-3.1855E-057	-7.7967E-050	8.1401E-050	1.9029E-043	1.7111E-048	5.7316E-001	0.0000E+000
6	0.1500	-8.6084E-053	-2.0742E-048	2.1655E-048	5.0622E-042	8.9514E-047	5.7316E-001	0.0000E+000
7	0.1625	-5.0447E-049	-2.2238E-047	2.3218E-047	5.4274E-041	1.8230E-045	5.7316E-001	0.0000E+000
8	0.1750	-1.9504E-045	-3.0054E-046	3.1378E-046	7.3347E-040	3.7195E-044	5.7317E-001	0.0000E+000
9	0.1875	-7.0387E-042	-4.1416E-045	4.3241E-045	1.0107E-038	7.5899E-043	5.7319E-001	0.0000E+000
10	0.1938	-6.8194E-039	-2.4469E-044	2.5582E-044	5.9794E-038	6.3744E-042	5.7322E-001	0.0000E+000
11	0.2000	-5.6772E-040	-4.8257E-044	1.8292E-043	4.2750E-037	5.7944E-041	5.7330E-001	0.0000E+000
12	0.2031	-1.0316E-038	-1.1546E-043	6.3937E-043	1.4937E-036	2.4269E-040	5.7339E-001	0.0000E+000
13	0.2047	-5.5293E-039	-2.2647E-043	1.4156E-042	3.3059E-036	5.9541E-040	5.7345E-001	0.0000E+000
14	0.2063	5.0842E-039	-5.0770E-043	3.4343E-042	8.0156E-036	1.5784E-039	5.7355E-001	0.0000E+000
15	0.2078	6.0768E-039	-1.2339E-042	8.6845E-042	2.0253E-035	4.3228E-039	5.7368E-001	0.0000E+000
16	0.2086	3.5502E-038	-2.0327E-042	1.4462E-041	3.3703E-035	7.5580E-039	5.7376E-001	0.0000E+000
17	0.2094	-4.8267E-039	-3.4761E-042	2.4863E-041	5.7890E-035	1.3647E-038	5.7385E-001	0.0000E+000
18	0.2102	-8.8359E-038	-6.1258E-042	4.3585E-041	1.0138E-034	2.5126E-038	5.7396E-001	0.0000E+000
19	0.2109	2.0074E-036	-1.0911E-041	7.7288E-041	1.7953E-034	4.6828E-038	5.7409E-001	0.0000E+000
20	0.2113	3.9442E-036	-1.4398E-041	1.0425E-040	2.4196E-034	6.4989E-038	5.7417E-001	0.0000E+000
21	0.2117	4.0427E-036	-1.8847E-041	1.4200E-040	3.2924E-034	9.1185E-038	5.7425E-001	0.0000E+000
22	0.2121	4.3305E-036	-2.3935E-041	1.9482E-040	4.5124E-034	1.2900E-037	5.7433E-001	0.0000E+000
23	0.2125	1.6384E-035	-2.9577E-041	2.6876E-040	6.2175E-034	1.8364E-037	5.7443E-001	0.0000E+000
24	0.2129	1.7935E-035	-4.1886E-041	3.7224E-040	8.5999E-034	2.6273E-037	5.7453E-001	0.0000E+000
25	0.2133	-2.2743E-035	-7.7794E-041	5.1705E-040	1.1928E-033	3.7738E-037	5.7463E-001	0.0000E+000
26	0.2137	4.0489E-036	-8.6435E-041	7.1969E-040	1.6575E-033	5.4394E-037	5.7475E-001	0.0000E+000
27	0.2141	-4.0913E-035	-9.4227E-041	1.0032E-039	2.3063E-033	7.8646E-037	5.7487E-001	0.0000E+000
28	0.2145	-2.6603E-035	-8.1539E-041	1.3999E-039	3.2118E-033	1.1405E-036	5.7501E-001	0.0000E+000
29	0.2148	-1.3043E-035	-5.2759E-041	1.9549E-039	4.4749E-033	1.6587E-036	5.7515E-001	0.0000E+000
30	0.2152	-5.7767E-036	-7.4289E-042	2.7313E-039	6.2362E-033	2.4192E-036	5.7530E-001	0.0000E+000
31	0.2156	-2.4346E-036	5.8205E-041	3.8174E-039	8.6908E-033	3.5387E-036	5.7546E-001	0.0000E+000
32	0.2164	-4.9652E-037	2.6999E-040	7.2874E-039	1.6491E-032	7.3728E-036	5.7582E-001	0.0000E+000
33	0.2172	-8.9635E-038	6.6054E-040	1.3532E-038	3.0391E-032	1.5054E-035	5.7622E-001	0.0000E+000
34	0.2180	1.4830E-038	1.3570E-039	2.4777E-038	5.5102E-032	3.0563E-035	5.7668E-001	0.0000E+000
35	0.2188	9.7240E-038	2.6114E-039	4.5049E-038	9.8907E-032	6.2046E-035	5.7718E-001	0.0000E+000
36	0.2195	2.7088E-037	4.8762E-039	8.1644E-038	1.7631E-031	1.2625E-034	5.7775E-001	0.0000E+000

117	0.4250	2.3792E-030	1.8133E-028	1.4864E-024	4.0213E-022	6.7134E-023	6.4792E-001	0.0000E+000
118	0.4375	2.2134E-030	2.1596E-028	1.6921E-024	4.4089E-022	7.1706E-023	6.4863E-001	0.0000E+000
119	0.4437	2.1353E-030	2.3436E-028	1.7993E-024	4.6078E-022	7.4001E-023	6.4896E-001	0.0000E+000
120	0.4500	2.0610E-030	2.5364E-028	1.9089E-024	4.8096E-022	7.6278E-023	6.4927E-001	0.0000E+000
121	0.4625	1.9251E-030	2.9450E-028	2.1314E-024	5.2157E-022	8.0715E-023	6.4982E-001	0.0000E+000
122	0.4688	1.8646E-030	3.1573E-028	2.2447E-024	5.4195E-022	8.2913E-023	6.5006E-001	0.0000E+000
123	0.4750	1.8110E-030	3.3743E-028	2.3573E-024	5.6209E-022	8.5061E-023	6.5027E-001	0.0000E+000
124	0.4812	1.7663E-030	3.5912E-028	2.4657E-024	5.8134E-022	8.7093E-023	6.5045E-001	0.0000E+000
125	0.4875	1.7326E-030	3.7968E-028	2.5619E-024	5.9827E-022	8.8830E-023	6.5059E-001	0.0000E+000
126	0.4906	1.7221E-030	3.8874E-028	2.5985E-024	6.0491E-022	8.9393E-023	6.5063E-001	0.0000E+000
127	0.4938	1.7115E-030	3.9635E-028	2.6292E-024	6.1011E-022	8.9877E-023	6.5066E-001	0.0000E+000
128	0.4969	1.7074E-030	4.0090E-028	2.6379E-024	6.1224E-022	8.9745E-023	6.5068E-001	0.0000E+000
129	0.5000	1.7074E-030	4.0090E-028	2.6379E-024	6.1224E-022	8.9745E-023	6.5068E-001	0.0000E+000

	X(cm)	MOLE FRACTIONS: C3H7	C3H8	CH2CHO	CH3CHO	K	KO	HKO
1	0.0000	-2.2545E-104	-3.0829E-102	-1.9655E-076	-7.0356E-072	7.9143E-019	1.1974E-019	3.3987E-011
2	0.0500	-1.5886E-102	-2.1812E-100	-1.1477E-074	-4.1250E-070	5.3639E-017	6.8722E-018	2.7816E-009
3	0.0750	-4.7895E-101	-5.9487E-099	-1.3960E-072	-9.3779E-069	5.6455E-017	7.2151E-018	4.1519E-009
4	0.1000	-1.7976E-099	-2.1151E-097	-1.7089E-070	-2.7668E-067	5.6973E-017	7.2626E-018	5.5179E-009
5	0.1250	-6.7887E-098	-7.5847E-096	-2.1734E-068	-8.2461E-066	5.7360E-017	7.2933E-018	6.8796E-009
6	0.1500	-2.5642E-096	-2.7206E-094	-2.7892E-066	-2.4582E-064	6.2495E-017	7.9262E-018	8.2382E-009
7	0.1625	-3.8238E-095	-3.8625E-093	-1.3660E-064	-2.9298E-063	1.5627E-016	1.9793E-017	8.9330E-009
8	0.1750	-7.1247E-094	-7.0057E-092	-5.5430E-063	-4.4223E-062	1.5400E-015	1.9497E-016	9.8344E-009
9	0.1875	-1.3457E-092	-1.2904E-090	-2.2438E-061	-6.7799E-061	2.2112E-014	2.8173E-015	1.3058E-008
10	0.1938	-1.0580E-091	-9.8801E-090	-3.5559E-060	-4.3815E-060	1.3740E-013	1.7828E-014	2.1416E-008
11	0.2000	-1.0135E-090	-9.3402E-089	-5.2046E-059	-3.4368E-059	7.0145E-013	9.6143E-014	5.7624E-008
12	0.2031	-4.5755E-090	-4.0810E-088	-3.1779E-058	-1.2819E-058	1.8009E-012	2.5982E-013	1.0468E-007
13	0.2047	-1.2435E-089	-1.0793E-087	-9.6981E-058	-2.9850E-058	2.9012E-012	4.3293E-013	1.4522E-007
14	0.2063	-3.8004E-089	-3.2113E-087	-3.1101E-057	-7.6868E-058	4.5972E-012	7.1034E-013	2.0863E-007
15	0.2078	-1.2168E-088	-9.9771E-087	-1.0065E-056	-2.0636E-057	7.2121E-012	1.1460E-012	3.0320E-007
16	0.2086	-2.3579E-088	-1.8864E-086	-1.9328E-056	-3.5590E-057	9.0545E-012	1.4534E-012	3.6359E-007
17	0.2094	-4.7963E-088	-3.7380E-086	-3.8259E-056	-6.3660E-057	1.1351E-011	1.8304E-012	4.3642E-007
18	0.2102	-1.0012E-087	-7.5918E-086	-7.6749E-056	-1.1631E-056	1.4197E-011	2.2831E-012	5.2224E-007
19	0.2109	-2.1176E-087	-1.5598E-085	-1.5467E-055	-2.1498E-056	1.7687E-011	2.8108E-012	6.2025E-007
20	0.2113	-3.1528E-087	-2.2818E-085	-2.2334E-055	-2.9658E-056	1.9705E-011	3.1036E-012	6.7269E-007
21	0.2117	-4.7688E-087	-3.3898E-085	-3.2602E-055	-4.1387E-056	2.1903E-011	3.4090E-012	7.2721E-007
22	0.2121	-7.2824E-087	-5.0860E-085	-4.7931E-055	-5.8242E-056	2.4268E-011	3.7208E-012	7.8290E-007
23	0.2125	-1.1176E-086	-7.6756E-085	-7.0777E-055	-8.2459E-056	2.6777E-011	4.0302E-012	8.3855E-007
24	0.2129	-1.7170E-086	-1.1613E-084	-1.0478E-054	-1.1724E-055	2.9391E-011	4.3249E-012	8.9258E-007
25	0.2133	-2.6339E-086	-1.7574E-084	-1.5535E-054	-1.6718E-055	3.2051E-011	4.5890E-012	9.4315E-007
26	0.2137	-4.0278E-086	-2.6561E-084	-2.3047E-054	-2.3884E-055	3.4683E-011	4.8025E-012	9.8818E-007
27	0.2141	-6.1406E-086	-4.0072E-084	-3.4197E-054	-3.4166E-055	3.7204E-011	4.9425E-012	1.0256E-006
28	0.2145	-9.3726E-086	-6.0459E-084	-5.0746E-054	-4.8909E-055	3.9534E-011	4.9848E-012	1.0536E-006
29	0.2148	-1.4351E-085	-9.1309E-084	-7.5286E-054	-7.0043E-055	4.1613E-011	4.9106E-012	1.0708E-006
30	0.2152	-2.2055E-085	-1.3808E-083	-1.1165E-053	-1.0032E-054	4.3417E-011	4.7154E-012	1.0768E-006
31	0.2156	-3.4011E-085	-2.0909E-083	-1.6548E-053	-1.4368E-054	4.4969E-011	4.4220E-012	1.0724E-006
32	0.2164	-7.7972E-085	-4.6209E-083	-3.5059E-053	-2.8648E-054	4.7404E-011	3.7505E-012	1.0363E-006
33	0.2172	-1.7249E-084	-9.7972E-083	-7.1643E-053	-5.5146E-054	4.9723E-011	3.2789E-012	9.8646E-007
34	0.2180	-3.7673E-084	-2.0407E-082	-1.4408E-052	-1.0423E-053	5.2397E-011	3.2357E-012	9.3864E-007
35	0.2188	-8.1874E-084	-4.2150E-082	-2.8791E-052	-1.9503E-053	5.5793E-011	3.5592E-012	9.0252E-007
36	0.2195	-1.7752E-083	-8.6641E-082	-5.7417E-052	-3.6271E-053	6.0283E-011	4.1192E-012	8.8241E-007
37	0.2203	-3.8441E-083	-1.7742E-081	-1.1455E-051	-6.7187E-053	6.6302E-011	4.8508E-012	8.7963E-007
38	0.2211	-8.3201E-083	-3.6191E-081	-2.2884E-051	-1.2407E-052	7.4362E-011	5.7564E-012	8.9410E-007
39	0.2219	-1.8018E-082	-7.3509E-081	-4.5772E-051	-2.2844E-052	8.5081E-011	6.8827E-012	9.2537E-007
40	0.2227	-3.9103E-082	-1.4858E-080	-9.1576E-051	-4.1935E-052	9.9274E-011	8.3227E-012	9.7353E-007
41	0.2234	-8.5207E-082	-2.9863E-080	-1.8282E-050	-7.6710E-052	1.1821E-010	1.0256E-011	1.0409E-006
42	0.2250	-3.4333E-081	-1.0392E-079	-6.2889E-050	-2.3049E-051	1.7853E-010	1.7433E-011	1.2565E-006
43	0.2266	-1.2556E-080	-3.1871E-079	-2.0100E-049	-6.3058E-051	3.0291E-010	4.2125E-011	1.6944E-006
44	0.2273	-2.5242E-080	-5.7368E-079	-3.8166E-049	-1.0669E-050	4.3000E-010	8.1923E-011	2.1472E-006
45	0.2277	-3.6774E-080	-7.8661E-079	-5.3621E-049	-1.4086E-050	5.3029E-010	1.2082E-010	2.5042E-006
46	0.2281	-5.4344E-080	-1.0934E-078	-7.5882E-049	-1.8761E-050	6.7099E-010	1.8306E-010	2.9990E-006
47	0.2285	-8.1002E-080	-1.5334E-078	-1.0764E-048	-2.5120E-050	8.6736E-010	2.8133E-010	3.6733E-006
48	0.2289	-1.2126E-079	-2.1613E-078	-1.5258E-048	-3.3715E-050	1.1367E-009	4.3229E-010	4.5672E-006
49	0.2291	-1.4896E-079	-2.5743E-078	-1.8191E-048	-3.9122E-050	1.3040E-009	5.3331E-010	5.1064E-006
50	0.2293	-1.8347E-079	-3.0736E-078	-2.1705E-048	-4.5449E-050	1.4968E-009	6.5399E-010	5.7151E-006
51	0.2295	-2.2637E-079	-3.6763E-078	-2.5904E-048	-5.2840E-050	1.7162E-009	7.9528E-010	6.3925E-006
52	0.2297	-2.7963E-079	-4.4026E-078	-3.0908E-048	-6.1457E-050	1.9622E-009	9.5663E-010	7.1341E-006
53	0.2299	-3.4564E-079	-5.2766E-078	-3.6857E-048	-7.1485E-050	2.2334E-009	1.1353E-009	7.9307E-006
54	0.2301	-4.2732E-079	-6.3265E-078	-4.3913E-048	-8.3133E-050	2.5267E-009	1.3257E-009	8.7684E-006
55	0.2303	-5.2822E-079	-7.5855E-078	-5.2260E-048	-9.6635E-050	2.8368E-009	1.5189E-009	9.6282E-006
56	0.2305	-6.5265E-079	-9.0925E-078	-6.2113E-048	-1.1226E-049	3.1566E-009	1.7027E-009	1.0487E-005
57	0.2307	-8.0578E-079	-1.0893E-077	-7.3715E-048	-1.3030E-049	3.4775E-009	1.8626E-009	1.1318E-005
58	0.2309	-9.9390E-079	-1.3041E-077	-8.7346E-048	-1.5109E-049	3.7900E-009	1.9837E-009	1.2095E-005
59	0.2311	-1.2245E-078	-1.5597E-077	-1.0333E-047	-1.7500E-049	4.0846E-009	2.0534E-009	1.2794E-005
60	0.2313	-1.5066E-078	-1.8633E-077	-1.2202E-047	-2.0244E-049	4.3533E-009	2.0653E-009	1.3397E-005
61	0.2314	-1.8510E-078	-2.2233E-077	-1.4383E-047	-2.3388E-049	4.5904E-009	2.0212E-009	1.3894E-005
62	0.2316	-2.2705E-078	-2.6491E-077	-1.6924E-047	-2.6982E-049	4.7934E-009	1.9325E-009	1.4284E-005
63	0.2318	-2.7804E-078	-3.1518E-077	-1.9878E-047	-3.1082E-049	4.9631E-009	1.8182E-009	1.4576E-005
64	0.2320	-3.3985E-078	-3.7438E-077	-2.3303E-047	-3.5750E-049	5.1028E-009	1.7000E-009	1.4786E-005

13	0.2047	1.4240E-005	1.8919E-012	1.2403E-015	1.0526E-017	1.7836E-042	2.3551E-010	-4.4428E-018
14	0.2063	1.3994E-005	3.6550E-012	2.4757E-015	1.2571E-017	3.0323E-043	4.0339E-010	-4.0586E-018
15	0.2078	1.3591E-005	7.0491E-012	4.9887E-015	1.5928E-017	3.0785E-044	7.2287E-010	-2.7111E-018
16	0.2086	1.3310E-005	9.7647E-012	6.9769E-015	1.8483E-017	5.1976E-045	9.6517E-010	-6.1374E-019
17	0.2094	1.2939E-005	1.3575E-011	9.8277E-015	2.2309E-017	2.0805E-044	1.3047E-009	4.4505E-018
18	0.2102	1.2452E-005	1.8807E-011	1.3794E-014	2.8313E-017	9.0874E-044	1.7711E-009	1.6676E-017
19	0.2109	1.1821E-005	2.5808E-011	1.9085E-014	3.8086E-017	3.1154E-043	2.3910E-009	4.6176E-017
20	0.2113	1.1440E-005	3.0082E-011	2.2238E-014	4.5383E-017	5.7599E-043	2.7622E-009	7.6541E-017
21	0.2117	1.0999E-005	3.4980E-011	2.5808E-014	5.5469E-017	1.0781E-042	3.1864E-009	1.2833E-016
22	0.2121	1.0488E-005	4.0537E-011	2.9785E-014	6.9571E-017	2.0334E-042	3.6657E-009	2.1661E-016
23	0.2125	9.8978E-006	4.6769E-011	3.4131E-014	8.9460E-017	3.8532E-042	4.2004E-009	3.6708E-016
24	0.2129	9.2204E-006	5.3667E-011	3.8776E-014	1.1767E-016	7.3154E-042	4.7885E-009	6.2345E-016
25	0.2133	8.4502E-006	6.1193E-011	4.3613E-014	1.5775E-016	1.3896E-041	5.4248E-009	1.0600E-015
26	0.2137	7.5883E-006	6.9272E-011	4.8504E-014	2.1460E-016	2.6385E-041	6.1012E-009	1.8033E-015
27	0.2141	6.6466E-006	7.7796E-011	5.3284E-014	2.9476E-016	5.0277E-041	6.8068E-009	3.0678E-015
28	0.2145	5.6519E-006	8.6623E-011	5.7781E-014	4.0668E-016	1.0102E-040	7.5286E-009	5.2181E-015
29	0.2148	4.6466E-006	9.5590E-011	6.1832E-014	5.6086E-016	3.3076E-040	8.2527E-009	8.8718E-015
30	0.2152	3.6857E-006	1.0453E-010	6.5315E-014	7.6980E-016	3.5762E-039	8.9652E-009	1.5068E-014
31	0.2156	2.8274E-006	1.1328E-010	6.8157E-014	1.0480E-015	-7.9461E-034	9.6541E-009	2.5347E-014
32	0.2164	1.5712E-006	1.2984E-010	7.1853E-014	1.8621E-015	-1.7699E-032	1.0929E-008	6.5108E-014
33	0.2172	8.9019E-007	1.4507E-010	7.3778E-014	3.0275E-015	-2.6096E-032	1.2077E-008	1.6163E-013
34	0.2180	5.9093E-007	1.5948E-010	7.4408E-014	4.5679E-015	-4.3278E-032	1.3119E-008	3.1648E-013
35	0.2188	4.7138E-007	1.7416E-010	7.3947E-014	6.4671E-015	9.4472E-032	1.4087E-008	7.3974E-013
36	0.2195	4.1986E-007	1.9062E-010	7.2419E-014	8.6659E-015	-2.8623E-031	1.5015E-008	9.1675E-013
37	0.2203	3.9231E-007	2.1067E-010	6.9804E-014	1.1061E-014	2.2013E-037	1.5935E-008	9.1811E-013
38	0.2211	3.7381E-007	2.3636E-010	6.6107E-014	1.3509E-014	3.9363E-037	1.6871E-008	9.1912E-013
39	0.2219	3.5899E-007	2.6997E-010	6.1398E-014	1.5837E-014	8.1337E-037	1.7844E-008	9.2022E-013
40	0.2227	3.4543E-007	3.1432E-010	5.5834E-014	1.7863E-014	1.8297E-036	1.8868E-008	9.2143E-013
41	0.2234	3.3189E-007	3.7365E-010	4.9699E-014	1.9427E-014	4.4671E-036	1.9948E-008	9.2275E-013
42	0.2250	3.0543E-007	5.6032E-010	3.7176E-014	2.0859E-014	3.3725E-035	2.2267E-008	9.2571E-013
43	0.2266	2.8074E-007	9.3627E-010	2.9229E-014	2.2241E-014	3.4503E-034	2.4683E-008	9.2909E-013
44	0.2273	2.6803E-007	1.3172E-009	3.1083E-014	2.5847E-014	1.3027E-033	2.6204E-008	9.3094E-013
45	0.2277	2.6101E-007	1.6145E-009	3.5828E-014	2.9928E-014	2.6936E-033	2.7234E-008	9.3191E-013
46	0.2281	2.5315E-007	2.0219E-009	4.5165E-014	3.6808E-014	5.8412E-033	2.8596E-008	9.3289E-013
47	0.2285	2.4419E-007	2.5759E-009	6.1379E-014	4.7841E-014	1.3242E-032	3.0418E-008	9.3390E-013
48	0.2289	2.3371E-007	3.3147E-009	8.7474E-014	6.4714E-014	3.1155E-032	3.2804E-008	9.3492E-013
49	0.2291	2.2768E-007	3.7649E-009	1.0546E-013	7.6030E-014	4.8301E-032	3.4212E-008	9.3544E-013
50	0.2293	2.2088E-007	4.2752E-009	1.2759E-013	8.9766E-014	7.5350E-032	3.5767E-008	9.3596E-013
51	0.2295	2.1315E-007	4.8465E-009	1.5425E-013	1.0618E-013	1.1805E-031	3.7437E-008	9.3648E-013
52	0.2297	2.0435E-007	5.4770E-009	1.8564E-013	1.2547E-013	1.8534E-031	3.9168E-008	9.3700E-013
53	0.2299	1.9435E-007	6.1615E-009	2.2161E-013	1.4773E-013	2.9099E-031	4.0881E-008	9.3752E-013
54	0.2301	1.8302E-007	6.8909E-009	2.6162E-013	1.7288E-013	4.5587E-031	4.2469E-008	9.3805E-013
55	0.2303	1.7032E-007	7.6520E-009	3.0453E-013	2.0067E-013	7.1109E-031	4.3805E-008	9.3857E-013
56	0.2305	1.5628E-007	8.4281E-009	3.4865E-013	2.3065E-013	1.1021E-030	4.4749E-008	9.3909E-013
57	0.2307	1.4106E-007	9.1995E-009	3.9177E-013	2.6214E-013	1.6942E-030	4.5163E-008	9.3960E-013
58	0.2309	1.2497E-007	9.9453E-009	4.3140E-013	2.9427E-013	2.5786E-030	4.4931E-008	9.4011E-013
59	0.2311	1.0850E-007	1.0645E-008	4.6507E-013	3.2607E-013	3.8808E-030	4.3977E-008	9.4061E-013
60	0.2313	9.2262E-008	1.1281E-008	4.9077E-013	3.5653E-013	5.7694E-030	4.2286E-008	9.4110E-013
61	0.2314	7.6932E-008	1.1841E-008	5.0733E-013	3.8474E-013	8.4670E-030	3.9908E-008	9.4158E-013
62	0.2316	6.3156E-008	1.2318E-008	5.1460E-013	4.0995E-013	1.2263E-029	3.6957E-008	9.4204E-013
63	0.2318	5.1418E-008	1.2710E-008	5.1349E-013	4.3167E-013	1.7527E-029	3.3597E-008	9.4249E-013
64	0.2320	4.1949E-008	1.3024E-008	5.0564E-013	4.4967E-013	2.4723E-029	3.0019E-008	9.4292E-013
65	0.2322	3.4699E-008	1.3266E-008	4.9305E-013	4.6397E-013	3.4415E-029	2.6410E-008	9.4332E-013
66	0.2324	2.9378E-008	1.3449E-008	4.7765E-013	4.7478E-013	4.7266E-029	2.2934E-008	9.4369E-013
67	0.2326	2.5563E-008	1.3582E-008	4.6099E-013	4.8242E-013	6.4015E-029	1.9710E-008	9.4403E-013
68	0.2328	2.2816E-008	1.3676E-008	4.4413E-013	4.8729E-013	8.5429E-029	1.6814E-008	9.4433E-013
69	0.2330	2.0766E-008	1.3737E-008	4.2770E-013	4.8979E-013	1.1223E-028	1.4275E-008	9.4459E-013
70	0.2332	1.9144E-008	1.3772E-008	4.1202E-013	4.9029E-013	1.4501E-028	1.2090E-008	9.4479E-013
71	0.2336	1.6702E-008	1.3778E-008	3.8333E-013	4.8634E-013	2.2976E-028	8.6938E-009	9.4500E-013
72	0.2344	1.3277E-008	1.3608E-008	3.3512E-013	4.6640E-013	4.7042E-028	4.6240E-009	9.4435E-013
73	0.2352	1.0914E-008	1.3281E-008	2.9496E-013	4.4004E-013	7.7563E-028	2.5357E-009	9.4148E-013
74	0.2359	9.2072E-009	1.2842E-008	2.6114E-013	4.1163E-013	1.1196E-027	1.4419E-009	9.3499E-013
75	0.2367	7.9363E-009	1.2330E-008	2.3250E-013	3.8357E-013	1.4966E-027	8.4786E-010	9.2289E-013
76	0.2375	6.9725E-009	1.1775E-008	2.0827E-013	3.5716E-013	1.9032E-027	5.1468E-010	9.0259E-013
77	0.2383	6.2335E-009	1.1199E-008	1.8787E-013	3.3311E-013	2.3257E-027	3.2227E-010	8.7120E-013
78	0.2391	5.6626E-009	1.0618E-008	1.7075E-013	3.1166E-013	2.7375E-027	2.0801E-010	8.2622E-013
79	0.2398	5.2199E-009	1.0043E-008	1.5637E-013	2.9275E-013	3.1014E-027	1.3830E-010	7.6661E-013
80	0.2406	4.8757E-009	9.4799E-009	1.4416E-013	2.7606E-013	3.3788E-027	9.4634E-011	6.9373E-013
81	0.2414	4.6083E-009	8.9336E-009	1.3350E-013	2.6098E-013	3.5413E-027	6.6569E-011	6.1164E-013
82	0.2422	4.4006E-009	8.4069E-009	1.2371E-013	2.4667E-013	3.5806E-027	4.8076E-011	5.2621E-013
83	0.2430	4.2397E-009	7.9021E-009	1.1410E-013	2.3208E-013	3.5095E-027	3.5594E-011	4.4338E-013
84	0.2437	4.1151E-009	7.4214E-009	1.0397E-013	2.1614E-013	3.3551E-027	2.6973E-011	3.6776E-013
85	0.2445	4.0184E-009	6.9671E-009	9.2850E-014	1.9799E-013	3.1491E-027	2.0888E-011	3.0191E-013
86	0.2453	3.9425E-009	6.5413E-009	8.0678E-014	1.7735E-013	2.9196E-027	1.6503E-011	2.4651E-013
87	0.2461	3.8818E-009	6.1460E-009	6.7928E-014	1.5478E-013	2.6876E-027	1.3281E-011	2.0102E-013
88	0.2469	3.8314E-009	5.7827E-009	5.5478E-014	1.3157E-013	2.4650E-027	1.0870E-011	1.6485E-013
89	0.2477	3.7874E-009	5.4524E-009	4.4236E-014	1.0929E-013	2.2636E-027	9.0357E-012	1.3532E-013
90	0.2484	3.7465E-009	5.1555E-009	3.4785E-014	8.9323E-014	2.0847E-027	7.6175E-012	1.1170E-013
91	0.2500	3.6653E-009	4.6599E-009	2.1557E-014	5.8963E-014	1.7952E-027	5.6228E-012	7.7645E-014
92	0.2516	3.5743E-009	4.2854E-009	1.3910E-014	3.9429E-014	1.5860E-027	4.3188E-012	5.5317E-014

41	0.2234	1.4641E-017	1.3494E-005
42	0.2250	1.9256E-017	1.3372E-005
43	0.2266	2.9346E-017	1.3064E-005
44	0.2273	3.9513E-017	1.2702E-005
45	0.2277	4.7145E-017	1.2399E-005
46	0.2281	5.7395E-017	1.1961E-005
47	0.2285	7.1295E-017	1.1346E-005
48	0.2289	9.0290E-017	1.0508E-005
49	0.2291	1.0230E-016	9.9938E-006
50	0.2293	1.1642E-016	9.4069E-006
51	0.2295	1.3301E-016	8.7470E-006
52	0.2297	1.5255E-016	8.0183E-006
53	0.2299	1.7557E-016	7.2293E-006
54	0.2301	2.0269E-016	6.3943E-006
55	0.2303	2.3467E-016	5.5328E-006
56	0.2305	2.7237E-016	4.6694E-006
57	0.2307	3.1682E-016	3.8318E-006
58	0.2309	3.6922E-016	3.0483E-006
59	0.2311	4.3096E-016	2.3447E-006
60	0.2313	5.0368E-016	1.7406E-006
61	0.2314	5.8928E-016	1.2468E-006
62	0.2316	6.8998E-016	8.6379E-007
63	0.2318	8.0835E-016	5.8235E-007
64	0.2320	9.4738E-016	3.8624E-007
65	0.2322	1.1106E-015	2.5586E-007
66	0.2324	1.3018E-015	1.7206E-007
67	0.2326	1.5258E-015	1.1889E-007
68	0.2328	1.7878E-015	8.4711E-008
69	0.2330	2.0939E-015	6.1964E-008
70	0.2332	2.4511E-015	4.6119E-008
71	0.2336	3.3519E-015	2.6544E-008
72	0.2344	6.1978E-015	9.2851E-009
73	0.2352	1.1223E-014	3.4000E-009
74	0.2359	1.9808E-014	1.3067E-009
75	0.2367	3.3914E-014	5.2738E-010
76	0.2375	5.6064E-014	2.2392E-010
77	0.2383	8.9043E-014	1.0016E-010
78	0.2391	1.3520E-013	4.7218E-011
79	0.2398	1.9542E-013	2.3454E-011
80	0.2406	2.6816E-013	1.2260E-011
81	0.2414	3.4923E-013	6.7317E-012
82	0.2422	4.3274E-013	3.8728E-012
83	0.2430	5.1271E-013	2.3278E-012
84	0.2437	5.8460E-013	1.4573E-012
85	0.2445	6.4588E-013	9.4703E-013
86	0.2453	6.9590E-013	6.3677E-013
87	0.2461	7.3526E-013	4.4155E-013
88	0.2469	7.6460E-013	3.1480E-013
89	0.2477	7.8667E-013	2.3008E-013
90	0.2484	8.0228E-013	1.7195E-013
91	0.2500	8.1882E-013	1.0179E-013
92	0.2516	8.2199E-013	6.3928E-014
93	0.2531	8.1648E-013	4.2122E-014
94	0.2562	7.9075E-013	2.0615E-014
95	0.2594	7.5535E-013	1.1289E-014
96	0.2625	7.1683E-013	6.8105E-015
97	0.2656	6.7878E-013	4.4771E-015
98	0.2688	6.4310E-013	3.1742E-015
99	0.2750	5.8239E-013	1.9244E-015
100	0.2812	5.3255E-013	1.3738E-015
101	0.2875	4.9184E-013	1.0893E-015
102	0.2938	4.5832E-013	9.2012E-016
103	0.3000	4.3045E-013	8.0581E-016
104	0.3063	4.0707E-013	7.1962E-016
105	0.3125	3.8736E-013	6.4893E-016
106	0.3188	3.7072E-013	5.8769E-016
107	0.3250	3.5672E-013	5.3298E-016
108	0.3313	3.4503E-013	4.8345E-016
109	0.3375	3.3540E-013	4.3847E-016
110	0.3438	3.2760E-013	3.9776E-016
111	0.3500	3.2146E-013	3.6115E-016
112	0.3625	3.1406E-013	3.0015E-016
113	0.3750	3.1081E-013	2.5116E-016
114	0.3875	3.1082E-013	2.1207E-016
115	0.4000	3.1332E-013	1.8087E-016
116	0.4125	3.1766E-013	1.5588E-016
117	0.4250	3.2335E-013	1.3572E-016
118	0.4375	3.2998E-013	1.1926E-016
119	0.4437	3.3348E-013	1.1207E-016
120	0.4500	3.3711E-013	1.0558E-016

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THIS IS THE FIRST CALL TO AREA
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1	0.0000	6.7300E+002	1.0000E+000	2.6408E+003	3.7867E-004	-1.7131E-005
2	0.1000	6.7300E+002	1.0000E+000	2.6408E+003	3.7867E-004	-1.7131E-005
3	0.2000	1.0748E+003	1.0000E+000	4.0872E+003	2.4467E-004	1.1639E+005
4	0.2500	1.6133E+003	1.0000E+000	5.8917E+003	1.6973E-004	1.8600E+005
5	0.3000	2.1518E+003	1.0000E+000	7.5584E+003	1.3230E-004	9.2193E+004
6	0.4000	2.5536E+003	1.0000E+000	8.7212E+003	1.1466E-004	5.6685E-002
7	0.5000	2.5536E+003	1.0000E+000	8.7212E+003	1.1466E-004	5.6685E-002

	X(cm)	MOLE FRACTIONS:					
		H2	H	O	O2	OH	H2O	HO2
1	0.0000	2.9585E-001	0.0000E+000	0.0000E+000	1.4793E-001	0.0000E+000	0.0000E+000	0.0000E+000
2	0.1000	2.9585E-001	0.0000E+000	0.0000E+000	1.4793E-001	0.0000E+000	0.0000E+000	0.0000E+000
3	0.2000	2.3823E-001	1.0941E-003	3.5843E-004	1.1804E-001	2.8048E-003	6.5088E-002	5.2855E-007
4	0.2500	1.6098E-001	2.5608E-003	8.3890E-004	7.7966E-002	6.5646E-003	1.5234E-001	1.2371E-006
5	0.3000	8.3735E-002	4.0274E-003	1.3194E-003	3.7897E-002	1.0324E-002	2.3959E-001	1.9456E-006
6	0.4000	2.6109E-002	5.1215E-003	1.6778E-003	8.0053E-003	1.3129E-002	3.0467E-001	2.4741E-006
7	0.5000	2.6109E-002	5.1215E-003	1.6778E-003	8.0053E-003	1.3129E-002	3.0467E-001	2.4741E-006

	X(cm)	MOLE FRACTIONS:						
		H2O2	C	CH	CH2	CH2(S)	CH3	CH4
1	0.0000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
2	0.1000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
3	0.2000	4.6246E-008	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
4	0.2500	1.0824E-007	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
5	0.3000	1.7023E-007	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
6	0.4000	2.1648E-007	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
7	0.5000	2.1648E-007	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000

	X(cm)	MOLE FRACTIONS:						
		CO	CO2	HCO	CH2O	CH2OH	CH3O	CH3OH
1	0.0000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
2	0.1000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
3	0.2000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
4	0.2500	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
5	0.3000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
6	0.4000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
7	0.5000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000

	X(cm)	MOLE FRACTIONS:						
		C2H	C2H2	C2H3	C2H4	C2H5	C2H6	HCCO
1	0.0000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
2	0.1000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
3	0.2000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
4	0.2500	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
5	0.3000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
6	0.4000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
7	0.5000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000

	X(cm)	MOLE FRACTIONS:						
		CH2CO	HCCOH	N	NH	NH2	NH3	NNH
1	0.0000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
2	0.1000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
3	0.2000	0.0000E+000	0.0000E+000	8.1373E-008	1.5360E-008	5.0935E-009	7.3241E-009	2.1974E-009
4	0.2500	0.0000E+000	0.0000E+000	1.9045E-007	3.5949E-008	1.1921E-008	1.7142E-008	5.1429E-009
5	0.3000	0.0000E+000	0.0000E+000	2.9953E-007	5.6539E-008	1.8749E-008	2.6960E-008	8.0884E-009
6	0.4000	0.0000E+000	0.0000E+000	3.8091E-007	7.1899E-008	2.3842E-008	3.4284E-008	1.0286E-008
7	0.5000	0.0000E+000	0.0000E+000	3.8091E-007	7.1899E-008	2.3842E-008	3.4284E-008	1.0286E-008

	X(cm)	MOLE FRACTIONS:						
		NO	NO2	N2O	HNO	CN	HCN	H2CN
1	0.0000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
2	0.1000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
3	0.2000	9.4870E-004	1.5663E-007	4.7708E-008	5.1291E-008	0.0000E+000	0.0000E+000	0.0000E+000
4	0.2500	2.2204E-003	3.6658E-007	1.1166E-007	1.2005E-007	0.0000E+000	0.0000E+000	0.0000E+000
5	0.3000	3.4921E-003	5.7654E-007	1.7561E-007	1.8880E-007	0.0000E+000	0.0000E+000	0.0000E+000
6	0.4000	4.4408E-003	7.3316E-007	2.2332E-007	2.4009E-007	0.0000E+000	0.0000E+000	0.0000E+000
7	0.5000	4.4408E-003	7.3316E-007	2.2332E-007	2.4009E-007	0.0000E+000	0.0000E+000	0.0000E+000

	X(cm)	MOLE FRACTIONS:						
		HCNN	HCNO	HOCN	HNCO	NCO	N2	AR
1	0.0000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	5.5620E-001	0.0000E+000
2	0.1000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	5.5620E-001	0.0000E+000
3	0.2000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	5.7343E-001	0.0000E+000
4	0.2500	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	5.9651E-001	0.0000E+000
5	0.3000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	6.1960E-001	0.0000E+000

5	0.3000	-7.1342E-019	-1.5697E-018	-3.6987E-024	-9.5949E-027	-1.6214E-030	-2.4509E-032	-2.1456E-032
6	0.4000	-1.5132E-018	-1.4557E-018	-4.1206E-024	-2.1385E-026	-1.3001E-030	-2.0903E-032	-2.4504E-032
7	0.5000	-1.5132E-018	-1.4557E-018	-4.1206E-024	-2.1385E-026	-1.3001E-030	-2.0903E-032	-2.4504E-032

	X(cm)	MOLE FRACTIONS: C2H	C2H2	C2H3	C2H4	C2H5	C2H6	HCCO
1	0.0000	-5.0127E-064	-6.9163E-056	-7.9612E-060	-1.3861E-056	-3.0534E-059	-5.7823E-058	-4.9013E-056
2	0.1000	-1.4794E-061	-2.0606E-053	-2.3932E-057	-4.1978E-054	-1.0035E-056	-1.9148E-055	-9.7266E-054
3	0.2000	-9.6085E-056	-5.4199E-051	-2.4073E-052	-1.1236E-051	-3.4428E-054	-5.1654E-053	-2.7626E-049
4	0.2500	-1.4685E-051	-4.5340E-049	-7.4658E-051	-7.1536E-051	-5.4736E-054	-7.1107E-054	-5.7015E-047
5	0.3000	-4.7652E-049	-2.0942E-047	-1.3347E-050	-4.1062E-051	-6.9915E-055	-1.3665E-055	-1.0942E-045
6	0.4000	-2.9295E-047	-6.1062E-046	-7.7756E-050	-1.5038E-050	-9.5242E-055	-3.0427E-056	-1.6678E-044
7	0.5000	-2.9295E-047	-6.1062E-046	-7.7756E-050	-1.5038E-050	-9.5242E-055	-3.0427E-056	-1.6678E-044

	X(cm)	MOLE FRACTIONS: CH2CO	HCCOH	N	NH	NH2	NH3	NNH
1	0.0000	-6.2157E-053	-2.6582E-059	2.9394E-014	1.5563E-014	5.2869E-016	1.6798E-015	6.2097E-015
2	0.1000	-2.1589E-050	-9.2327E-057	5.3377E-012	2.3853E-012	8.2632E-014	3.5547E-013	1.5796E-012
3	0.2000	-7.9968E-048	-3.2565E-054	4.7410E-009	1.1271E-009	1.8314E-011	4.4003E-011	4.8544E-009
4	0.2500	-3.1267E-046	-4.2658E-051	7.3517E-008	1.7641E-008	1.8915E-010	7.8564E-011	5.5297E-008
5	0.3000	-1.3103E-045	-1.8188E-049	7.6440E-008	2.4989E-008	8.0020E-010	2.9685E-010	7.0844E-008
6	0.4000	-9.6899E-045	-8.9283E-048	3.0425E-007	3.3104E-008	2.5432E-009	1.1490E-009	6.3779E-008
7	0.5000	-9.6899E-045	-8.9283E-048	3.0425E-007	3.3104E-008	2.5432E-009	1.1490E-009	6.3779E-008

	X(cm)	MOLE FRACTIONS: NO	NO2	N2O	HNO	CN	HCN	H2CN
1	0.0000	5.7882E-012	6.3242E-013	7.8161E-014	7.3857E-015	-1.9814E-044	-3.6079E-037	-2.5672E-039
2	0.1000	1.4527E-009	1.7904E-010	2.4433E-011	1.8309E-012	-5.0136E-042	-1.0801E-034	-7.7512E-037
3	0.2000	3.5210E-007	1.2691E-010	6.6713E-009	2.2643E-010	-1.0338E-036	-2.8008E-032	-1.5635E-034
4	0.2500	5.9513E-006	5.8359E-010	4.4377E-008	1.7688E-009	-9.9464E-033	-2.1745E-030	-9.1666E-034
5	0.3000	1.3132E-005	1.0422E-009	6.5403E-008	2.5983E-009	-2.6554E-030	-1.3061E-028	-5.4648E-033
6	0.4000	5.2224E-005	5.6691E-009	1.2097E-007	5.6087E-009	-5.7145E-029	-1.7208E-027	-1.9231E-032
7	0.5000	5.2224E-005	5.6691E-009	1.2097E-007	5.6087E-009	-5.7145E-029	-1.7208E-027	-1.9231E-032

	X(cm)	MOLE FRACTIONS: HCNN	HCNO	HOCN	HNCO	NCO	N2	AR
1	0.0000	-4.8829E-043	-2.4184E-042	-4.1894E-041	-3.9861E-036	-1.2051E-038	5.5622E-001	0.0000E+000
2	0.1000	-9.6902E-041	-7.5293E-040	-1.3043E-038	-1.2410E-033	-3.7359E-036	5.5704E-001	0.0000E+000
3	0.2000	-1.0233E-035	-2.1264E-037	-3.6925E-036	-3.3675E-031	-3.1987E-033	5.8243E-001	0.0000E+000
4	0.2500	-6.5256E-035	-8.9798E-036	-5.0838E-033	-2.0272E-029	-1.2780E-030	5.9696E-001	0.0000E+000
5	0.3000	-2.6551E-035	-6.1681E-035	-7.0998E-031	-3.5271E-028	-8.5012E-029	6.0274E-001	0.0000E+000
6	0.4000	-1.0066E-034	-4.9781E-033	-1.8073E-029	-3.1902E-027	-9.0201E-028	6.0861E-001	0.0000E+000
7	0.5000	-1.0066E-034	-4.9781E-033	-1.8073E-029	-3.1902E-027	-9.0201E-028	6.0861E-001	0.0000E+000

	X(cm)	MOLE FRACTIONS: C3H7	C3H8	CH2CHO	CH3CHO	K	KO	HKO
1	0.0000	6.1789E-084	2.3258E-082	-2.8890E-054	-3.2977E-055	5.2015E-015	1.3871E-015	5.6500E-010
2	0.1000	2.6085E-081	9.8586E-080	-1.0077E-051	-1.1551E-052	2.1107E-012	4.7530E-013	2.7736E-007
3	0.2000	3.8176E-078	3.7983E-077	-4.0976E-049	-1.0174E-050	5.9334E-009	1.7413E-009	1.5323E-005
4	0.2500	5.5270E-079	1.0158E-078	-1.5321E-048	-9.1211E-051	6.2207E-009	3.1560E-009	1.5758E-005
5	0.3000	1.6830E-080	6.2654E-081	-6.1884E-049	-6.2395E-051	3.6610E-007	1.2131E-007	1.5424E-005
6	0.4000	2.7221E-080	6.4193E-082	-9.4606E-049	-1.5798E-050	4.6060E-006	3.3965E-007	1.1105E-005
7	0.5000	2.7221E-080	6.4193E-082	-9.4606E-049	-1.5798E-050	4.6060E-006	3.3965E-007	1.1105E-005

	X(cm)	MOLE FRACTIONS: KO2	HK	K2O	K2O2	K2CO3	K2H2O2	KHCO3
1	0.0000	1.4677E-005	8.9702E-014	2.7415E-017	3.3220E-018	2.0484E-043	7.5509E-012	-5.4546E-021
2	0.1000	2.5286E-006	2.3274E-011	1.5005E-014	1.8471E-015	1.1615E-040	4.2055E-009	-3.0045E-018
3	0.2000	2.1627E-008	1.4192E-008	6.6297E-013	7.8324E-013	-2.3887E-033	5.5828E-009	-3.1160E-018
4	0.2500	3.0966E-009	5.4730E-009	1.5322E-014	4.4159E-014	-5.9726E-033	4.3355E-012	-1.9124E-019
5	0.3000	1.2556E-009	1.8358E-008	1.1306E-014	6.4935E-015	-1.3616E-032	1.1792E-013	-5.5722E-022
6	0.4000	3.5647E-010	3.2540E-008	1.3382E-014	9.1367E-016	-1.7404E-032	1.1749E-014	-1.3383E-023
7	0.5000	3.5647E-010	3.2540E-008	1.3382E-014	9.1367E-016	-1.7404E-032	1.1749E-014	-1.3383E-023

	X(cm)	MOLE FRACTIONS: KCO3	KO3
1	0.0000	5.3793E-025	2.1948E-008
2	0.1000	2.9601E-022	1.1910E-005
3	0.2000	-2.6817E-020	1.2477E-008
4	0.2500	-2.5975E-018	4.4088E-014
5	0.3000	-9.7119E-019	3.7165E-016
6	0.4000	-3.1449E-019	4.8164E-017
7	0.5000	-3.1449E-019	4.8164E-017

TWOPNT: SUCCESS. PROBLEM SOLVED.

PREMIX: FINISHED FIXED TEMPERATURE CASE,ADDING THE ENERGY EQUATION.

TWOPNT: DOUBLE PRECISION (TWO POINT BOUNDARY VALUE PROBLEM) SOLVER,
VERSION 3.30 OF APRIL 1998 BY DR. JOSEPH F. GRCAR.

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          SEARCH    -2.89    0.00   6 SEARCH STEPS

          REFINE    -2.89           0.13 AND 0.77 RATIOS, 125 GRID POINTS
          SEARCH    -2.77    0.00   9 SEARCH STEPS

          REFINE    -2.77           0.10 AND 0.69 RATIOS, 127 GRID POINTS
          SEARCH    -5.35    0.00   4 SEARCH STEPS

          REFINE    -5.35           0.10 AND 0.57 RATIOS, 129 GRID POINTS
          SEARCH    -4.38    0.00   3 SEARCH STEPS

          REFINE    -4.38           0.10 AND 0.43 RATIOS

TWOPNT:  FINAL SOLUTION:
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	X(cm)	T(K)	AREA(cm^2)	V(cm/s)	RHO(g/cm^3)	HDOT(cal/s/cm^3)
1	0.0000	6.7300E+002	1.0000E+000	9.1903E+002	3.7867E-004	-7.8054E-006
2	0.0250	6.7300E+002	1.0000E+000	9.1903E+002	3.7867E-004	3.8266E-005
3	0.0500	6.7300E+002	1.0000E+000	9.1903E+002	3.7867E-004	4.2798E-005
4	0.0750	6.7300E+002	1.0000E+000	9.1903E+002	3.7867E-004	4.3356E-005
5	0.0875	6.7300E+002	1.0000E+000	9.1903E+002	3.7867E-004	4.3461E-005
6	0.1000	6.7300E+002	1.0000E+000	9.1903E+002	3.7867E-004	4.3538E-005
7	0.1250	6.7300E+002	1.0000E+000	9.1903E+002	3.7867E-004	4.3786E-005
8	0.1500	6.7300E+002	1.0000E+000	9.1903E+002	3.7867E-004	4.9411E-005
9	0.1625	6.7300E+002	1.0000E+000	9.1903E+002	3.7867E-004	1.5238E-004
10	0.1750	6.7300E+002	1.0000E+000	9.1903E+002	3.7867E-004	1.6474E-003
11	0.1875	6.7302E+002	1.0000E+000	9.1903E+002	3.7867E-004	2.3736E-002
12	0.1938	6.7306E+002	1.0000E+000	9.1905E+002	3.7867E-004	1.4972E-001
13	0.2000	6.7323E+002	1.0000E+000	9.1916E+002	3.7862E-004	8.3438E-001
14	0.2031	6.7345E+002	1.0000E+000	9.1934E+002	3.7855E-004	2.3558E+000
15	0.2047	6.7366E+002	1.0000E+000	9.1953E+002	3.7847E-004	4.0861E+000
16	0.2063	6.7399E+002	1.0000E+000	9.1984E+002	3.7834E-004	7.1244E+000
17	0.2078	6.7451E+002	1.0000E+000	9.2037E+002	3.7812E-004	1.2523E+001
18	0.2086	6.7488E+002	1.0000E+000	9.2075E+002	3.7797E-004	1.6762E+001
19	0.2094	6.7536E+002	1.0000E+000	9.2126E+002	3.7776E-004	2.2516E+001
20	0.2102	6.7597E+002	1.0000E+000	9.2192E+002	3.7749E-004	3.0317E+001
21	0.2105	6.7634E+002	1.0000E+000	9.2232E+002	3.7732E-004	3.5230E+001
22	0.2109	6.7676E+002	1.0000E+000	9.2278E+002	3.7714E-004	4.0965E+001
23	0.2113	6.7723E+002	1.0000E+000	9.2331E+002	3.7692E-004	4.7651E+001
24	0.2117	6.7777E+002	1.0000E+000	9.2392E+002	3.7667E-004	5.5434E+001
25	0.2121	6.7838E+002	1.0000E+000	9.2462E+002	3.7639E-004	6.4475E+001
26	0.2125	6.7907E+002	1.0000E+000	9.2541E+002	3.7606E-004	7.4951E+001
27	0.2129	6.7985E+002	1.0000E+000	9.2631E+002	3.7570E-004	8.7049E+001
28	0.2133	6.8073E+002	1.0000E+000	9.2734E+002	3.7528E-004	1.0096E+002
29	0.2137	6.8172E+002	1.0000E+000	9.2850E+002	3.7481E-004	1.1688E+002
30	0.2141	6.8283E+002	1.0000E+000	9.2981E+002	3.7429E-004	1.3496E+002
31	0.2145	6.8407E+002	1.0000E+000	9.3128E+002	3.7369E-004	1.5538E+002
32	0.2148	6.8546E+002	1.0000E+000	9.3294E+002	3.7303E-004	1.7828E+002
33	0.2152	6.8701E+002	1.0000E+000	9.3480E+002	3.7229E-004	2.0384E+002
34	0.2156	6.8873E+002	1.0000E+000	9.3688E+002	3.7146E-004	2.3230E+002
35	0.2164	6.9276E+002	1.0000E+000	9.4176E+002	3.6954E-004	2.9866E+002
36	0.2172	6.9760E+002	1.0000E+000	9.4766E+002	3.6723E-004	3.7908E+002
37	0.2180	7.0336E+002	1.0000E+000	9.5473E+002	3.6452E-004	4.7491E+002
38	0.2188	7.1016E+002	1.0000E+000	9.6309E+002	3.6135E-004	5.8696E+002
39	0.2195	7.1810E+002	1.0000E+000	9.7288E+002	3.5772E-004	7.1567E+002
40	0.2203	7.2728E+002	1.0000E+000	9.8422E+002	3.5360E-004	8.6112E+002
41	0.2211	7.3780E+002	1.0000E+000	9.9722E+002	3.4898E-004	1.0230E+003
42	0.2219	7.4975E+002	1.0000E+000	1.0120E+003	3.4389E-004	1.2003E+003
43	0.2234	7.7808E+002	1.0000E+000	1.0470E+003	3.3238E-004	1.5883E+003
44	0.2250	8.1177E+002	1.0000E+000	1.0884E+003	3.1973E-004	2.0110E+003
45	0.2258	8.3054E+002	1.0000E+000	1.1114E+003	3.1313E-004	2.2333E+003
46	0.2266	8.5072E+002	1.0000E+000	1.1360E+003	3.0636E-004	2.4597E+003
47	0.2270	8.6134E+002	1.0000E+000	1.1489E+003	3.0292E-004	2.5746E+003
48	0.2273	8.7232E+002	1.0000E+000	1.1622E+003	2.9945E-004	2.6907E+003
49	0.2277	8.8367E+002	1.0000E+000	1.1759E+003	2.9596E-004	2.8083E+003
50	0.2281	8.9537E+002	1.0000E+000	1.1900E+003	2.9244E-004	2.9278E+003
51	0.2283	9.0136E+002	1.0000E+000	1.1972E+003	2.9068E-004	2.9886E+003
52	0.2285	9.0744E+002	1.0000E+000	1.2045E+003	2.8892E-004	3.0501E+003
53	0.2287	9.1360E+002	1.0000E+000	1.2120E+003	2.8715E-004	3.1124E+003
54	0.2289	9.1986E+002	1.0000E+000	1.2195E+003	2.8538E-004	3.1756E+003
55	0.2291	9.2620E+002	1.0000E+000	1.2271E+003	2.8361E-004	3.2396E+003
56	0.2293	9.3263E+002	1.0000E+000	1.2348E+003	2.8184E-004	3.3043E+003
57	0.2295	9.3914E+002	1.0000E+000	1.2426E+003	2.8006E-004	3.3695E+003
58	0.2297	9.4573E+002	1.0000E+000	1.2505E+003	2.7830E-004	3.4349E+003
59	0.2299	9.5241E+002	1.0000E+000	1.2585E+003	2.7653E-004	3.5001E+003
60	0.2301	9.5916E+002	1.0000E+000	1.2666E+003	2.7477E-004	3.5647E+003
61	0.2303	9.6598E+002	1.0000E+000	1.2747E+003	2.7301E-004	3.6283E+003
62	0.2305	9.7288E+002	1.0000E+000	1.2830E+003	2.7125E-004	3.6906E+003
63	0.2307	9.7985E+002	1.0000E+000	1.2913E+003	2.6951E-004	3.7514E+003
64	0.2309	9.8688E+002	1.0000E+000	1.2997E+003	2.6777E-004	3.8106E+003

93	0.2500	6.5429E-002	6.0624E-002	1.3673E-002	4.5390E-002	1.2025E-002	2.0469E-001	3.3038E-005
94	0.2516	6.1176E-002	6.0436E-002	1.3967E-002	4.1884E-002	1.2765E-002	2.1066E-001	2.9907E-005
95	0.2531	5.7980E-002	5.9911E-002	1.4157E-002	3.9110E-002	1.3428E-002	2.1541E-001	2.7383E-005
96	0.2562	5.4031E-002	5.8149E-002	1.4283E-002	3.5365E-002	1.4531E-002	2.2203E-001	2.3791E-005
97	0.2594	5.1855E-002	5.5981E-002	1.4207E-002	3.2917E-002	1.5423E-002	2.2656E-001	2.1292E-005
98	0.2625	5.0658E-002	5.3699E-002	1.4007E-002	3.1260E-002	1.6150E-002	2.2985E-001	1.9470E-005
99	0.2656	4.9977E-002	5.1456E-002	1.3736E-002	3.0076E-002	1.6749E-002	2.3242E-001	1.8071E-005
100	0.2688	4.9551E-002	4.9325E-002	1.3430E-002	2.9175E-002	1.7248E-002	2.3455E-001	1.6945E-005
101	0.2750	4.9023E-002	4.5481E-002	1.2783E-002	2.7875E-002	1.8007E-002	2.3806E-001	1.5225E-005
102	0.2812	4.8558E-002	4.2123E-002	1.2147E-002	2.6830E-002	1.8582E-002	2.4115E-001	1.3861E-005
103	0.2875	4.8068E-002	3.9171E-002	1.1541E-002	2.5927E-002	1.9023E-002	2.4398E-001	1.2727E-005
104	0.2938	4.7540E-002	3.6553E-002	1.0970E-002	2.5115E-002	1.9362E-002	2.4663E-001	1.1760E-005
105	0.3000	4.6977E-002	3.4209E-002	1.0434E-002	2.4370E-002	1.9620E-002	2.4914E-001	1.0919E-005
106	0.3063	4.6388E-002	3.2096E-002	9.9310E-003	2.3678E-002	1.9812E-002	2.5152E-001	1.0180E-005
107	0.3125	4.5782E-002	3.0181E-002	9.4591E-003	2.3032E-002	1.9949E-002	2.5379E-001	9.5252E-006
108	0.3188	4.5164E-002	2.8440E-002	9.0169E-003	2.2424E-002	2.0039E-002	2.5595E-001	8.9424E-006
109	0.3250	4.4541E-002	2.6851E-002	8.6030E-003	2.1852E-002	2.0090E-002	2.5802E-001	8.4218E-006
110	0.3313	4.3918E-002	2.5399E-002	8.2160E-003	2.1311E-002	2.0107E-002	2.6000E-001	7.9557E-006
111	0.3375	4.3300E-002	2.4072E-002	7.8549E-003	2.0800E-002	2.0097E-002	2.6188E-001	7.5380E-006
112	0.3438	4.2690E-002	2.2857E-002	7.5184E-003	2.0317E-002	2.0063E-002	2.6367E-001	7.1636E-006
113	0.3500	4.2092E-002	2.1746E-002	7.2057E-003	1.9861E-002	2.0010E-002	2.6538E-001	6.8284E-006
114	0.3625	4.0941E-002	1.9813E-002	6.6514E-003	1.9041E-002	1.9859E-002	2.6850E-001	6.2669E-006
115	0.3750	3.9845E-002	1.8164E-002	6.1673E-003	1.8303E-002	1.9666E-002	2.7134E-001	5.8082E-006
116	0.3875	3.8810E-002	1.6751E-002	5.7442E-003	1.7638E-002	1.9447E-002	2.7392E-001	5.4316E-006
117	0.4000	3.7840E-002	1.5534E-002	5.3734E-003	1.7038E-002	1.9214E-002	2.7627E-001	5.1207E-006
118	0.4125	3.6932E-002	1.4480E-002	5.0476E-003	1.6496E-002	1.8974E-002	2.7840E-001	4.8624E-006
119	0.4250	3.6088E-002	1.3563E-002	4.7606E-003	1.6004E-002	1.8734E-002	2.8035E-001	4.6462E-006
120	0.4375	3.5305E-002	1.2762E-002	4.5069E-003	1.5557E-002	1.8497E-002	2.8212E-001	4.4641E-006
121	0.4500	3.4586E-002	1.2062E-002	4.2824E-003	1.5148E-002	1.8268E-002	2.8373E-001	4.3097E-006
122	0.4625	3.3938E-002	1.1453E-002	4.0842E-003	1.4773E-002	1.8051E-002	2.8520E-001	4.1779E-006
123	0.4750	3.3377E-002	1.0933E-002	3.9112E-003	1.4426E-002	1.7851E-002	2.8651E-001	4.0653E-006
124	0.4812	3.3145E-002	1.0711E-002	3.8350E-003	1.4260E-002	1.7763E-002	2.8710E-001	4.0154E-006
125	0.4875	3.2964E-002	1.0527E-002	3.7697E-003	1.4104E-002	1.7689E-002	2.8761E-001	3.9715E-006
126	0.4906	3.2897E-002	1.0455E-002	3.7429E-003	1.4033E-002	1.7660E-002	2.8783E-001	3.9526E-006
127	0.4938	3.2851E-002	1.0401E-002	3.7221E-003	1.3971E-002	1.7640E-002	2.8800E-001	3.9371E-006
128	0.4969	3.2827E-002	1.0371E-002	3.7097E-003	1.3930E-002	1.7628E-002	2.8810E-001	3.9273E-006
129	0.5000	3.2827E-002	1.0371E-002	3.7097E-003	1.3930E-002	1.7628E-002	2.8810E-001	3.9273E-006

	X(cm)	MOLE FRACTIONS:						
		H2O2	C	CH	CH2	CH2(S)	CH3	CH4
1	0.0000	1.2083E-015	2.4258E-077	8.5001E-069	3.9269E-060	4.6874E-061	1.3503E-050	7.2296E-050
2	0.0250	2.7192E-014	3.8689E-076	1.1967E-067	7.9860E-059	9.5326E-060	2.8018E-049	1.5040E-048
3	0.0500	7.9990E-014	1.1236E-074	3.1577E-066	1.9147E-057	2.2857E-058	6.5601E-048	3.0780E-047
4	0.0750	1.6040E-013	2.7093E-073	7.5306E-065	4.5159E-056	5.3910E-057	1.5434E-046	6.2793E-046
5	0.0875	2.0812E-013	2.6050E-072	7.2270E-064	4.3260E-055	5.1638E-056	1.4770E-045	5.2563E-045
6	0.1000	2.6442E-013	2.9917E-071	8.2600E-063	4.9384E-054	5.8948E-055	1.6845E-044	5.5044E-044
7	0.1250	4.4352E-013	4.2870E-069	2.6562E-061	1.5809E-052	1.8811E-053	5.3652E-043	1.6107E-042
8	0.1500	1.4697E-012	1.3661E-064	1.5670E-059	6.8944E-051	4.4857E-052	1.2750E-041	3.3001E-041
9	0.1625	8.6488E-012	2.1039E-060	9.7850E-056	7.2306E-048	5.1188E-051	1.2206E-040	2.7316E-040
10	0.1750	9.0557E-011	2.1610E-056	1.3474E-051	1.1033E-044	1.2212E-048	1.3923E-039	2.8360E-039
11	0.1875	1.0256E-009	2.2031E-052	1.6322E-047	1.6920E-041	1.7405E-045	1.6149E-038	3.0143E-038
12	0.1938	4.8048E-009	7.3403E-049	1.9311E-044	9.7440E-039	-2.0743E-043	8.2787E-038	1.4234E-037
13	0.2000	2.5430E-008	7.9362E-046	1.1587E-041	1.2736E-037	1.7516E-041	4.8037E-037	7.9878E-037
14	0.2031	5.9536E-008	-2.7966E-045	1.9346E-038	1.7296E-035	2.7181E-038	1.4480E-036	2.3007E-036
15	0.2047	9.4962E-008	9.3856E-044	4.4495E-040	4.2145E-034	1.6722E-038	1.2134E-035	3.4515E-036
16	0.2063	1.5731E-007	3.0001E-042	6.6134E-039	3.0672E-035	5.5125E-039	2.3812E-035	5.9307E-036
17	0.2078	2.6226E-007	-1.8634E-042	7.8896E-038	1.4565E-034	-1.0551E-038	3.1618E-035	1.0137E-035
18	0.2086	3.3712E-007	1.4785E-041	5.8467E-038	-1.2971E-034	-5.3266E-039	3.2664E-035	1.3575E-035
19	0.2094	4.3407E-007	1.1710E-041	1.3929E-038	1.4100E-034	-8.5987E-039	3.4314E-035	1.7684E-035
20	0.2102	5.5733E-007	-2.2485E-040	1.6812E-037	3.0126E-034	1.6421E-038	3.7522E-035	2.2841E-035
21	0.2105	6.3019E-007	2.3310E-040	5.4129E-038	1.2497E-034	1.0396E-038	3.9224E-035	2.5936E-035
22	0.2109	7.1217E-007	2.5979E-040	3.9380E-038	4.0394E-035	1.0291E-038	4.3516E-035	2.9365E-035
23	0.2113	8.0396E-007	9.2221E-041	2.8751E-038	2.4215E-035	2.9304E-039	4.8697E-035	3.3110E-035
24	0.2117	9.0616E-007	1.3192E-040	6.3668E-038	3.9718E-035	-2.2140E-039	5.6673E-035	3.7057E-035
25	0.2121	1.0193E-006	-2.3872E-040	4.1863E-037	1.1985E-034	-1.8649E-038	6.8441E-035	4.1060E-035
26	0.2125	1.1438E-006	8.0083E-040	1.3815E-036	4.0538E-034	-3.2552E-038	8.4469E-035	4.4952E-035
27	0.2129	1.2800E-006	6.9479E-039	2.9874E-037	1.3927E-033	1.3250E-037	1.0156E-034	4.7828E-035
28	0.2133	1.4280E-006	4.8046E-039	1.0373E-036	5.3054E-034	6.5996E-038	1.0935E-034	4.9242E-035
29	0.2137	1.5878E-006	3.0424E-039	5.4408E-037	2.2154E-034	3.2724E-038	1.1725E-034	4.7212E-035
30	0.2141	1.7593E-006	3.1972E-039	4.5772E-037	1.5953E-034	2.7818E-038	1.3036E-034	3.9887E-035
31	0.2145	1.9421E-006	8.4775E-039	1.0628E-036	3.2392E-034	5.0725E-038	1.5250E-034	2.4486E-035
32	0.2148	2.1358E-006	2.8964E-038	3.6266E-036	1.0362E-033	1.3977E-037	1.8525E-034	-3.2717E-036
33	0.2152	2.3397E-006	7.0513E-038	8.6261E-036	3.5816E-033	3.8462E-037	2.3750E-034	-4.3967E-035
34	0.2156	2.5534E-006	9.2034E-038	-1.6153E-035	8.8262E-033	-9.9426E-037	2.1310E-034	-1.1778E-034
35	0.2164	3.0074E-006	1.0089E-037	8.4251E-036	1.6173E-033	2.3068E-037	2.2248E-034	-3.0655E-034
36	0.2172	3.4872E-006	3.5260E-038	2.1392E-036	2.8982E-034	7.0404E-038	1.5763E-034	-6.9044E-034
37	0.2180	3.9863E-006	1.0272E-038	4.8479E-037	5.1603E-035	3.1761E-038	9.7367E-035	-1.3692E-033
38	0.2188	4.4979E-006	2.8896E-039	1.0773E-037	9.0968E-036	1.6386E-038	5.2961E-035	-2.5016E-033
39	0.2195	5.0152E-006	7.7912E-040	2.3098E-038	1.5551E-036	1.8555E-039	2.1040E-035	-4.3339E-033
40	0.2203	5.5293E-006	1.0334E-040	2.3392E-039	1.2337E-037	-2.0908E-038	-5.0730E-036	-7.2503E-033

121	0.4500	2.4648E-007	-5.7661E-030	-2.3740E-030	-3.0059E-030	-3.2101E-031	-9.6753E-030	-1.7392E-030
122	0.4625	2.4380E-007	-6.0694E-030	-2.3624E-030	-3.0074E-030	-3.0687E-031	-9.2627E-030	-1.7014E-030
123	0.4750	2.4178E-007	-6.3986E-030	-2.3584E-030	-3.0200E-030	-2.9678E-031	-8.9570E-030	-1.6805E-030
124	0.4812	2.4097E-007	-6.5802E-030	-2.3618E-030	-3.0359E-030	-2.9316E-031	-8.8522E-030	-1.6749E-030
125	0.4875	2.4029E-007	-6.7733E-030	-2.3742E-030	-3.0551E-030	-2.9137E-031	-8.7923E-030	-1.6756E-030
126	0.4906	2.4001E-007	-6.8623E-030	-2.3808E-030	-3.0677E-030	-2.9102E-031	-8.7794E-030	-1.6771E-030
127	0.4938	2.3977E-007	-6.9391E-030	-2.3877E-030	-3.0794E-030	-2.9092E-031	-8.7672E-030	-1.6791E-030
128	0.4969	2.3962E-007	-6.9634E-030	-2.3898E-030	-3.0833E-030	-2.9075E-031	-8.7615E-030	-1.6806E-030
129	0.5000	2.3962E-007	-6.9623E-030	-2.3898E-030	-3.0833E-030	-2.9075E-031	-8.7615E-030	-1.6806E-030

	X(cm)	MOLE FRACTIONS: CO	CO2	HCO	CH2O	CH2OH	CH3O	CH3OH
1	0.0000	-3.2389E-057	-1.0359E-049	-8.2230E-058	-2.3873E-048	-2.5589E-059	3.3251E-056	-1.6879E-051
2	0.0250	-7.3111E-056	-2.8742E-048	-2.1862E-056	-6.3940E-047	-6.9536E-058	9.0357E-055	-4.6084E-050
3	0.0500	-2.0641E-054	-8.1455E-047	-6.1713E-055	-1.7129E-045	-2.0512E-056	4.0850E-053	-1.2584E-048
4	0.0750	-5.5681E-053	-1.5455E-046	-1.6642E-053	-4.5884E-044	-5.5595E-055	1.4101E-051	-3.4363E-047
5	0.0875	-6.0247E-052	-1.3199E-046	-1.7989E-052	-4.9512E-043	-6.0120E-054	1.5585E-050	-3.7753E-046
6	0.1000	-8.2039E-051	4.3573E-046	-2.4510E-051	-6.7363E-042	-8.1925E-053	2.0466E-049	-5.2343E-045
7	0.1250	-2.9116E-049	4.2779E-044	-9.5235E-050	-2.6061E-040	-3.1859E-051	7.7567E-048	-2.0659E-043
8	0.1500	1.2200E-046	5.2797E-044	-3.7793E-048	-7.0609E-039	-9.6970E-050	9.4101E-047	-5.7054E-042
9	0.1625	2.3766E-043	-8.3333E-044	-7.5121E-045	-7.6218E-038	-3.1865E-048	-1.3434E-044	-6.2697E-041
10	0.1750	3.1075E-040	-6.6008E-042	-3.4807E-041	-1.0370E-036	-4.6519E-046	-1.2120E-042	-8.6861E-040
11	0.1875	5.0427E-037	-3.2272E-039	-1.6241E-037	-1.4384E-035	-9.0329E-044	-1.0180E-040	-1.2221E-038
12	0.1938	4.6288E-034	-4.2644E-038	-2.8435E-034	-8.5588E-035	-3.3661E-042	-3.3610E-039	-7.2224E-038
13	0.2000	-1.2449E-033	-2.3154E-037	4.5144E-035	-6.1486E-034	-1.2801E-040	-8.0685E-038	-4.9035E-037
14	0.2031	1.5577E-034	-6.3787E-037	-4.3318E-036	-2.1660E-033	-9.4738E-040	-7.8001E-037	-1.4017E-036
15	0.2047	1.9341E-034	-1.0972E-036	-3.6486E-035	-1.6949E-033	-1.6484E-039	-5.7761E-038	-1.2670E-036
16	0.2063	4.1364E-034	-1.9148E-036	1.8039E-035	-1.1904E-033	-2.9194E-039	4.9158E-037	-5.4807E-037
17	0.2078	1.3436E-034	-3.4744E-036	6.0654E-037	-7.3318E-034	-2.0699E-039	1.7746E-036	6.6298E-037
18	0.2086	-1.9855E-034	-4.8893E-036	-2.0539E-035	-3.4572E-034	-1.4226E-039	2.6222E-036	1.5779E-036
19	0.2094	-1.2196E-033	-7.3345E-036	-6.7328E-035	-2.1324E-034	-5.7693E-040	3.4213E-036	2.8269E-036
20	0.2102	-6.1396E-033	-1.2394E-035	-2.8877E-035	4.5594E-035	5.1721E-040	4.5373E-036	4.4363E-036
21	0.2105	-1.8215E-032	-1.7483E-035	-5.2229E-036	2.2282E-034	1.3873E-039	5.2805E-036	5.4367E-036
22	0.2109	-5.0379E-032	-2.6684E-035	-1.0542E-036	3.7222E-034	2.8219E-039	6.1486E-036	6.5642E-036
23	0.2113	-1.3640E-031	-4.4425E-035	9.2877E-038	5.4881E-034	4.9059E-039	7.1786E-036	7.8639E-036
24	0.2117	-3.6173E-031	-8.0490E-035	3.9559E-037	7.8220E-034	7.9615E-039	8.4522E-036	9.3493E-036
25	0.2121	-9.3947E-031	-1.5710E-034	3.1807E-036	1.1049E-033	1.3307E-038	1.0013E-035	1.1041E-035
26	0.2125	-2.3818E-030	-3.2622E-034	3.3197E-036	1.5711E-033	2.2077E-038	1.1994E-035	1.2973E-035
27	0.2129	-5.8711E-030	-7.1339E-034	-4.0510E-037	2.2698E-033	2.2461E-038	1.4235E-035	1.5076E-035
28	0.2133	-1.4008E-029	-1.6333E-033	2.4740E-036	2.5551E-033	3.8426E-038	1.6175E-035	1.7279E-035
29	0.2137	-3.2173E-029	-3.9061E-033	-4.0832E-036	2.7643E-033	4.9644E-038	1.8252E-035	1.9469E-035
30	0.2141	-7.0817E-029	-9.7606E-033	-1.7137E-035	2.9809E-033	6.1579E-038	2.0550E-035	2.1495E-035
31	0.2145	-1.4869E-028	-2.5501E-032	-4.2506E-035	3.2315E-033	7.6793E-038	2.3124E-035	2.3110E-035
32	0.2148	-2.9686E-028	-3.2736E-032	-9.4664E-035	3.4712E-033	1.0062E-037	2.5910E-035	2.3908E-035
33	0.2152	-5.6278E-028	-1.2829E-031	-2.2584E-034	3.7277E-033	1.3461E-037	2.7397E-035	2.5117E-035
34	0.2156	-1.0146E-027	-1.8725E-031	-4.7356E-034	3.0231E-033	2.2700E-037	2.4212E-035	2.4283E-035
35	0.2164	-2.7553E-027	-4.1910E-031	-1.6128E-033	1.7238E-033	9.3207E-038	2.5658E-035	3.1590E-035
36	0.2172	-6.4414E-027	-9.7074E-031	-4.8308E-033	-2.6816E-033	-1.3761E-037	2.1405E-035	3.5015E-035
37	0.2180	-1.3747E-026	-2.4965E-030	-1.2849E-032	-1.0932E-032	-7.2145E-037	1.4445E-035	3.3298E-035
38	0.2188	-2.7780E-026	-5.1907E-030	-3.2100E-032	-2.5796E-032	-2.1478E-036	6.6630E-036	2.4383E-035
39	0.2195	-5.4293E-026	-1.0761E-029	-7.7015E-032	-5.2565E-032	-5.4670E-036	-1.5571E-036	5.3385E-036
40	0.2203	-1.0379E-025	-2.2955E-029	-1.7934E-031	-1.0079E-031	-1.2985E-035	-1.1245E-035	-2.8921E-035
41	0.2211	-1.9519E-025	-5.1019E-029	-4.0744E-031	-1.8747E-031	-2.9675E-035	-2.4742E-035	-8.6968E-035
42	0.2219	-3.6207E-025	-1.1870E-028	-9.0792E-031	-3.4236E-031	-6.6253E-035	-4.5814E-035	-1.8269E-034
43	0.2234	-1.0962E-024	-7.2376E-028	-3.7899E-030	-1.0078E-030	-2.7763E-034	-1.2679E-034	-5.5110E-034
44	0.2250	-3.0229E-024	-4.8420E-027	-1.3776E-029	-2.6434E-030	-9.8875E-034	-3.0237E-034	-1.3123E-033
45	0.2258	-5.0989E-024	-1.2819E-026	-2.6308E-029	-4.2703E-030	-1.8323E-033	-4.6094E-034	-1.9597E-033
46	0.2266	-8.6329E-024	-3.4483E-026	-4.9850E-029	-6.9029E-030	-3.3524E-033	-7.0020E-034	-2.9070E-033
47	0.2270	-1.1301E-023	-5.6841E-026	-6.8790E-029	-8.7894E-030	-4.5217E-033	-8.6222E-034	-3.5333E-033
48	0.2273	-1.4838E-023	-9.4160E-026	-9.4983E-029	-1.1208E-029	-6.0894E-033	-1.0620E-033	-4.2945E-033
49	0.2277	-1.9505E-023	-1.5686E-025	-1.3097E-028	-1.4284E-029	-8.1695E-033	-1.3058E-033	-5.2132E-033
50	0.2281	-2.5638E-023	-2.6319E-025	-1.8005E-028	-1.8166E-029	-1.0900E-032	-1.6009E-033	-6.3133E-033
51	0.2283	-2.9414E-023	-3.4218E-025	-2.1107E-028	-2.0475E-029	-1.2569E-032	-1.7706E-033	-6.9410E-033
52	0.2285	-3.3761E-023	-4.4663E-025	-2.4743E-028	-2.3072E-029	-1.4480E-032	-1.9573E-033	-7.6278E-033
53	0.2287	-3.8760E-023	-5.8581E-025	-2.8995E-028	-2.5989E-029	-1.6663E-032	-2.1622E-033	-8.3778E-033
54	0.2289	-4.4500E-023	-7.7302E-025	-3.3958E-028	-2.9259E-029	-1.9149E-032	-2.3866E-033	-9.1950E-033
55	0.2291	-5.1082E-023	-1.0277E-024	-3.9741E-028	-3.2915E-029	-2.1973E-032	-2.6317E-033	-1.0084E-032
56	0.2293	-5.8618E-023	-1.3788E-024	-4.6467E-028	-3.6994E-029	-2.5172E-032	-2.8987E-033	-1.1047E-032
57	0.2295	-6.7235E-023	-1.8705E-024	-5.4276E-028	-4.1537E-029	-2.8786E-032	-3.1888E-033	-1.2091E-032
58	0.2297	-7.7073E-023	-2.5711E-024	-6.3324E-028	-4.6584E-029	-3.2857E-032	-3.5033E-033	-1.3217E-032
59	0.2299	-8.8285E-023	-3.5885E-024	-7.3788E-028	-5.2180E-029	-3.7430E-032	-3.8433E-033	-1.4430E-032
60	0.2301	-1.0105E-022	-5.0955E-024	-8.5865E-028	-5.8372E-029	-4.2553E-032	-4.2101E-033	-1.5734E-032
61	0.2303	-1.1554E-022	-7.3702E-024	-9.9776E-028	-6.5210E-029	-4.8278E-032	-4.6048E-033	-1.7132E-032
62	0.2305	-1.3199E-022	-1.0859E-023	-1.1577E-027	-7.2745E-029	-5.4658E-032	-5.0286E-033	-1.8627E-032
63	0.2307	-1.5062E-022	-1.6265E-023	-1.3412E-027	-8.1032E-029	-6.1749E-032	-5.4827E-033	-2.0222E-032
64	0.2309	-1.7168E-022	-2.4644E-023	-1.5514E-027	-9.0130E-029	-6.9610E-032	-5.9682E-033	-2.1920E-032
65	0.2311	-1.9547E-022	-3.7464E-023	-1.7917E-027	-1.0010E-028	-7.8306E-032	-6.4862E-033	-2.3724E-032
66	0.2313	-2.2231E-022	-5.6527E-023	-2.0661E-027	-1.1101E-028	-8.7900E-032	-7.0380E-033	-2.5635E-032
67	0.2314	-2.5255E-022	-8.3718E-023	-2.3789E-027	-1.2292E-028	-9.8461E-032	-7.6245E-033	-2.7655E-032
68	0.2316	-2.8660E-022	-1.2076E-022	-2.7350E-027	-1.3591E-028	-1.1006E-031	-8.2470E-033	-2.9786E-032

97	0.2594	9.1319E-054	1.3644E-051	1.0237E-053	6.2722E-054	3.0559E-057	1.5934E-057	1.5661E-049
98	0.2625	1.7443E-053	2.3034E-051	1.3570E-053	7.8125E-054	3.4434E-057	1.5286E-057	2.4573E-049
99	0.2656	2.9769E-053	3.5511E-051	1.6791E-053	9.1700E-054	3.6934E-057	1.4221E-057	3.5433E-049
100	0.2688	4.6633E-053	5.1071E-051	1.9765E-053	1.0315E-053	3.8296E-057	1.3003E-057	4.7936E-049
101	0.2750	9.5187E-053	9.1129E-051	2.4848E-053	1.2020E-053	3.8767E-057	1.0675E-057	7.6791E-049
102	0.2812	1.6294E-052	1.4036E-050	2.8356E-053	1.2918E-053	3.6890E-057	8.5406E-058	1.0815E-048
103	0.2875	2.4849E-052	1.9649E-050	3.0505E-053	1.3216E-053	3.3883E-057	6.7639E-058	1.4003E-048
104	0.2938	3.4923E-052	2.5726E-050	3.1597E-053	1.3118E-053	3.0516E-057	5.3487E-058	1.7106E-048
105	0.3000	4.6208E-052	3.2073E-050	3.1907E-053	1.2773E-053	2.7189E-057	4.2403E-058	2.0038E-048
106	0.3063	5.8393E-052	3.8538E-050	3.1661E-053	1.2288E-053	2.4095E-057	3.3772E-058	2.2751E-048
107	0.3125	7.1201E-052	4.5014E-050	3.1039E-053	1.1733E-053	2.1313E-057	2.7058E-058	2.5227E-048
108	0.3188	8.4392E-052	5.1426E-050	3.0179E-053	1.1156E-053	1.8861E-057	2.1830E-058	2.7469E-048
109	0.3250	9.7778E-052	5.7736E-050	2.9182E-053	1.0587E-053	1.6727E-057	1.7749E-058	2.9494E-048
110	0.3313	1.1121E-051	6.3921E-050	2.8125E-053	1.0044E-053	1.4886E-057	1.4555E-058	3.1327E-048
111	0.3375	1.2458E-051	6.9980E-050	2.7057E-053	9.5377E-054	1.3303E-057	1.2047E-058	3.2996E-048
112	0.3438	1.3778E-051	7.5913E-050	2.6014E-053	9.0727E-054	1.1948E-057	1.0069E-058	3.4530E-048
113	0.3500	1.5071E-051	8.1706E-050	2.5013E-053	8.6499E-054	1.0788E-057	8.5030E-059	3.5948E-048
114	0.3625	1.7463E-051	9.2528E-050	2.3142E-053	7.9173E-054	8.9463E-058	6.2744E-059	3.8404E-048
115	0.3750	1.9731E-051	1.0319E-049	2.1493E-053	7.3240E-054	7.5617E-058	4.8066E-059	4.0796E-048
116	0.3875	2.1876E-051	1.1401E-049	2.0013E-053	6.8422E-054	6.4964E-058	3.8178E-059	4.3349E-048
117	0.4000	2.3924E-051	1.2554E-049	1.8628E-053	6.4470E-054	5.6501E-058	3.1400E-059	4.6362E-048
118	0.4125	2.5977E-051	1.3868E-049	1.7242E-053	6.1090E-054	4.9331E-058	2.6524E-059	5.0231E-048
119	0.4250	2.8205E-051	1.5441E-049	1.5775E-053	5.8052E-054	4.2848E-058	2.2862E-059	5.5151E-048
120	0.4375	3.0827E-051	1.7267E-049	1.4191E-053	5.4886E-054	3.6433E-058	1.9672E-059	6.0624E-048
121	0.4500	3.3827E-051	1.8908E-049	1.2578E-053	5.0756E-054	2.9801E-058	1.6333E-059	6.3978E-048
122	0.4625	3.7008E-051	1.9090E-049	1.1152E-053	4.3823E-054	2.2562E-058	1.1868E-059	5.8527E-048
123	0.4750	3.9420E-051	1.3250E-049	8.2615E-054	2.5733E-054	9.6958E-059	4.6173E-060	2.3273E-048
124	0.4812	2.8330E-051	-9.7005E-050	1.1798E-054	6.4956E-056	-7.3677E-059	-1.5595E-060	-6.0228E-048
125	0.4875	-1.1236E-050	-1.5234E-048	3.2241E-054	6.0712E-054	-3.0361E-058	-1.0036E-059	-4.6549E-047
126	0.4906	-3.7387E-050	-4.1877E-048	1.4206E-052	5.4470E-053	-1.2866E-057	-3.1361E-059	-1.5437E-046
127	0.4938	-9.5058E-050	-9.2942E-048	2.8880E-052	1.4584E-052	-2.5643E-057	-7.4005E-059	-2.9637E-046
128	0.4969	-2.3712E-049	-1.8254E-047	1.4675E-051	4.6345E-052	-1.5957E-056	-3.2728E-058	-7.0999E-046
129	0.5000	-2.3712E-049	-1.8254E-047	1.4675E-051	4.6345E-052	-1.5957E-056	-3.2728E-058	-7.0999E-046

	X(cm)	MOLE FRACTIONS:						
		CH2CO	HCCOH	N	NH	NH2	NH3	NNH
1	0.0000	-2.8157E-080	2.7369E-088	1.1704E-033	6.9907E-028	8.0892E-030	2.8794E-029	3.2690E-019
2	0.0250	-8.7477E-079	8.6677E-087	1.9542E-032	9.9518E-027	1.1728E-028	5.5581E-028	7.5249E-018
3	0.0500	-2.7177E-077	2.7440E-085	1.1408E-030	1.6772E-026	5.7650E-028	8.5670E-027	8.2834E-018
4	0.0750	-8.4431E-076	8.6840E-084	8.0686E-029	5.6922E-026	1.0491E-026	1.5258E-025	8.3756E-018
5	0.0875	-1.0466E-074	1.0951E-082	2.2126E-027	5.4490E-025	1.1328E-025	1.1405E-024	8.3906E-018
6	0.1000	-1.6474E-073	1.7544E-081	5.0769E-026	6.8904E-024	1.2577E-024	1.0648E-023	8.4004E-018
7	0.1250	-7.4313E-072	8.0596E-080	3.3353E-024	2.4958E-022	3.8129E-023	2.7329E-022	8.4364E-018
8	0.1500	-2.3319E-070	2.5729E-078	2.3723E-022	8.7779E-021	1.0229E-021	4.6402E-021	9.4423E-018
9	0.1625	-2.8915E-069	3.2421E-077	6.5069E-021	1.2392E-019	1.0816E-020	2.9726E-020	2.8029E-017
10	0.1750	-4.5514E-068	5.1887E-076	1.4932E-019	1.6579E-018	1.1500E-019	2.3455E-019	2.9781E-016
11	0.1875	-7.2892E-067	8.4451E-075	3.4168E-018	2.2193E-017	1.2000E-018	1.7839E-018	4.2680E-015
12	0.1938	-4.9242E-066	5.7863E-074	3.1842E-017	1.2812E-016	5.4497E-018	5.8016E-018	2.6640E-014
13	0.2000	-4.0696E-065	4.8514E-073	2.7809E-016	7.5760E-016	2.6484E-017	2.1922E-017	1.4328E-013
14	0.2031	-1.5966E-064	1.9234E-072	1.1067E-015	2.2403E-015	6.7214E-017	4.6184E-017	3.8831E-013
15	0.2047	-3.9275E-064	4.6979E-072	2.4653E-015	4.1913E-015	1.1513E-016	7.1844E-017	6.5182E-013
16	0.2063	-1.0748E-063	1.2746E-071	5.6448E-015	8.1227E-015	2.0512E-016	1.1851E-016	1.0865E-012
17	0.2078	-3.0538E-063	3.6131E-071	1.3036E-014	1.6034E-014	3.7330E-016	2.0365E-016	1.8036E-012
18	0.2086	-5.4639E-063	6.4588E-071	2.0365E-014	2.3007E-014	5.1166E-016	2.7252E-016	2.3357E-012
19	0.2094	-1.0170E-062	1.2026E-070	3.2222E-014	3.3418E-014	7.0907E-016	3.7137E-016	3.0266E-012
20	0.2102	-1.9368E-062	2.2920E-070	5.1334E-014	4.8971E-014	9.9031E-016	5.1364E-016	3.9231E-012
21	0.2105	-2.7274E-062	3.2282E-070	6.5241E-014	5.9642E-014	1.1755E-015	6.0838E-016	4.4709E-012
22	0.2109	-3.8957E-062	4.6125E-070	8.3254E-014	7.2922E-014	1.3997E-015	7.2470E-016	5.0973E-012
23	0.2113	-5.6207E-062	6.6595E-070	1.0656E-013	8.9454E-014	1.6709E-015	8.6768E-016	5.8134E-012
24	0.2117	-8.1656E-062	9.6869E-070	1.3667E-013	1.1004E-013	1.9990E-015	1.0436E-015	6.6322E-012
25	0.2121	-1.1908E-061	1.4165E-069	1.7554E-013	1.3570E-013	2.3955E-015	1.2603E-015	7.5688E-012
26	0.2125	-1.7482E-061	2.0788E-069	2.2568E-013	1.6769E-013	2.8746E-015	1.5274E-015	8.6403E-012
27	0.2129	-2.5730E-061	3.0588E-069	2.9029E-013	2.0759E-013	3.4532E-015	1.8568E-015	9.8668E-012
28	0.2133	-3.8140E-061	4.5090E-069	3.7347E-013	2.5739E-013	4.1514E-015	2.2634E-015	1.1271E-011
29	0.2137	-5.6565E-061	6.6551E-069	4.8046E-013	3.1951E-013	4.9935E-015	2.7656E-015	1.2881E-011
30	0.2141	-8.3942E-061	9.8322E-069	6.1797E-013	3.9698E-013	6.0085E-015	3.3861E-015	1.4726E-011
31	0.2145	-1.2459E-060	1.4536E-068	7.9452E-013	4.9347E-013	7.2313E-015	4.1530E-015	1.6844E-011
32	0.2148	-1.8416E-060	2.1504E-068	1.0210E-012	6.1341E-013	8.7033E-015	5.1014E-015	1.9276E-011
33	0.2152	-2.6525E-060	3.1828E-068	1.3111E-012	7.6211E-013	1.0474E-014	6.2744E-015	2.2070E-011
34	0.2156	-3.7357E-060	4.7134E-068	1.6826E-012	9.4588E-013	1.2603E-014	7.7256E-015	2.5286E-011
35	0.2164	-6.9532E-060	9.9876E-068	2.7357E-012	1.4408E-012	1.8148E-014	1.1660E-014	3.3205E-011
36	0.2172	-7.4210E-060	2.0421E-067	4.3804E-012	2.1580E-012	2.5911E-014	1.7422E-014	4.3663E-011
37	0.2180	-6.2327E-060	4.1140E-067	6.9411E-012	3.1855E-012	3.6763E-014	2.5842E-014	5.7520E-011
38	0.2188	-3.5142E-060	8.2470E-067	1.0914E-011	4.6470E-012	5.1928E-014	3.8117E-014	7.5928E-011
39	0.2195	1.6552E-060	1.6537E-066	1.7054E-011	6.7187E-012	7.3119E-014	5.5960E-014	1.0043E-010
40	0.2203	1.1886E-059	3.3278E-066	2.6510E-011	9.6557E-012	1.0275E-013	8.1802E-014	1.3310E-010
41	0.2211	3.3269E-059	6.7367E-066	4.1013E-011	1.3831E-011	1.4423E-013	1.1907E-013	1.7665E-010
42	0.2219	7.9691E-059	1.3748E-065	6.3160E-011	1.9797E-011	2.0238E-013	1.7254E-013	2.3470E-010
43	0.2234	3.4177E-058	5.0391E-065	1.4171E-010	3.9488E-011	3.8857E-013	3.4732E-013	4.1224E-010
44	0.2250	1.3631E-057	1.7701E-064	2.9996E-010	7.6766E-011	7.2672E-013	6.5656E-013	7.1446E-010

45	0.2258	2.9992E-057	3.6591E-064	4.3457E-010	1.0719E-010	9.9806E-013	8.9329E-013	9.3530E-010
46	0.2266	6.6738E-057	7.8612E-064	6.2762E-010	1.4965E-010	1.3744E-012	1.2132E-012	1.2193E-009
47	0.2270	1.0184E-056	1.1970E-063	7.5378E-010	1.7691E-010	1.6158E-012	1.4135E-012	1.3897E-009
48	0.2273	1.5646E-056	1.8534E-063	9.0488E-010	2.0915E-010	1.9015E-012	1.6474E-012	1.5821E-009
49	0.2277	2.4083E-056	2.9076E-063	1.0849E-009	2.4715E-010	2.2387E-012	1.9197E-012	1.7986E-009
50	0.2281	3.7023E-056	4.6087E-063	1.2981E-009	2.9175E-010	2.6353E-012	2.2353E-012	2.0418E-009
51	0.2283	4.6034E-056	5.8562E-063	1.4190E-009	3.1686E-010	2.8592E-012	2.4114E-012	2.1742E-009
52	0.2285	5.7309E-056	7.4746E-063	1.5505E-009	3.4405E-010	3.1021E-012	2.6012E-012	2.3143E-009
53	0.2287	7.1384E-056	9.5750E-063	1.6933E-009	3.7345E-010	3.3655E-012	2.8055E-012	2.4624E-009
54	0.2289	8.8912E-056	1.2303E-062	1.8481E-009	4.0521E-010	3.6506E-012	3.0251E-012	2.6190E-009
55	0.2291	1.1069E-055	1.5847E-062	2.0158E-009	4.3947E-010	3.9590E-012	3.2610E-012	2.7843E-009
56	0.2293	1.3770E-055	2.0454E-062	2.1971E-009	4.7637E-010	4.2922E-012	3.5139E-012	2.9588E-009
57	0.2295	1.7110E-055	2.6446E-062	2.3928E-009	5.1607E-010	4.6518E-012	3.7850E-012	3.1427E-009
58	0.2297	2.1234E-055	3.4242E-062	2.6037E-009	5.5873E-010	5.0395E-012	4.0751E-012	3.3365E-009
59	0.2299	2.6312E-055	4.4385E-062	2.8307E-009	6.0451E-010	5.4569E-012	4.3851E-012	3.5405E-009
60	0.2301	3.2554E-055	5.7586E-062	3.0746E-009	6.5356E-010	5.9059E-012	4.7160E-012	3.7551E-009
61	0.2303	4.0208E-055	7.4762E-062	3.3362E-009	7.0605E-010	6.3882E-012	5.0689E-012	3.9807E-009
62	0.2305	4.9573E-055	9.7110E-062	3.6164E-009	7.6214E-010	6.9057E-012	5.4445E-012	4.2175E-009
63	0.2307	6.1008E-055	1.2618E-061	3.9161E-009	8.2202E-010	7.4603E-012	5.8439E-012	4.4661E-009
64	0.2309	7.4940E-055	1.6397E-061	4.2361E-009	8.8584E-010	8.0539E-012	6.2680E-012	4.7266E-009
65	0.2311	9.1880E-055	2.1310E-061	4.5773E-009	9.5378E-010	8.6883E-012	6.7177E-012	4.9996E-009
66	0.2313	1.1244E-054	2.7692E-061	4.9406E-009	1.0260E-009	9.3657E-012	7.1939E-012	5.2852E-009
67	0.2314	1.3733E-054	3.5978E-061	5.3268E-009	1.1027E-009	1.0088E-011	7.6975E-012	5.5838E-009
68	0.2316	1.6742E-054	4.6732E-061	5.7367E-009	1.1841E-009	1.0857E-011	8.2292E-012	5.8957E-009
69	0.2318	2.0373E-054	6.0682E-061	6.1712E-009	1.2702E-009	1.1675E-011	8.7898E-012	6.2213E-009
70	0.2320	2.4748E-054	7.8770E-061	6.6311E-009	1.3614E-009	1.2544E-011	9.3800E-012	6.5607E-009
71	0.2322	3.0009E-054	1.0222E-060	7.1172E-009	1.4578E-009	1.3465E-011	1.0001E-011	6.9142E-009
72	0.2324	3.6327E-054	1.3260E-060	7.6302E-009	1.5595E-009	1.4442E-011	1.0652E-011	7.2822E-009
73	0.2328	5.2734E-054	2.2027E-060	8.7394E-009	1.7797E-009	1.6564E-011	1.2048E-011	8.0621E-009
74	0.2336	1.0504E-053	5.5940E-060	1.1291E-008	2.2883E-009	2.1503E-011	1.5205E-011	9.8025E-009
75	0.2344	1.9820E-053	1.3534E-059	1.4279E-008	2.8903E-009	2.7383E-011	1.8797E-011	1.1783E-008
76	0.2352	3.6105E-053	3.1601E-059	1.7706E-008	3.5890E-009	3.4225E-011	2.2778E-011	1.4001E-008
77	0.2359	6.4084E-053	7.1492E-059	2.1555E-008	4.3837E-009	4.1995E-011	2.7071E-011	1.6442E-008
78	0.2367	1.1141E-052	1.5695E-058	2.5790E-008	5.2692E-009	5.0600E-011	3.1573E-011	1.9085E-008
79	0.2375	1.9031E-052	3.3462E-058	3.0359E-008	6.2363E-009	5.9890E-011	3.6159E-011	2.1898E-008
80	0.2383	3.1988E-052	6.9297E-058	3.5190E-008	7.2717E-009	6.9675E-011	4.0697E-011	2.4843E-008
81	0.2391	5.2919E-052	1.3937E-057	4.0203E-008	8.3594E-009	7.9733E-011	4.5056E-011	2.7874E-008
82	0.2398	8.6126E-052	2.7206E-057	4.5307E-008	9.4814E-009	8.9840E-011	4.9117E-011	3.0946E-008
83	0.2406	1.3775E-051	5.1521E-057	5.0407E-008	1.0619E-008	9.9784E-011	5.2788E-011	3.4010E-008
84	0.2414	2.1628E-051	9.4597E-057	5.5411E-008	1.1753E-008	1.0939E-010	5.6006E-011	3.7022E-008
85	0.2422	3.3300E-051	1.6836E-056	6.0229E-008	1.2866E-008	1.1852E-010	5.8741E-011	3.9939E-008
86	0.2430	5.0244E-051	2.9048E-056	6.4782E-008	1.3943E-008	1.2709E-010	6.0994E-011	4.2727E-008
87	0.2437	7.4273E-051	4.8616E-056	6.9000E-008	1.4972E-008	1.3507E-010	6.2796E-011	4.5356E-008
88	0.2445	1.0759E-050	7.9001E-056	7.2830E-008	1.5941E-008	1.4248E-010	6.4197E-011	4.7805E-008
89	0.2453	1.5281E-050	1.2482E-055	7.6229E-008	1.6844E-008	1.4935E-010	6.5264E-011	5.0059E-008
90	0.2461	2.1299E-050	1.9210E-055	7.9172E-008	1.7675E-008	1.5577E-010	6.6071E-011	5.2109E-008
91	0.2469	2.9176E-050	2.8876E-055	8.1644E-008	1.8433E-008	1.6180E-010	6.6694E-011	5.3953E-008
92	0.2484	5.1830E-050	6.0430E-055	8.5166E-008	1.9719E-008	1.7307E-010	6.7618E-011	5.7018E-008
93	0.2500	8.4868E-050	1.1412E-054	8.7099E-008	2.0739E-008	1.8394E-010	6.8590E-011	5.9365E-008
94	0.2516	1.3041E-049	1.9899E-054	8.7681E-008	2.1518E-008	1.9486E-010	6.9919E-011	6.1087E-008
95	0.2531	1.9042E-049	3.2554E-054	8.7192E-008	2.2088E-008	2.0609E-010	7.1798E-011	6.2286E-008
96	0.2562	3.6064E-049	7.4823E-054	8.3826E-008	2.2697E-008	2.3001E-010	7.7541E-011	6.3405E-008
97	0.2594	5.8553E-049	1.4310E-053	7.9156E-008	2.2863E-008	2.5546E-010	8.5433E-011	6.3533E-008
98	0.2625	8.5555E-049	2.4138E-053	7.4134E-008	2.2740E-008	2.8168E-010	9.5005E-011	6.3073E-008
99	0.2656	1.1580E-048	3.7151E-053	6.9285E-008	2.2440E-008	3.0787E-010	1.0574E-010	6.2278E-008
100	0.2688	1.4803E-048	5.3363E-053	6.4854E-008	2.2035E-008	3.3340E-010	1.1718E-010	6.1300E-008
101	0.2750	2.1496E-048	9.5089E-053	5.7508E-008	2.1068E-008	3.8082E-010	1.4097E-010	5.9088E-008
102	0.2812	2.7793E-048	1.4728E-052	5.1896E-008	2.0042E-008	4.2412E-010	1.6510E-010	5.6797E-008
103	0.2875	3.3362E-048	2.0839E-052	4.7723E-008	1.9020E-008	4.6339E-010	1.8919E-010	5.4528E-008
104	0.2938	3.8103E-048	2.7707E-052	4.4709E-008	1.8034E-008	4.9898E-010	2.1308E-010	5.2318E-008
105	0.3000	4.2030E-048	3.5230E-052	4.2635E-008	1.7098E-008	5.3133E-010	2.3674E-010	5.0184E-008
106	0.3063	4.5222E-048	4.3336E-052	4.1333E-008	1.6218E-008	5.6087E-010	2.6021E-010	4.8134E-008
107	0.3125	4.7785E-048	5.1978E-052	4.0676E-008	1.5398E-008	5.8803E-010	2.8355E-010	4.6171E-008
108	0.3188	4.9830E-048	6.1126E-052	4.0557E-008	1.4640E-008	6.1322E-010	3.0682E-010	4.4298E-008
109	0.3250	5.1461E-048	7.0770E-052	4.0890E-008	1.3946E-008	6.3682E-010	3.3013E-010	4.2517E-008
110	0.3313	5.2771E-048	8.0903E-052	4.1598E-008	1.3314E-008	6.5920E-010	3.5355E-010	4.0827E-008
111	0.3375	5.3835E-048	9.1529E-052	4.2616E-008	1.2745E-008	6.8073E-010	3.7720E-010	3.9229E-008
112	0.3438	5.4715E-048	1.0265E-051	4.3884E-008	1.2235E-008	7.0172E-010	4.0118E-010	3.7723E-008
113	0.3500	5.5453E-048	1.1423E-051	4.5342E-008	1.1783E-008	7.2240E-010	4.2553E-010	3.6308E-008
114	0.3625	5.6511E-048	1.3815E-051	4.8588E-008	1.1045E-008	7.6321E-010	4.7526E-010	3.3753E-008
115	0.3750	5.7493E-048	1.6460E-051	5.2133E-008	1.0480E-008	8.0570E-010	5.2797E-010	3.1486E-008
116	0.3875	5.8592E-048	1.9474E-051	5.5797E-008	1.0065E-008	8.5119E-010	5.8462E-010	2.9475E-008
117	0.4000	6.0101E-048	2.3091E-051	5.9446E-008	9.7733E-009	9.0041E-010	6.4588E-010	2.7693E-008
118	0.4125	6.2218E-048	2.7720E-051	6.2991E-008	9.5836E-009	9.5373E-010	7.1217E-010	2.6111E-008
119	0.4250	6.5019E-048	3.3878E-051	6.6378E-008	9.4763E-009	1.0112E-009	7.8371E-010	2.4705E-008
120	0.4375	6.7655E-048	4.1746E-051	6.9577E-008	9.4352E-009	1.0726E-009	8.6052E-010	2.3455E-008
121	0.4500	6.7318E-048	4.9763E-051	7.2582E-008	9.4480E-009	1.1378E-009	9.4250E-010	2.2345E-008
122	0.4625	5.8898E-048	5.1891E-051	7.5408E-008	9.5060E-009	1.2065E-009	1.0294E-009	2.1367E-008
123	0.4750	2.7947E-048	1.3442E-051	7.8104E-008	9.6064E-009	1.2787E-009	1.1208E-009	2.0525E-008
124	0.4812	-2.0736E-048	-1.6975E-050	7.9441E-008	9.6748E-009	1.3161E-009	1.1675E-009	2.0166E-008

125	0.4875	-1.9734E-047	-1.3556E-049	8.0756E-008	9.7563E-009	1.3533E-009	1.2134E-009	1.9871E-008
126	0.4906	-4.8695E-047	-4.5497E-049	8.1376E-008	9.7996E-009	1.3705E-009	1.2344E-009	1.9757E-008
127	0.4938	-9.5074E-047	-9.0555E-049	8.1919E-008	9.8404E-009	1.3853E-009	1.2522E-009	1.9673E-008
128	0.4969	-1.7144E-046	-2.1365E-048	8.2283E-008	9.8693E-009	1.3950E-009	1.2639E-009	1.9627E-008
129	0.5000	-1.7144E-046	-2.1365E-048	8.2283E-008	9.8693E-009	1.3950E-009	1.2639E-009	1.9627E-008

	X(cm)	MOLE FRACTIONS: NO	NO2	N2O	HNO	CN	HCN	H2CN
1	0.0000	2.1111E-027	7.8017E-031	2.8329E-022	4.8100E-029	-3.0451E-071	-2.6854E-057	-3.9605E-059
2	0.0250	4.7972E-026	1.9905E-029	7.9529E-021	1.0801E-027	-6.9742E-070	-7.2303E-056	-1.0752E-057
3	0.0500	2.0482E-025	5.0556E-028	1.6474E-020	4.0141E-027	-1.9195E-068	-1.9429E-054	-3.3077E-056
4	0.0750	2.5351E-024	1.2876E-026	2.5158E-020	4.5807E-026	-5.1689E-067	-5.2190E-053	-1.0215E-054
5	0.0875	2.1703E-023	1.3264E-025	2.9526E-020	4.2743E-025	-5.5968E-066	-5.6444E-052	-1.2593E-053
6	0.1000	2.4428E-022	1.7194E-024	3.3921E-020	5.0465E-024	-7.6477E-065	-7.7054E-051	-1.8684E-052
7	0.1250	7.7658E-021	6.3200E-023	4.2984E-020	1.6716E-022	-2.9743E-063	-2.9918E-049	-7.8762E-051
8	0.1500	1.7008E-019	1.6298E-021	5.6907E-020	3.9396E-021	-8.0966E-062	-8.1189E-048	-2.4511E-049
9	0.1625	1.4575E-018	1.6792E-020	1.0321E-019	3.4599E-020	-8.9671E-061	-8.7721E-047	-3.0224E-048
10	0.1750	1.5583E-017	2.1754E-019	5.7611E-019	3.5531E-019	-1.6817E-059	-1.1965E-045	-4.4843E-047
11	0.1875	1.6668E-016	2.8632E-018	5.3465E-018	3.4740E-018	-1.5670E-057	-1.6637E-044	-6.7396E-046
12	0.1938	7.6570E-016	1.5836E-017	2.0635E-017	1.3815E-017	-1.0391E-055	-9.9185E-044	-4.3012E-045
13	0.2000	4.2100E-015	1.0315E-016	9.1785E-017	6.3484E-017	-9.1603E-054	-7.1575E-043	-3.2605E-044
14	0.2031	1.1901E-014	3.1028E-016	2.0442E-016	1.5159E-016	-1.4624E-052	-2.5200E-042	-1.1881E-043
15	0.2047	2.2686E-014	6.0611E-016	3.2750E-016	2.5719E-016	-6.2579E-052	-5.2839E-042	-2.6984E-043
16	0.2063	4.6884E-014	1.2792E-015	5.6732E-016	4.7094E-016	-3.7466E-051	-1.2344E-041	-6.7087E-043
17	0.2078	1.0129E-013	2.7779E-015	1.0435E-015	9.0762E-016	-2.0573E-050	-3.0722E-041	-1.7345E-042
18	0.2086	1.5402E-013	4.1739E-015	1.4623E-015	1.2990E-015	-5.1331E-050	-5.1229E-041	-2.9238E-042
19	0.2094	2.4030E-013	6.3956E-015	2.1209E-015	1.9078E-015	-1.3114E-049	-8.8491E-041	-5.0890E-042
20	0.2102	3.8163E-013	9.8977E-015	3.1714E-015	2.8583E-015	-3.4253E-049	-1.5573E-040	-9.0275E-042
21	0.2105	4.8617E-013	1.2379E-014	3.9386E-015	3.5345E-015	-5.6531E-049	-2.0967E-040	-1.2204E-041
22	0.2109	6.2439E-013	1.5568E-014	4.9554E-015	4.4056E-015	-9.3302E-049	-2.8543E-040	-1.6675E-041
23	0.2113	8.0719E-013	1.9651E-014	6.3087E-015	5.5284E-015	-1.5550E-048	-3.9179E-040	-2.2967E-041
24	0.2117	1.0490E-012	2.4862E-014	8.1161E-015	6.9758E-015	-2.6067E-048	-5.4097E-040	-3.1817E-041
25	0.2121	1.3689E-012	3.1486E-014	1.0536E-014	8.8417E-015	-4.3704E-048	-7.5006E-040	-4.4259E-041
26	0.2125	1.7920E-012	3.9865E-014	1.3782E-014	1.1246E-014	-7.2857E-048	-1.0438E-039	-6.1742E-041
27	0.2129	2.3518E-012	5.0414E-014	1.8138E-014	1.4341E-014	-1.2341E-047	-1.4564E-039	-8.6293E-041
28	0.2133	3.0920E-012	6.3618E-014	2.3977E-014	1.8321E-014	-2.0643E-047	-2.0390E-039	-1.2075E-040
29	0.2137	4.0705E-012	8.0048E-014	3.1792E-014	2.3430E-014	-3.4717E-047	-2.8558E-039	-1.6906E-040
30	0.2141	5.3634E-012	1.0036E-013	4.2223E-014	2.9977E-014	-5.8065E-047	-3.9996E-039	-2.3677E-040
31	0.2145	7.0706E-012	1.2530E-013	5.6093E-014	3.8346E-014	-9.6350E-047	-5.6005E-039	-3.3153E-040
32	0.2148	9.3229E-012	1.5570E-013	7.4463E-014	4.9016E-014	-1.5853E-046	-7.8406E-039	-4.6406E-040
33	0.2152	1.2291E-011	1.9247E-013	9.8692E-014	6.2578E-014	-2.6078E-046	-1.0973E-038	-6.4915E-040
34	0.2156	1.6200E-011	2.3655E-013	1.3053E-013	7.9759E-014	-4.6791E-046	-1.5363E-038	-9.0734E-040
35	0.2164	2.7707E-011	3.4957E-013	2.2379E-013	1.2764E-013	-1.1671E-045	-2.9599E-038	-1.7269E-039
36	0.2172	4.6308E-011	4.9710E-013	3.7095E-013	1.9892E-013	-3.0327E-045	-5.5113E-038	-3.1800E-039
37	0.2180	7.6192E-011	6.8386E-013	6.0152E-013	3.0325E-013	-7.5669E-045	-1.0061E-037	-5.7375E-039
38	0.2188	1.2390E-010	9.1451E-013	9.6228E-013	4.5360E-013	-1.8458E-044	-1.8140E-037	-1.0201E-038
39	0.2195	1.9954E-010	1.1940E-012	1.5277E-012	6.6739E-013	-4.4435E-044	-3.2433E-037	-1.7913E-038
40	0.2203	3.1863E-010	1.5283E-012	2.4166E-012	9.6809E-013	-1.0610E-043	-5.7610E-037	-3.1095E-038
41	0.2211	5.0474E-010	1.9238E-012	3.8176E-012	1.3872E-012	-2.5241E-043	-1.0174E-036	-5.3343E-038
42	0.2219	7.9323E-010	2.3852E-012	6.0290E-012	1.9658E-012	-6.0539E-043	-1.7870E-036	-9.0370E-038
43	0.2234	1.8317E-009	3.4673E-012	1.4262E-011	3.7475E-012	-3.0647E-042	-5.0077E-036	-2.3487E-037
44	0.2250	3.8684E-009	4.6902E-012	3.0897E-011	6.6390E-012	-1.4369E-041	-1.2792E-035	-5.3808E-037
45	0.2258	5.5523E-009	5.4232E-012	4.4926E-011	8.7361E-012	-3.2601E-041	-2.0711E-035	-8.0031E-037
46	0.2266	7.9665E-009	6.3077E-012	6.5542E-011	1.1486E-011	-7.5413E-041	-3.3970E-035	-1.1902E-036
47	0.2270	9.5491E-009	6.8285E-012	7.9319E-011	1.3174E-011	-1.1758E-040	-4.3900E-035	-1.4529E-036
48	0.2273	1.1462E-008	7.4186E-012	9.6265E-011	1.5123E-011	-1.8514E-040	-5.7086E-035	-1.7772E-036
49	0.2277	1.3765E-008	8.0866E-012	1.1704E-010	1.7368E-011	-2.9412E-040	-7.4552E-035	-2.1757E-036
50	0.2281	1.6528E-008	8.8417E-012	1.4241E-010	1.9945E-011	-4.7009E-040	-9.7628E-035	-2.6631E-036
51	0.2283	1.8112E-008	9.2565E-012	1.5716E-010	2.1375E-011	-5.9818E-040	-1.1192E-034	-2.9465E-036
52	0.2285	1.9852E-008	9.6999E-012	1.7353E-010	2.2910E-011	-7.6300E-040	-1.2848E-034	-3.2611E-036
53	0.2287	2.1760E-008	1.0174E-011	1.9168E-010	2.4557E-011	-9.7535E-040	-1.4764E-034	-3.6098E-036
54	0.2289	2.3852E-008	1.0679E-011	2.1180E-010	2.6324E-011	-1.2492E-039	-1.6979E-034	-3.9958E-036
55	0.2291	2.6143E-008	1.1219E-011	2.3408E-010	2.8218E-011	-1.6024E-039	-1.9540E-034	-4.4225E-036
56	0.2293	2.8649E-008	1.1795E-011	2.5871E-010	3.0246E-011	-2.0583E-039	-2.2498E-034	-4.8936E-036
57	0.2295	3.1388E-008	1.2408E-011	2.8593E-010	3.2416E-011	-2.6465E-039	-2.5911E-034	-5.4132E-036
58	0.2297	3.4378E-008	1.3062E-011	3.1598E-010	3.4737E-011	-3.4055E-039	-2.9846E-034	-5.9853E-036
59	0.2299	3.7640E-008	1.3757E-011	3.4912E-010	3.7217E-011	-4.3844E-039	-3.4381E-034	-6.6144E-036
60	0.2301	4.1194E-008	1.4497E-011	3.8562E-010	3.9866E-011	-5.6462E-039	-3.9603E-034	-7.3053E-036
61	0.2303	4.5063E-008	1.5283E-011	4.2580E-010	4.2694E-011	-7.2716E-039	-4.5612E-034	-8.0629E-036
62	0.2305	4.9270E-008	1.6119E-011	4.6996E-010	4.5710E-011	-9.3635E-039	-5.2521E-034	-8.8927E-036
63	0.2307	5.3841E-008	1.7007E-011	5.1846E-010	4.8925E-011	-1.2053E-038	-6.0460E-034	-9.8002E-036
64	0.2309	5.8801E-008	1.7950E-011	5.7167E-010	5.2350E-011	-1.5509E-038	-6.9575E-034	-1.0791E-035
65	0.2311	6.4178E-008	1.8951E-011	6.2998E-010	5.5996E-011	-1.9943E-038	-8.0034E-034	-1.1872E-035
66	0.2313	7.0002E-008	2.0012E-011	6.9382E-010	5.9874E-011	-2.5628E-038	-9.2026E-034	-1.3050E-035
67	0.2314	7.6304E-008	2.1138E-011	7.6364E-010	6.3996E-011	-3.2909E-038	-1.0577E-033	-1.4330E-035
68	0.2316	8.3115E-008	2.2332E-011	8.3991E-010	6.8375E-011	-4.2230E-038	-1.2150E-033	-1.5721E-035
69	0.2318	9.0469E-008	2.3598E-011	9.2316E-010	7.3022E-011	-5.4156E-038	-1.3951E-033	-1.7230E-035
70	0.2320	9.8402E-008	2.4938E-011	1.0139E-009	7.7950E-011	-6.9418E-038	-1.6009E-033	-1.8864E-035
71	0.2322	1.0695E-007	2.6358E-011	1.1128E-009	8.3172E-011	-8.8968E-038	-1.8362E-033	-2.0631E-035
72	0.2324	1.1615E-007	2.7860E-011	1.2203E-009	8.8701E-011	-1.1406E-037	-2.1048E-033	-2.2540E-035

73	0.2328	1.3665E-007	3.1122E-011	1.4635E-009	1.0071E-010	-1.8585E-037	-2.7556E-033	-2.6803E-035
74	0.2336	1.8641E-007	3.8658E-011	2.0694E-009	1.2856E-010	-4.6473E-037	-4.5999E-033	-3.7167E-035
75	0.2344	2.4880E-007	4.7526E-011	2.8480E-009	1.6151E-010	-1.1140E-036	-7.4490E-033	-5.0122E-035
76	0.2352	3.2563E-007	5.7876E-011	3.8266E-009	2.0001E-010	-2.5729E-036	-1.1817E-032	-6.6179E-035
77	0.2359	4.1860E-007	6.9841E-011	5.0290E-009	2.4438E-010	-5.7457E-036	-1.8463E-032	-8.6053E-035
78	0.2367	5.2923E-007	8.3526E-011	6.4732E-009	2.9477E-010	-1.2433E-035	-2.8497E-032	-1.1071E-034
79	0.2375	6.5870E-007	9.8995E-011	8.1690E-009	3.5119E-010	-2.6096E-035	-4.3525E-032	-1.4142E-034
80	0.2383	8.0785E-007	1.1627E-010	1.0116E-008	4.1345E-010	-5.3153E-035	-6.5847E-032	-1.7981E-034
81	0.2391	9.7712E-007	1.3534E-010	1.2302E-008	4.8116E-010	-1.0505E-034	-9.8701E-032	-2.2789E-034
82	0.2398	1.1665E-006	1.5614E-010	1.4705E-008	5.5381E-010	-2.0140E-034	-1.4659E-031	-2.8814E-034
83	0.2406	1.3756E-006	1.7859E-010	1.7292E-008	6.3073E-010	-3.7440E-034	-2.1567E-031	-3.6353E-034
84	0.2414	1.6037E-006	2.0255E-010	2.0023E-008	7.1118E-010	-6.7471E-034	-3.1418E-031	-4.5758E-034
85	0.2422	1.8496E-006	2.2790E-010	2.2852E-008	7.9439E-010	-1.1787E-033	-4.5298E-031	-5.7440E-034
86	0.2430	2.1120E-006	2.5448E-010	2.5732E-008	8.7955E-010	-1.9967E-033	-6.4613E-031	-7.1867E-034
87	0.2437	2.3893E-006	2.8214E-010	2.8616E-008	9.6590E-010	-3.2823E-033	-9.1143E-031	-8.9570E-034
88	0.2445	2.6800E-006	3.1073E-010	3.1460E-008	1.0527E-009	-5.2413E-033	-1.2712E-030	-1.1114E-033
89	0.2453	2.9822E-006	3.4008E-010	3.4226E-008	1.1394E-009	-8.1412E-033	-1.7528E-030	-1.3723E-033
90	0.2461	3.2943E-006	3.7007E-010	3.6881E-008	1.2252E-009	-1.2321E-032	-2.3897E-030	-1.6857E-033
91	0.2469	3.6146E-006	4.0056E-010	3.9397E-008	1.3098E-009	-1.8214E-032	-3.2227E-030	-2.0586E-033
92	0.2484	4.2751E-006	4.6278E-010	4.3948E-008	1.4739E-009	-3.6926E-032	-5.6225E-030	-2.9965E-033
93	0.2500	4.9482E-006	5.2540E-010	4.7888E-008	1.6289E-009	-6.8203E-032	-9.2128E-030	-4.1712E-033
94	0.2516	5.6247E-006	5.8766E-010	5.1229E-008	1.7733E-009	-1.1702E-031	-1.4384E-029	-5.6097E-033
95	0.2531	6.2966E-006	6.4894E-010	5.4020E-008	1.9066E-009	-1.8915E-031	-2.1604E-029	-7.3423E-033
96	0.2562	7.6071E-006	7.6723E-010	5.8125E-008	2.1391E-009	-4.2614E-031	-4.3952E-029	-1.1698E-032
97	0.2594	8.8592E-006	8.7799E-010	6.1043E-008	2.3327E-009	-8.1416E-031	-7.7738E-029	-1.6692E-032
98	0.2625	1.0045E-005	9.8055E-010	6.3145E-008	2.4931E-009	-1.3894E-030	-1.2514E-028	-2.2173E-032
99	0.2656	1.1161E-005	1.0752E-009	6.4699E-008	2.6260E-009	-2.1815E-030	-1.8783E-028	-2.7986E-032
100	0.2688	1.2210E-005	1.1625E-009	6.5891E-008	2.7363E-009	-3.2128E-030	-2.6710E-028	-3.4008E-032
101	0.2750	1.4100E-005	1.3175E-009	6.7574E-008	2.9030E-009	-6.0514E-030	-4.8011E-028	-4.6523E-032
102	0.2812	1.5806E-005	1.4562E-009	6.8882E-008	3.0226E-009	-9.8681E-030	-7.5114E-028	-5.7441E-032
103	0.2875	1.7361E-005	1.5839E-009	7.0008E-008	3.1088E-009	-1.4617E-029	-1.0748E-027	-6.6625E-032
104	0.2938	1.8796E-005	1.7045E-009	7.1051E-008	3.1708E-009	-2.0200E-029	-1.4434E-027	-7.4056E-032
105	0.3000	2.0135E-005	1.8210E-009	7.2069E-008	3.2150E-009	-2.6490E-029	-1.8487E-027	-7.9818E-032
106	0.3063	2.1397E-005	1.9361E-009	7.3096E-008	3.2464E-009	-3.3358E-029	-2.2827E-027	-8.4077E-032
107	0.3125	2.2601E-005	2.0515E-009	7.4156E-008	3.2685E-009	-4.0676E-029	-2.7386E-027	-8.7046E-032
108	0.3188	2.3759E-005	2.1690E-009	7.5264E-008	3.2845E-009	-4.8333E-029	-3.2107E-027	-8.8950E-032
109	0.3250	2.4884E-005	2.2898E-009	7.6435E-008	3.2968E-009	-5.6234E-029	-3.6947E-027	-9.0008E-032
110	0.3313	2.5984E-005	2.4148E-009	7.7677E-008	3.3072E-009	-6.4305E-029	-4.1873E-027	-9.0416E-032
111	0.3375	2.7069E-005	2.5449E-009	7.8994E-008	3.3174E-009	-7.2488E-029	-4.6864E-027	-9.0348E-032
112	0.3438	2.8143E-005	2.6806E-009	8.0391E-008	3.3288E-009	-8.0736E-029	-5.1902E-027	-8.9947E-032
113	0.3500	2.9213E-005	2.8222E-009	8.1864E-008	3.3423E-009	-8.9000E-029	-5.6970E-027	-8.9327E-032
114	0.3625	3.1352E-005	3.1231E-009	8.5023E-008	3.3801E-009	-1.0527E-028	-6.7089E-027	-8.7833E-032
115	0.3750	3.3510E-005	3.4493E-009	8.8450E-008	3.4306E-009	-1.2156E-028	-7.7354E-027	-8.6135E-032
116	0.3875	3.5697E-005	3.8004E-009	9.2122E-008	3.4954E-009	-1.3799E-028	-8.7885E-027	-8.4578E-032
117	0.4000	3.7915E-005	4.1752E-009	9.5998E-008	3.5743E-009	-1.5463E-028	-9.8765E-027	-8.3303E-032
118	0.4125	4.0166E-005	4.5719E-009	1.0003E-007	3.6665E-009	-1.7152E-028	-1.1005E-026	-8.2350E-032
119	0.4250	4.2448E-005	4.9884E-009	1.0417E-007	3.7708E-009	-1.8869E-028	-1.2176E-026	-8.1715E-032
120	0.4375	4.4759E-005	5.4223E-009	1.0837E-007	3.8858E-009	-2.0612E-028	-1.3391E-026	-8.1373E-032
121	0.4500	4.7095E-005	5.8710E-009	1.1259E-007	4.0102E-009	-2.2383E-028	-1.4650E-026	-8.1324E-032
122	0.4625	4.9452E-005	6.3306E-009	1.1675E-007	4.1428E-009	-2.4188E-028	-1.5951E-026	-8.1572E-032
123	0.4750	5.1824E-005	6.7948E-009	1.2079E-007	4.2830E-009	-2.6044E-028	-1.7297E-026	-8.2238E-032
124	0.4812	5.3005E-005	7.0235E-009	1.2273E-007	4.3556E-009	-2.7005E-028	-1.7981E-026	-8.2728E-032
125	0.4875	5.4158E-005	7.2419E-009	1.2452E-007	4.4287E-009	-2.7958E-028	-1.8666E-026	-8.3566E-032
126	0.4906	5.4696E-005	7.3411E-009	1.2532E-007	4.4636E-009	-2.8418E-028	-1.8989E-026	-8.4148E-032
127	0.4938	5.5165E-005	7.4254E-009	1.2600E-007	4.4943E-009	-2.8804E-028	-1.9274E-026	-8.4632E-032
128	0.4969	5.5485E-005	7.4813E-009	1.2646E-007	4.5153E-009	-2.9058E-028	-1.9464E-026	-8.5328E-032
129	0.5000	5.5485E-005	7.4813E-009	1.2646E-007	4.5153E-009	-2.9058E-028	-1.9464E-026	-8.5328E-032

	X(cm)	MOLE FRACTIONS: HCNN	HCNO	HOCN	HNCO	NCO	N2	AR
1	0.0000	3.1853E-070	-4.2320E-061	-1.8459E-062	-4.4746E-056	-2.3929E-062	5.5620E-001	0.0000E+000
2	0.0250	5.7847E-069	-1.1835E-059	-5.1618E-061	-1.2513E-054	-6.6640E-061	5.5620E-001	0.0000E+000
3	0.0500	1.5262E-067	-3.3094E-058	-1.4435E-059	-3.4992E-053	-3.6367E-059	5.5620E-001	0.0000E+000
4	0.0750	3.6395E-066	-9.2547E-057	-4.0366E-058	-9.7851E-052	-2.0030E-057	5.5620E-001	0.0000E+000
5	0.0875	3.4933E-065	-1.0395E-055	-4.5339E-057	-1.0991E-050	-4.2875E-056	5.5620E-001	0.0000E+000
6	0.1000	3.9946E-064	-1.4753E-054	-6.4349E-056	-1.5599E-049	-9.1915E-055	5.5620E-001	0.0000E+000
7	0.1250	1.4928E-062	-5.9686E-053	-2.6033E-054	-6.3107E-048	-5.6403E-053	5.5620E-001	0.0000E+000
8	0.1500	3.1709E-059	-1.6875E-051	-7.3604E-053	-1.7842E-046	-3.1104E-051	5.5621E-001	0.0000E+000
9	0.1625	1.7442E-055	-1.8961E-050	-8.2703E-052	-2.0048E-045	-6.6590E-050	5.5621E-001	0.0000E+000
10	0.1750	6.3840E-052	-2.6913E-049	-1.1738E-050	-2.8454E-044	-1.4276E-048	5.5621E-001	0.0000E+000
11	0.1875	2.1574E-048	-3.8921E-048	-1.6976E-049	-4.1149E-043	-3.0609E-047	5.5622E-001	0.0000E+000
12	0.1938	1.9359E-045	-2.4021E-047	-1.0477E-048	-2.5395E-042	-2.6900E-046	5.5625E-001	0.0000E+000
13	0.2000	8.0416E-043	-1.7987E-046	-7.8445E-048	-1.9011E-041	-2.5617E-045	5.5632E-001	0.0000E+000
14	0.2031	7.4766E-041	-6.5242E-046	-2.8432E-047	-6.8872E-041	-1.1165E-044	5.5640E-001	0.0000E+000
15	0.2047	-4.9611E-040	-8.5267E-046	-6.4762E-047	-1.5679E-040	-2.8266E-044	5.5647E-001	0.0000E+000
16	0.2063	-6.4958E-040	-1.7779E-045	-1.6234E-046	-3.9273E-040	-7.7615E-044	5.5656E-001	0.0000E+000
17	0.2078	-6.0285E-039	-3.2955E-045	-4.2442E-046	-1.0257E-039	-2.2048E-043	5.5668E-001	0.0000E+000
18	0.2086	-1.7319E-040	-2.8588E-045	-7.2125E-046	-1.7415E-039	-3.9474E-043	5.5676E-001	0.0000E+000
19	0.2094	2.0962E-039	-2.6249E-045	-1.2682E-045	-3.0587E-039	-7.3183E-043	5.5685E-001	0.0000E+000
20	0.2102	2.8178E-039	-1.8120E-045	-2.2762E-045	-5.4822E-039	-1.3853E-042	5.5696E-001	0.0000E+000

21	0.2105	3.5117E-039	-3.5241E-047	-3.0988E-045	-7.4567E-039	-1.9440E-042	5.5702E-001	0.0000E+000
22	0.2109	3.2411E-039	1.8655E-045	-4.2677E-045	-1.0259E-038	-2.7629E-042	5.5709E-001	0.0000E+000
23	0.2113	1.1397E-039	3.6565E-045	-5.9288E-045	-1.4236E-038	-3.9640E-042	5.5717E-001	0.0000E+000
24	0.2117	-2.5293E-040	6.0868E-045	-8.2889E-045	-1.9879E-038	-5.7281E-042	5.5725E-001	0.0000E+000
25	0.2121	1.1152E-038	9.0521E-045	-1.1642E-044	-2.7884E-038	-8.3230E-042	5.5733E-001	0.0000E+000
26	0.2125	4.3052E-038	9.3466E-045	-1.6407E-044	-3.9236E-038	-1.2147E-041	5.5742E-001	0.0000E+000
27	0.2129	9.7412E-038	1.1640E-044	-2.3175E-044	-5.5331E-038	-1.7796E-041	5.5753E-001	0.0000E+000
28	0.2133	5.5907E-038	2.3850E-045	-3.2790E-044	-7.8143E-038	-2.6160E-041	5.5763E-001	0.0000E+000
29	0.2137	3.2468E-038	-2.2937E-044	-4.6447E-044	-1.1046E-037	-3.8581E-041	5.5775E-001	0.0000E+000
30	0.2141	2.9830E-038	-6.5530E-044	-6.5845E-044	-1.5624E-037	-5.7082E-041	5.5788E-001	0.0000E+000
31	0.2145	5.8629E-038	-1.3227E-043	-9.3394E-044	-2.2104E-037	-8.4726E-041	5.5801E-001	0.0000E+000
32	0.2148	1.3284E-037	-2.4384E-043	-1.3252E-043	-3.1274E-037	-1.2616E-040	5.5815E-001	0.0000E+000
33	0.2152	1.1635E-037	-4.4342E-043	-1.8807E-043	-4.4241E-037	-1.8846E-040	5.5831E-001	0.0000E+000
34	0.2156	-2.5307E-037	-1.0749E-042	-2.6696E-043	-6.2569E-037	-2.8235E-040	5.5847E-001	0.0000E+000
35	0.2164	2.8603E-037	-2.6240E-043	-5.2396E-043	-1.2188E-036	-6.1371E-040	5.5883E-001	0.0000E+000
36	0.2172	1.0425E-037	-5.3164E-044	-9.9754E-043	-2.2981E-036	-1.3032E-039	5.5924E-001	0.0000E+000
37	0.2180	2.6648E-038	-4.8204E-044	-1.8711E-042	-4.2568E-036	-2.7490E-039	5.5970E-001	0.0000E+000
38	0.2188	6.1207E-039	-1.4791E-043	-3.4850E-042	-7.7994E-036	-5.7976E-039	5.6022E-001	0.0000E+000
39	0.2195	1.3149E-039	-3.6233E-043	-6.4726E-042	-1.4182E-035	-1.2258E-038	5.6079E-001	0.0000E+000
40	0.2203	1.7963E-040	-7.6929E-043	-1.2020E-041	-2.5630E-035	-2.6016E-038	5.6143E-001	0.0000E+000
41	0.2211	-2.6166E-040	-1.5339E-042	-2.2360E-041	-4.6064E-035	-5.5437E-038	5.6213E-001	0.0000E+000
42	0.2219	-8.5100E-040	-2.9773E-042	-4.1740E-041	-8.2331E-035	-1.1863E-037	5.6290E-001	0.0000E+000
43	0.2234	-4.4334E-039	-9.7330E-042	-1.3177E-040	-2.3747E-034	-4.6335E-037	5.6463E-001	0.0000E+000
44	0.2250	-1.8608E-038	-2.9678E-041	-3.9840E-040	-6.2060E-034	-1.6606E-036	5.6664E-001	0.0000E+000
45	0.2258	-3.7424E-038	-5.4652E-041	-7.4397E-040	-1.0164E-033	-3.2692E-036	5.6775E-001	0.0000E+000
46	0.2266	-7.2992E-038	-1.0263E-040	-1.4324E-039	-1.6873E-033	-6.4760E-036	5.6893E-001	0.0000E+000
47	0.2270	-1.0160E-037	-1.4292E-040	-2.0375E-039	-2.1942E-033	-9.2202E-036	5.6954E-001	0.0000E+000
48	0.2273	-1.4063E-037	-2.0058E-040	-2.9333E-039	-2.8719E-033	-1.3190E-035	5.7017E-001	0.0000E+000
49	0.2277	-1.9329E-037	-2.8270E-040	-4.2598E-039	-3.7751E-033	-1.8902E-035	5.7082E-001	0.0000E+000
50	0.2281	-2.6351E-037	-3.9917E-040	-6.2261E-039	-4.9747E-033	-2.7071E-035	5.7147E-001	0.0000E+000
51	0.2283	-3.0704E-037	-4.7542E-040	-7.5665E-039	-5.7205E-033	-3.2444E-035	5.7181E-001	0.0000E+000
52	0.2285	-3.5718E-037	-5.6700E-040	-9.2214E-039	-6.5866E-033	-3.8913E-035	5.7214E-001	0.0000E+000
53	0.2287	-4.1476E-037	-6.7684E-040	-1.1264E-038	-7.5914E-033	-4.6690E-035	5.7248E-001	0.0000E+000
54	0.2289	-4.8069E-037	-8.0838E-040	-1.3786E-038	-8.7562E-033	-5.6023E-035	5.7282E-001	0.0000E+000
55	0.2291	-5.5594E-037	-9.6567E-040	-1.6898E-038	-1.0105E-032	-6.7206E-035	5.7316E-001	0.0000E+000
56	0.2293	-6.4158E-037	-1.1535E-039	-2.0739E-038	-1.1665E-032	-8.0584E-035	5.7350E-001	0.0000E+000
57	0.2295	-7.3873E-037	-1.3775E-039	-2.5480E-038	-1.3469E-032	-9.6561E-035	5.7385E-001	0.0000E+000
58	0.2297	-8.4862E-037	-1.6442E-039	-3.1329E-038	-1.5550E-032	-1.1561E-034	5.7419E-001	0.0000E+000
59	0.2299	-9.7254E-037	-1.9612E-039	-3.8547E-038	-1.7952E-032	-1.3828E-034	5.7454E-001	0.0000E+000
60	0.2301	-1.1119E-036	-2.3377E-039	-4.7452E-038	-2.0718E-032	-1.6521E-034	5.7489E-001	0.0000E+000
61	0.2303	-1.2681E-036	-2.7840E-039	-5.8438E-038	-2.3902E-032	-1.9715E-034	5.7524E-001	0.0000E+000
62	0.2305	-1.4427E-036	-3.3123E-039	-7.1987E-038	-2.7564E-032	-2.3497E-034	5.7558E-001	0.0000E+000
63	0.2307	-1.6375E-036	-3.9369E-039	-8.8695E-038	-3.1770E-032	-2.7965E-034	5.7593E-001	0.0000E+000
64	0.2309	-1.8540E-036	-4.6741E-039	-1.0929E-037	-3.6596E-032	-3.3236E-034	5.7628E-001	0.0000E+000
65	0.2311	-2.0941E-036	-5.5430E-039	-1.3468E-037	-4.2129E-032	-3.9445E-034	5.7663E-001	0.0000E+000
66	0.2313	-2.3598E-036	-6.5657E-039	-1.6596E-037	-4.8465E-032	-4.6747E-034	5.7697E-001	0.0000E+000
67	0.2314	-2.6530E-036	-7.7677E-039	-2.0448E-037	-5.5715E-032	-5.5324E-034	5.7732E-001	0.0000E+000
68	0.2316	-2.9760E-036	-9.1785E-039	-2.5192E-037	-6.4001E-032	-6.5384E-034	5.7766E-001	0.0000E+000
69	0.2318	-3.3308E-036	-1.0832E-038	-3.1033E-037	-7.3463E-032	-7.7174E-034	5.7801E-001	0.0000E+000
70	0.2320	-3.7200E-036	-1.2768E-038	-3.8220E-037	-8.4258E-032	-9.0978E-034	5.7835E-001	0.0000E+000
71	0.2322	-4.1459E-036	-1.5031E-038	-4.7065E-037	-9.6561E-032	-1.0713E-033	5.7869E-001	0.0000E+000
72	0.2324	-4.6112E-036	-1.7673E-038	-5.7947E-037	-1.1057E-031	-1.2604E-033	5.7902E-001	0.0000E+000
73	0.2328	-5.6663E-036	-2.4273E-038	-8.7218E-037	-1.4437E-031	-1.7352E-033	5.7969E-001	0.0000E+000
74	0.2336	-8.3005E-036	-4.3962E-038	-1.8757E-036	-2.3917E-031	-3.1790E-033	5.8099E-001	0.0000E+000
75	0.2344	-1.1720E-035	-7.6140E-038	-3.8822E-036	-3.8252E-031	-5.6163E-033	5.8224E-001	0.0000E+000
76	0.2352	-1.6093E-035	-1.2764E-037	-7.8114E-036	-5.9649E-031	-9.6686E-033	5.8345E-001	0.0000E+000
77	0.2359	-2.1632E-035	-2.0837E-037	-1.5316E-035	-9.1192E-031	-1.6312E-032	5.8460E-001	0.0000E+000
78	0.2367	-2.8598E-035	-3.3235E-037	-2.9278E-035	-1.3711E-030	-2.7062E-032	5.8570E-001	0.0000E+000
79	0.2375	-3.7294E-035	-5.1893E-037	-5.4555E-035	-2.0312E-030	-4.4229E-032	5.8674E-001	0.0000E+000
80	0.2383	-4.8049E-035	-7.9410E-037	-9.9067E-035	-2.9677E-030	-7.1269E-032	5.8773E-001	0.0000E+000
81	0.2391	-6.1196E-035	-1.1915E-036	-1.7527E-034	-4.2781E-030	-1.1320E-031	5.8867E-001	0.0000E+000
82	0.2398	-7.7041E-035	-1.7534E-036	-3.0206E-034	-6.0854E-030	-1.7712E-031	5.8956E-001	0.0000E+000
83	0.2406	-9.5830E-035	-2.5307E-036	-5.0705E-034	-8.5398E-030	-2.7269E-031	5.9040E-001	0.0000E+000
84	0.2414	-1.1772E-034	-3.5821E-036	-8.2916E-034	-1.1820E-029	-4.1263E-031	5.9121E-001	0.0000E+000
85	0.2422	-1.4275E-034	-4.9733E-036	-1.3212E-033	-1.6132E-029	-6.1316E-031	5.9198E-001	0.0000E+000
86	0.2430	-1.7085E-034	-6.7748E-036	-2.0525E-033	-2.1708E-029	-8.9426E-031	5.9272E-001	0.0000E+000
87	0.2437	-2.0182E-034	-9.0596E-036	-3.1111E-033	-2.8804E-029	-1.2799E-030	5.9342E-001	0.0000E+000
88	0.2445	-2.3540E-034	-1.1901E-035	-4.6057E-033	-3.7692E-029	-1.7979E-030	5.9410E-001	0.0000E+000
89	0.2453	-2.7121E-034	-1.5369E-035	-6.6672E-033	-4.8666E-029	-2.4801E-030	5.9475E-001	0.0000E+000
90	0.2461	-3.0884E-034	-1.9532E-035	-9.4511E-033	-6.2034E-029	-3.3624E-030	5.9536E-001	0.0000E+000
91	0.2469	-3.4778E-034	-2.4453E-035	-1.3144E-032	-7.8127E-029	-4.4849E-030	5.9596E-001	0.0000E+000
92	0.2484	-4.2764E-034	-3.6767E-035	-2.4000E-032	-1.1956E-028	-7.6048E-030	5.9708E-001	0.0000E+000
93	0.2500	-5.0405E-034	-5.2102E-035	-4.0568E-032	-1.7332E-028	-1.2080E-029	5.9811E-001	0.0000E+000
94	0.2516	-5.7424E-034	-7.0401E-035	-6.4529E-032	-2.4066E-028	-1.8206E-029	5.9906E-001	0.0000E+000
95	0.2531	-6.3700E-034	-9.1514E-035	-9.7724E-032	-3.2270E-028	-2.6274E-029	5.9995E-001	0.0000E+000
96	0.2562	-7.3940E-034	-1.4161E-034	-1.9926E-031	-5.3461E-028	-4.9281E-029	6.0156E-001	0.0000E+000
97	0.2594	-8.0343E-034	-1.9787E-034	-3.5415E-031	-7.9802E-028	-8.1854E-029	6.0301E-001	0.0000E+000
98	0.2625	-8.3745E-034	-2.5797E-034	-5.7242E-031	-1.1084E-027	-1.2471E-028	6.0433E-001	0.0000E+000
99	0.2656	-8.5074E-034	-3.2041E-034	-8.6241E-031	-1.4600E-027	-1.7800E-028	6.0554E-001	0.0000E+000
100	0.2688	-8.5065E-034	-3.8439E-034	-1.2308E-030	-1.8466E-027	-2.4132E-028	6.0667E-001	0.0000E+000

101	0.2750	-8.3191E-034	-5.1686E-034	-2.2252E-030	-2.7096E-027	-3.9507E-028	6.0872E-001	0.0000E+000
102	0.2812	-7.9712E-034	-6.5632E-034	-3.5768E-030	-3.6510E-027	-5.7924E-028	6.1057E-001	0.0000E+000
103	0.2875	-7.5862E-034	-8.0857E-034	-5.3163E-030	-4.6572E-027	-7.8770E-028	6.1224E-001	0.0000E+000
104	0.2938	-7.2203E-034	-9.8144E-034	-7.4677E-030	-5.7196E-027	-1.0144E-027	6.1378E-001	0.0000E+000
105	0.3000	-6.8948E-034	-1.1838E-033	-1.0050E-029	-6.8332E-027	-1.2540E-027	6.1521E-001	0.0000E+000
106	0.3063	-6.6148E-034	-1.4252E-033	-1.3080E-029	-7.9954E-027	-1.5023E-027	6.1653E-001	0.0000E+000
107	0.3125	-6.3781E-034	-1.7155E-033	-1.6568E-029	-9.2053E-027	-1.7558E-027	6.1776E-001	0.0000E+000
108	0.3188	-6.1798E-034	-2.0647E-033	-2.0524E-029	-1.0463E-026	-2.0122E-027	6.1891E-001	0.0000E+000
109	0.3250	-6.0138E-034	-2.4827E-033	-2.4955E-029	-1.1769E-026	-2.2698E-027	6.1999E-001	0.0000E+000
110	0.3313	-5.8738E-034	-2.9790E-033	-2.9864E-029	-1.3124E-026	-2.5274E-027	6.2100E-001	0.0000E+000
111	0.3375	-5.7544E-034	-3.5625E-033	-3.5253E-029	-1.4529E-026	-2.7846E-027	6.2195E-001	0.0000E+000
112	0.3438	-5.6503E-034	-4.2410E-033	-4.1120E-029	-1.5985E-026	-3.0411E-027	6.2283E-001	0.0000E+000
113	0.3500	-5.5573E-034	-5.0207E-033	-4.7448E-029	-1.7490E-026	-3.2961E-027	6.2365E-001	0.0000E+000
114	0.3625	-5.3846E-034	-6.9014E-033	-6.1301E-029	-2.0613E-026	-3.7932E-027	6.2514E-001	0.0000E+000
115	0.3750	-5.2277E-034	-9.2330E-033	-7.7014E-029	-2.3963E-026	-4.2955E-027	6.2646E-001	0.0000E+000
116	0.3875	-5.0778E-034	-1.2076E-032	-9.4713E-029	-2.7582E-026	-4.8087E-027	6.2763E-001	0.0000E+000
117	0.4000	-4.9308E-034	-1.5473E-032	-1.1448E-028	-3.1493E-026	-5.3364E-027	6.2867E-001	0.0000E+000
118	0.4125	-4.7858E-034	-1.9461E-032	-1.3638E-028	-3.5710E-026	-5.8812E-027	6.2961E-001	0.0000E+000
119	0.4250	-4.6437E-034	-2.4068E-032	-1.6045E-028	-4.0239E-026	-6.4436E-027	6.3044E-001	0.0000E+000
120	0.4375	-4.5065E-034	-2.9316E-032	-1.8668E-028	-4.5077E-026	-7.0239E-027	6.3119E-001	0.0000E+000
121	0.4500	-4.3781E-034	-3.5218E-032	-2.1503E-028	-5.0226E-026	-7.6193E-027	6.3185E-001	0.0000E+000
122	0.4625	-4.2609E-034	-4.1772E-032	-2.4547E-028	-5.5645E-026	-8.2331E-027	6.3243E-001	0.0000E+000
123	0.4750	-4.1665E-034	-4.8977E-032	-2.7769E-028	-6.1300E-026	-8.8633E-027	6.3292E-001	0.0000E+000
124	0.4812	-4.1316E-034	-5.2717E-032	-2.9400E-028	-6.4159E-026	-9.1799E-027	6.3311E-001	0.0000E+000
125	0.4875	-4.1163E-034	-5.6492E-032	-3.1004E-028	-6.6977E-026	-9.4876E-027	6.3326E-001	0.0000E+000
126	0.4906	-4.1137E-034	-5.8288E-032	-3.1735E-028	-6.8269E-026	-9.6238E-027	6.3331E-001	0.0000E+000
127	0.4938	-4.1139E-034	-5.9866E-032	-3.2366E-028	-6.9347E-026	-9.7466E-027	6.3334E-001	0.0000E+000
128	0.4969	-4.1106E-034	-6.0898E-032	-3.2736E-028	-6.9987E-026	-9.7989E-027	6.3336E-001	0.0000E+000
129	0.5000	-4.1106E-034	-6.0898E-032	-3.2736E-028	-6.9987E-026	-9.7989E-027	6.3336E-001	0.0000E+000

	X(cm)	MOLE FRACTIONS: C3H7	C3H8	CH2CHO	CH3CHO	K	KO	HKO
1	0.0000	1.2913E-111	2.7730E-110	-1.2688E-086	-1.1390E-082	1.5924E-018	2.3860E-019	3.2466E-011
2	0.0250	4.8815E-110	1.0905E-108	-3.9577E-085	-3.5535E-081	5.7583E-017	7.3208E-018	1.4137E-009
3	0.0500	1.9429E-108	4.2773E-107	-2.9984E-083	-1.1087E-079	6.3554E-017	8.0606E-018	2.7925E-009
4	0.0750	7.7428E-107	1.6752E-105	-3.0938E-081	-3.4588E-078	6.4432E-017	8.1509E-018	4.1678E-009
5	0.0875	1.2149E-105	2.5821E-104	-1.4001E-079	-4.3042E-077	6.4633E-017	8.1657E-018	4.8544E-009
6	0.1000	2.3890E-104	5.0965E-103	-5.5533E-078	-6.8021E-076	6.4795E-017	8.1755E-018	5.5401E-009
7	0.1250	1.3567E-102	2.9078E-101	-6.4808E-076	-3.0807E-074	6.5244E-017	8.2110E-018	6.9074E-009
8	0.1500	5.4447E-101	1.1424E-099	-8.1131E-074	-9.6938E-073	7.3212E-017	9.1905E-018	8.2726E-009
9	0.1625	8.5443E-100	1.7534E-098	-3.8763E-072	-1.2009E-071	2.1757E-016	2.7275E-017	8.9758E-009
10	0.1750	1.6800E-098	3.4462E-097	-1.5556E-070	-1.8787E-070	2.3118E-015	2.8975E-016	9.9483E-009
11	0.1875	3.3466E-097	6.8656E-096	-6.2250E-069	-2.9452E-069	3.2850E-014	4.1504E-015	1.3938E-008
12	0.1938	2.7602E-096	5.6385E-095	-9.7370E-068	-1.8829E-068	2.0020E-013	2.5860E-014	2.4575E-008
13	0.2000	2.8057E-095	5.7369E-094	-1.4226E-066	-1.4306E-067	1.0018E-012	1.3790E-013	7.0742E-008
14	0.2031	1.3243E-094	2.6535E-093	-8.5858E-066	-4.9349E-067	2.5333E-012	3.6854E-013	1.2996E-007
15	0.2047	2.3843E-094	7.7511E-093	-2.6089E-065	-1.0684E-066	4.0546E-012	6.1028E-013	1.8031E-007
16	0.2063	5.8838E-094	2.3817E-092	-8.3689E-065	-2.5317E-066	6.3942E-012	9.9381E-013	2.5810E-007
17	0.2078	1.4660E-093	6.5930E-092	-2.6974E-064	-6.1240E-066	9.9913E-012	1.5851E-012	3.7214E-007
18	0.2086	2.2603E-093	1.1542E-091	-5.1306E-064	-9.6954E-066	1.2514E-011	1.9944E-012	4.4354E-007
19	0.2094	3.7043E-093	2.1502E-091	-1.0051E-063	-1.5652E-065	1.5641E-011	2.4866E-012	5.2797E-007
20	0.2102	6.3740E-093	4.1414E-091	-1.9880E-063	-2.5291E-065	1.9479E-011	3.0615E-012	6.2488E-007
21	0.2105	8.6756E-093	5.9243E-091	-2.8370E-063	-3.2075E-065	2.1704E-011	3.3809E-012	6.7699E-007
22	0.2109	1.2246E-092	8.7106E-091	-4.0891E-063	-4.0670E-065	2.4133E-011	3.7149E-012	7.3148E-007
23	0.2113	1.7819E-092	1.3068E-090	-5.9257E-063	-5.1304E-065	2.6758E-011	4.0570E-012	7.8753E-007
24	0.2117	2.6798E-092	1.9967E-090	-8.6020E-063	-6.4021E-065	2.9557E-011	4.3978E-012	8.4403E-007
25	0.2121	4.1596E-092	3.0985E-090	-1.2472E-062	-7.8455E-065	3.2494E-011	4.7246E-012	8.9954E-007
26	0.2125	6.6524E-092	4.9008E-090	-1.8017E-062	-9.3455E-065	3.5512E-011	5.0206E-012	9.5228E-007
27	0.2129	1.0954E-091	7.8518E-090	-2.5869E-062	-1.0647E-064	3.8534E-011	5.2650E-012	1.0003E-006
28	0.2133	1.8533E-091	1.2702E-089	-3.6806E-062	-1.1242E-064	4.1471E-011	5.4337E-012	1.0413E-006
29	0.2137	3.1656E-091	2.0705E-089	-5.1714E-062	-1.0235E-064	4.4230E-011	5.5012E-012	1.0735E-006
30	0.2141	5.4242E-091	3.3883E-089	-7.1403E-062	-6.0812E-065	4.6735E-011	5.4461E-012	1.0953E-006
31	0.2145	9.2975E-091	5.5553E-089	-9.6185E-062	3.7642E-065	4.8940E-011	5.2591E-012	1.1059E-006
32	0.2148	1.5936E-090	9.1191E-089	-1.2492E-061	2.3354E-064	5.0848E-011	4.9534E-012	1.1056E-006
33	0.2152	2.6966E-090	1.5022E-088	-1.5329E-061	5.8912E-064	5.2511E-011	4.5700E-012	1.0957E-006
34	0.2156	4.5276E-090	2.4829E-088	-1.6197E-061	1.1979E-063	5.4019E-011	4.1742E-012	1.0785E-006
35	0.2164	1.1493E-089	6.2914E-088	-4.4568E-061	3.7330E-063	5.6814E-011	3.6642E-012	1.0303E-006
36	0.2172	2.8382E-089	1.4893E-087	-6.4529E-061	9.7130E-063	5.9998E-011	3.5726E-012	9.8302E-007
37	0.2180	6.8110E-089	3.3986E-087	-6.3740E-061	2.2964E-062	6.4052E-011	3.8794E-012	9.4755E-007
38	0.2188	1.5985E-088	7.5614E-087	-2.6599E-061	5.0662E-062	6.9449E-011	4.4545E-012	9.2914E-007
39	0.2195	3.6990E-088	1.6536E-086	7.4724E-061	1.0633E-061	7.6732E-011	5.2227E-012	9.2951E-007
40	0.2203	8.4985E-088	3.5726E-086	2.9731E-060	2.1554E-061	8.6535E-011	6.1817E-012	9.4874E-007
41	0.2211	1.9492E-087	7.6482E-086	7.6155E-060	4.2668E-061	9.9626E-011	7.3806E-012	9.8628E-007
42	0.2219	4.4826E-087	1.6246E-085	1.7190E-059	8.3109E-061	1.1702E-010	8.9189E-012	1.0421E-006
43	0.2234	1.9583E-086	6.1537E-085	6.6298E-059	2.7281E-060	1.7026E-010	1.3835E-011	1.2149E-006
44	0.2250	7.6983E-086	2.0305E-084	2.2955E-058	8.0200E-060	2.6527E-010	2.5847E-011	1.5005E-006
45	0.2258	1.6286E-085	3.8316E-084	4.5891E-058	1.4178E-059	3.4903E-010	4.1638E-011	1.7554E-006
46	0.2266	3.5413E-085	7.4381E-084	9.2718E-058	2.5531E-059	4.9004E-010	7.9099E-011	2.1937E-006
47	0.2270	5.3516E-085	1.0564E-083	1.3394E-057	3.4688E-059	6.0042E-010	1.1573E-010	2.5380E-006
48	0.2273	8.1929E-085	1.5198E-083	1.9463E-057	4.7494E-059	7.5524E-010	1.7460E-010	3.0172E-006

49	0.2277	1.2631E-084	2.2032E-083	2.8309E-057	6.5289E-059	9.7208E-010	2.6817E-010	3.6741E-006
50	0.2281	1.9522E-084	3.2057E-083	4.1098E-057	8.9856E-059	1.2712E-009	4.1312E-010	4.5517E-006
51	0.2283	2.4371E-084	3.8796E-083	4.9588E-057	1.0557E-058	1.4580E-009	5.1076E-010	5.0843E-006
52	0.2285	3.0507E-084	4.7073E-083	5.9881E-057	1.2418E-058	1.6743E-009	6.2794E-010	5.6885E-006
53	0.2287	3.8256E-084	5.7222E-083	7.2325E-057	1.4616E-058	1.9214E-009	7.6578E-010	6.3639E-006
54	0.2289	4.8026E-084	6.9644E-083	8.7328E-057	1.7210E-058	2.1997E-009	9.2389E-010	7.1062E-006
55	0.2291	6.0321E-084	8.4823E-083	1.0537E-056	2.0262E-058	2.5078E-009	1.0997E-009	7.9067E-006
56	0.2293	7.5766E-084	1.0333E-082	1.2699E-056	2.3847E-058	2.8419E-009	1.2876E-009	8.7511E-006
57	0.2295	9.5133E-084	1.2587E-082	1.5286E-056	2.8050E-058	3.1963E-009	1.4787E-009	9.6195E-006
58	0.2297	1.1937E-083	1.5325E-082	1.8372E-056	3.2965E-058	3.5625E-009	1.6607E-009	1.0488E-005
59	0.2299	1.4964E-083	1.8646E-082	2.2044E-056	3.8703E-058	3.9303E-009	1.8187E-009	1.1328E-005
60	0.2301	1.8736E-083	2.2664E-082	2.6403E-056	4.5386E-058	4.2883E-009	1.9376E-009	1.2113E-005
61	0.2303	2.3427E-083	2.7518E-082	3.1564E-056	5.3153E-058	4.6254E-009	2.0049E-009	1.2817E-005
62	0.2305	2.9248E-083	3.3367E-082	3.7662E-056	6.2161E-058	4.9320E-009	2.0142E-009	1.3421E-005
63	0.2307	3.6454E-083	4.0401E-082	4.4848E-056	7.2586E-058	5.2016E-009	1.9683E-009	1.3915E-005
64	0.2309	4.5355E-083	4.8841E-082	5.3299E-056	8.4626E-058	5.4314E-009	1.8795E-009	1.4299E-005
65	0.2311	5.6323E-083	5.8947E-082	6.3214E-056	9.8499E-058	5.6227E-009	1.7675E-009	1.4584E-005
66	0.2313	6.9806E-083	7.1018E-082	7.4821E-056	1.1445E-057	5.7798E-009	1.6544E-009	1.4787E-005
67	0.2314	8.6343E-083	8.5405E-082	8.8381E-056	1.3276E-057	5.9088E-009	1.5585E-009	1.4926E-005
68	0.2316	1.0658E-082	1.0251E-081	1.0419E-055	1.5371E-057	6.0161E-009	1.4901E-009	1.5020E-005
69	0.2318	1.3128E-082	1.2280E-081	1.2257E-055	1.7765E-057	6.1070E-009	1.4507E-009	1.5085E-005
70	0.2320	1.6138E-082	1.4682E-081	1.4391E-055	2.0493E-057	6.1855E-009	1.4353E-009	1.5132E-005
71	0.2322	1.9797E-082	1.7517E-081	1.6861E-055	2.3596E-057	6.2544E-009	1.4364E-009	1.5168E-005
72	0.2324	2.4239E-082	2.0857E-081	1.9711E-055	2.7116E-057	6.3153E-009	1.4466E-009	1.5196E-005
73	0.2328	3.5950E-082	2.9287E-081	2.6692E-055	3.5546E-057	6.4165E-009	1.4837E-009	1.5240E-005
74	0.2336	7.4038E-082	5.4517E-081	4.6481E-055	5.8669E-057	6.5541E-009	1.5694E-009	1.5301E-005
75	0.2344	1.4145E-081	9.4430E-081	7.6642E-055	9.2012E-057	6.6246E-009	1.6533E-009	1.5346E-005
76	0.2352	2.5582E-081	1.5518E-080	1.2201E-054	1.3918E-056	6.6427E-009	1.7349E-009	1.5385E-005
77	0.2359	4.4231E-081	2.4435E-080	1.8942E-054	2.0492E-056	6.6218E-009	1.8137E-009	1.5419E-005
78	0.2367	7.3562E-081	3.7096E-080	2.8847E-054	2.9538E-056	6.5736E-009	1.8902E-009	1.5452E-005
79	0.2375	1.1821E-080	5.4545E-080	4.3252E-054	4.1847E-056	6.5077E-009	1.9652E-009	1.5482E-005
80	0.2383	1.8422E-080	7.7952E-080	6.3978E-054	5.8409E-056	6.4314E-009	2.0395E-009	1.5510E-005
81	0.2391	2.7923E-080	1.0860E-079	9.3440E-054	8.0434E-056	6.3500E-009	2.1137E-009	1.5537E-005
82	0.2398	4.1259E-080	1.4783E-079	1.3474E-053	1.0935E-055	6.2673E-009	2.1882E-009	1.5563E-005
83	0.2406	5.9545E-080	1.9698E-079	1.9172E-053	1.4678E-055	6.1860E-009	2.2634E-009	1.5587E-005
84	0.2414	8.4059E-080	2.5733E-079	2.6894E-053	1.9451E-055	6.1081E-009	2.3394E-009	1.5610E-005
85	0.2422	1.1621E-079	3.2995E-079	3.7164E-053	2.5445E-055	6.0354E-009	2.4166E-009	1.5632E-005
86	0.2430	1.5749E-079	4.1570E-079	5.0560E-053	3.2857E-055	5.9698E-009	2.4953E-009	1.5652E-005
87	0.2437	2.0945E-079	5.1512E-079	6.7702E-053	4.1893E-055	5.9131E-009	2.5758E-009	1.5672E-005
88	0.2445	2.7361E-079	6.2844E-079	8.9237E-053	5.2764E-055	5.8675E-009	2.6588E-009	1.5691E-005
89	0.2453	3.5144E-079	7.5557E-079	1.1583E-052	6.5696E-055	5.8354E-009	2.7448E-009	1.5709E-005
90	0.2461	4.4428E-079	8.9608E-079	1.4818E-052	8.0931E-055	5.8194E-009	2.8346E-009	1.5727E-005
91	0.2469	5.5316E-079	1.0489E-078	1.8699E-052	9.8722E-055	5.8221E-009	2.9289E-009	1.5743E-005
92	0.2484	8.2085E-079	1.3848E-078	2.8521E-052	1.4264E-054	5.8914E-009	3.1339E-009	1.5774E-005
93	0.2500	1.1332E-078	1.7147E-078	4.0600E-052	1.9603E-054	6.0676E-009	3.3705E-009	1.5803E-005
94	0.2516	1.4765E-078	2.0168E-078	5.4812E-052	2.5941E-054	6.3712E-009	3.6474E-009	1.5829E-005
95	0.2531	1.8394E-078	2.2811E-078	7.0983E-052	3.3363E-054	6.8206E-009	3.9734E-009	1.5852E-005
96	0.2562	2.5957E-078	2.6938E-078	1.0839E-051	5.1876E-054	8.2019E-009	4.7985E-009	1.5894E-005
97	0.2594	3.2000E-078	2.8202E-078	1.4528E-051	7.2795E-054	1.0377E-008	5.9301E-009	1.5930E-005
98	0.2625	3.6083E-078	2.7292E-078	1.7856E-051	9.4861E-054	1.3486E-008	7.4321E-009	1.5961E-005
99	0.2656	3.8384E-078	2.5137E-078	2.0650E-051	1.1685E-053	1.7660E-008	9.3581E-009	1.5988E-005
100	0.2688	3.9292E-078	2.2459E-078	2.2860E-051	1.3776E-053	2.3012E-008	1.1747E-008	1.6010E-005
101	0.2750	3.8741E-078	1.7296E-078	2.5792E-051	1.7461E-053	3.7422E-008	1.7912E-008	1.6044E-005
102	0.2812	3.5681E-078	1.2710E-078	2.6702E-051	2.0087E-053	5.7908E-008	2.6214E-008	1.6064E-005
103	0.2875	3.1663E-078	9.1655E-079	2.6259E-051	2.1699E-053	8.5412E-008	3.6662E-008	1.6071E-005
104	0.2938	2.7563E-078	6.5915E-079	2.5011E-051	2.2484E-053	1.2083E-007	4.9077E-008	1.6064E-005
105	0.3000	2.3762E-078	4.7657E-079	2.3340E-051	2.2643E-053	1.6500E-007	6.3103E-008	1.6043E-005
106	0.3063	2.0397E-078	3.4788E-079	2.1494E-051	2.2356E-053	2.1864E-007	7.8243E-008	1.6009E-005
107	0.3125	1.7491E-078	2.5700E-079	1.9630E-051	2.1768E-053	2.8235E-007	9.3913E-008	1.5963E-005
108	0.3188	1.5020E-078	1.9244E-079	1.7842E-051	2.0992E-053	3.5653E-007	1.0952E-007	1.5904E-005
109	0.3250	1.2935E-078	1.4621E-079	1.6180E-051	2.0111E-053	4.4132E-007	1.2452E-007	1.5832E-005
110	0.3313	1.1186E-078	1.1278E-079	1.4667E-051	1.9185E-053	5.3667E-007	1.3847E-007	1.5750E-005
111	0.3375	9.7220E-079	8.8363E-080	1.3307E-051	1.8255E-053	6.4223E-007	1.5106E-007	1.5657E-005
112	0.3438	8.4993E-079	7.0345E-080	1.2096E-051	1.7347E-053	7.5737E-007	1.6212E-007	1.5554E-005
113	0.3500	7.4780E-079	5.6913E-080	1.1025E-051	1.6478E-053	8.8100E-007	1.7155E-007	1.5443E-005
114	0.3625	5.9092E-079	3.9170E-080	9.2443E-052	1.4873E-053	1.1452E-006	1.8555E-007	1.5205E-005
115	0.3750	4.7965E-079	2.8500E-080	7.8431E-052	1.3470E-053	1.4336E-006	1.9439E-007	1.4943E-005
116	0.3875	4.0127E-079	2.1923E-080	6.7186E-052	1.2243E-053	1.7389E-006	1.9911E-007	1.4664E-005
117	0.4000	3.4711E-079	1.7821E-080	5.7957E-052	1.1165E-053	2.0543E-006	2.0074E-007	1.4375E-005
118	0.4125	3.1146E-079	1.5301E-080	4.9970E-052	1.0176E-053	2.3737E-006	2.0015E-007	1.4081E-005
119	0.4250	2.8965E-079	1.3804E-080	4.2682E-052	9.2328E-054	2.6921E-006	1.9802E-007	1.3787E-005
120	0.4375	2.7535E-079	1.2824E-080	3.5528E-052	8.2496E-054	3.0054E-006	1.9487E-007	1.3497E-005
121	0.4500	2.5672E-079	1.1646E-080	2.8294E-052	7.1414E-054	3.3105E-006	1.9110E-007	1.3213E-005
122	0.4625	2.1224E-079	9.0477E-081	2.1692E-052	5.9023E-054	3.6049E-006	1.8699E-007	1.2939E-005
123	0.4750	9.9575E-080	2.5030E-081	1.3119E-052	3.9187E-054	3.8865E-006	1.8278E-007	1.2674E-005
124	0.4812	-5.6797E-080	-6.7121E-081	7.5127E-054	2.1426E-054	4.0217E-006	1.8073E-007	1.2546E-005
125	0.4875	-5.1516E-079	-3.3929E-080	-3.2124E-052	1.1187E-053	4.1472E-006	1.7885E-007	1.2426E-005
126	0.4906	-1.6515E-078	-9.3236E-080	-1.7470E-053	4.6573E-053	4.2030E-006	1.7803E-007	1.2371E-005
127	0.4938	-2.3374E-078	-1.3133E-079	-1.4540E-051	1.1167E-052	4.2490E-006	1.7737E-007	1.2325E-005
128	0.4969	-6.7947E-078	-3.3869E-079	3.2405E-051	3.2550E-052	4.2785E-006	1.7695E-007	1.2295E-005

129	0.5000	-6.7947E-078	-3.3869E-079	3.2405E-051	3.2550E-052	4.2785E-006	1.7695E-007	1.2295E-005

	X(cm)	MOLE FRACTIONS: KO2	HK	K2O	K2O2	K2CO3	K2H2O2	KHCO3
1	0.0000	1.4700E-005	4.6409E-023	1.6460E-023	2.9842E-021	-3.7197E-050	1.7235E-015	-2.8613E-030
2	0.0250	1.4699E-005	1.0888E-021	7.9730E-022	1.4679E-019	-1.8651E-048	8.4921E-014	-1.3946E-028
3	0.0500	1.4697E-005	2.1055E-021	2.4721E-021	4.2800E-019	4.3512E-044	3.9840E-013	-3.8697E-027
4	0.0750	1.4696E-005	2.9412E-021	4.9848E-021	8.4536E-019	-9.0228E-047	1.0855E-012	-7.1152E-027
5	0.0875	1.4695E-005	3.5965E-021	6.4528E-021	1.0887E-018	-7.6868E-047	1.5527E-012	-7.8259E-027
6	0.1000	1.4694E-005	8.1702E-021	8.1322E-021	1.3667E-018	2.5393E-046	2.1624E-012	8.0705E-027
7	0.1250	1.4693E-005	1.8489E-019	1.2359E-020	2.0579E-018	1.6381E-042	4.0434E-012	8.4493E-025
8	0.1500	1.4692E-005	5.5800E-018	1.9020E-020	2.8842E-018	2.5971E-043	6.7277E-012	-1.6296E-024
9	0.1625	1.4691E-005	6.8284E-017	4.1282E-020	3.3338E-018	-4.8892E-042	8.3176E-012	-6.7356E-023
10	0.1750	1.4689E-005	9.5404E-016	3.7783E-019	3.8395E-018	1.8787E-040	1.0358E-011	-1.6644E-021
11	0.1875	1.4679E-005	1.3438E-014	6.1786E-018	4.5801E-018	-4.4902E-040	1.5061E-011	-4.2525E-020
12	0.1938	1.4648E-005	8.0182E-014	4.1582E-017	5.3186E-018	2.6996E-039	2.5605E-011	-1.4633E-019
13	0.2000	1.4501E-005	5.3493E-013	3.5415E-016	7.3806E-018	-7.8700E-043	9.1887E-011	-2.4749E-019
14	0.2031	1.4297E-005	1.5963E-012	1.0631E-015	9.3866E-018	-1.3416E-043	2.0237E-010	-2.6582E-019
15	0.2047	1.4110E-005	2.9586E-012	1.9498E-015	1.0972E-017	-2.8366E-044	3.1973E-010	-2.6874E-019
16	0.2063	1.3795E-005	5.7051E-012	3.8543E-015	1.3550E-017	-4.7310E-045	5.5002E-010	-2.7084E-019
17	0.2078	1.3279E-005	1.0947E-011	7.6526E-015	1.8061E-017	-1.4659E-045	9.8129E-010	-2.7723E-019
18	0.2086	1.2921E-005	1.5075E-011	1.0571E-014	2.1688E-017	-1.4790E-045	1.3003E-009	-2.8741E-019
19	0.2094	1.2453E-005	2.0793E-011	1.4637E-014	2.7345E-017	-1.7919E-045	1.7366E-009	-3.1268E-019
20	0.2102	1.1846E-005	2.8509E-011	2.0080E-014	3.6479E-017	-2.7324E-045	2.3157E-009	-3.7547E-019
21	0.2105	1.1482E-005	3.3250E-011	2.3333E-014	4.3232E-017	-3.4328E-045	2.6627E-009	-4.4182E-019
22	0.2109	1.1060E-005	3.8714E-011	2.7032E-014	5.2514E-017	-4.6586E-045	3.0600E-009	-5.5738E-019
23	0.2113	1.0574E-005	4.4950E-011	3.1172E-014	6.5426E-017	-7.1619E-045	3.5104E-009	-7.5865E-019
24	0.2117	1.0013E-005	5.1987E-011	3.5723E-014	8.3551E-017	-1.2162E-044	4.0151E-009	-1.1091E-018
25	0.2121	9.3694E-006	5.9829E-011	4.0619E-014	1.0915E-016	-2.0960E-044	4.5733E-009	-1.7190E-018
26	0.2125	8.6374E-006	6.8445E-011	4.5760E-014	1.4539E-016	-3.7451E-044	5.1811E-009	-2.7801E-018
27	0.2129	7.8163E-006	7.7764E-011	5.1008E-014	1.9666E-016	-6.9620E-044	5.8320E-009	-4.6256E-018
28	0.2133	6.9143E-006	8.7675E-011	5.6193E-014	2.6882E-016	-1.3185E-043	6.5167E-009	-7.8334E-018
29	0.2137	5.9522E-006	9.8023E-011	6.1134E-014	3.6945E-016	-2.6448E-043	7.2234E-009	-1.3406E-017
30	0.2141	4.9659E-006	1.0863E-010	6.5657E-014	5.0793E-016	-8.3383E-043	7.9392E-009	-2.3081E-017
31	0.2145	4.0037E-006	1.1929E-010	6.9621E-014	6.9537E-016	-7.3463E-042	8.6512E-009	-3.9847E-017
32	0.2148	3.1191E-006	1.2982E-010	7.2942E-014	9.4423E-016	-9.2804E-041	9.3476E-009	-6.8367E-017
33	0.2152	2.3590E-006	1.4008E-010	7.5603E-014	1.2680E-015	-1.2511E-041	1.0019E-008	-6.7800E-017
34	0.2156	1.7516E-006	1.4996E-010	7.7638E-014	1.6811E-015	-6.5738E-044	1.0660E-008	-6.7252E-017
35	0.2164	1.0111E-006	1.6842E-010	8.0014E-014	2.8215E-015	1.0120E-035	1.1834E-008	-6.6750E-017
36	0.2172	6.6750E-007	1.8591E-010	8.0962E-014	4.3495E-015	1.2631E-035	1.2904E-008	-5.7331E-017
37	0.2180	5.2529E-007	2.0375E-010	8.0724E-014	6.2545E-015	-4.1788E-042	1.3904E-008	-5.7331E-017
38	0.2188	4.6364E-007	2.2383E-010	7.9339E-014	8.4816E-015	-7.8055E-042	1.4869E-008	-5.7379E-017
39	0.2195	4.3122E-007	2.4845E-010	7.6783E-014	1.0929E-014	-1.3667E-041	1.5832E-008	-5.7433E-017
40	0.2203	4.0983E-007	2.8015E-010	7.3048E-014	1.3448E-014	-2.5893E-041	1.6823E-008	-5.7493E-017
41	0.2211	3.9284E-007	3.2182E-010	6.8188E-014	1.5854E-014	-5.4647E-041	1.7864E-008	-5.7559E-017
42	0.2219	3.7737E-007	3.7702E-010	6.2348E-014	1.7932E-014	-1.2472E-040	1.8970E-008	-5.7632E-017
43	0.2234	3.4879E-007	5.4386E-010	4.8593E-014	2.0368E-014	-8.2684E-040	2.1395E-008	-5.7798E-017
44	0.2250	3.2252E-007	8.3555E-010	3.5932E-014	2.0937E-014	-7.0932E-039	2.3869E-008	-5.7991E-017
45	0.2258	3.0872E-007	1.0927E-009	3.2220E-014	2.1738E-014	-2.3479E-038	2.5128E-008	-5.8098E-017
46	0.2266	2.9378E-007	1.5180E-009	3.3320E-014	2.4629E-014	-8.8579E-038	2.6549E-008	-5.8212E-017
47	0.2270	2.8561E-007	1.8485E-009	3.7655E-014	2.8090E-014	-1.8281E-037	2.7468E-008	-5.8272E-017
48	0.2273	2.7653E-007	2.3022E-009	4.6619E-014	3.4091E-014	-3.9638E-037	2.8661E-008	-5.8333E-017
49	0.2277	2.6620E-007	2.9222E-009	6.2600E-014	4.3928E-014	-9.0052E-037	3.0253E-008	-5.8396E-017
50	0.2281	2.5417E-007	3.7543E-009	8.8795E-014	5.9251E-014	-2.1283E-036	3.2354E-008	-5.8460E-017
51	0.2283	2.4727E-007	4.2645E-009	1.0707E-013	6.9663E-014	-3.3090E-036	3.3605E-008	-5.8492E-017
52	0.2285	2.3950E-007	4.8453E-009	1.2975E-013	8.2418E-014	-5.1853E-036	3.4998E-008	-5.8525E-017
53	0.2287	2.3070E-007	5.4986E-009	1.5730E-013	9.7796E-014	-8.1627E-036	3.6505E-008	-5.8557E-017
54	0.2289	2.2072E-007	6.2226E-009	1.8999E-013	1.1601E-013	-1.2886E-035	3.8080E-008	-5.8590E-017
55	0.2291	2.0940E-007	7.0117E-009	2.2774E-013	1.3719E-013	-2.0349E-035	3.9646E-008	-5.8623E-017
56	0.2293	1.9664E-007	7.8553E-009	2.7001E-013	1.6130E-013	-3.2072E-035	4.1104E-008	-5.8656E-017
57	0.2295	1.8240E-007	8.7381E-009	3.1567E-013	1.8812E-013	-5.0348E-035	4.2329E-008	-5.8689E-017
58	0.2297	1.6673E-007	9.6398E-009	3.6291E-013	2.1721E-013	-7.8511E-035	4.3184E-008	-5.8721E-017
59	0.2299	1.4984E-007	1.0537E-008	4.0939E-013	2.4794E-013	-1.2140E-034	4.3530E-008	-5.8754E-017
60	0.2301	1.3209E-007	1.1404E-008	4.5237E-013	2.7944E-013	-1.8582E-034	4.3251E-008	-5.8786E-017
61	0.2303	1.1404E-007	1.2217E-008	4.8918E-013	3.1074E-013	-2.8105E-034	4.2271E-008	-5.8818E-017
62	0.2305	9.6380E-008	1.2953E-008	5.1761E-013	3.4084E-013	-4.1970E-034	4.0571E-008	-5.8849E-017
63	0.2307	7.9869E-008	1.3599E-008	5.3637E-013	3.6882E-013	-6.1829E-034	3.8203E-008	-5.8880E-017
64	0.2309	6.5193E-008	1.4145E-008	5.4531E-013	3.9393E-013	-8.9826E-034	3.5281E-008	-5.8909E-017
65	0.2311	5.2843E-008	1.4593E-008	5.4540E-013	4.1566E-013	-1.2869E-033	3.1971E-008	-5.8938E-017
66	0.2313	4.3015E-008	1.4948E-008	5.3841E-013	4.3380E-013	-1.8179E-033	2.8462E-008	-5.8965E-017
67	0.2314	3.5593E-008	1.5221E-008	5.2645E-013	4.4834E-013	-2.5322E-033	2.4942E-008	-5.8991E-017
68	0.2316	3.0211E-008	1.5426E-008	5.1151E-013	4.5949E-013	-3.4764E-033	2.1569E-008	-5.9015E-017
69	0.2318	2.6380E-008	1.5575E-008	4.9517E-013	4.6756E-013	-4.7014E-033	1.8459E-008	-5.9037E-017
70	0.2320	2.3622E-008	1.5679E-008	4.7850E-013	4.7292E-013	-6.2576E-033	1.5681E-008	-5.9057E-017
71	0.2322	2.1551E-008	1.5746E-008	4.6212E-013	4.7596E-013	-8.1896E-033	1.3260E-008	-5.9074E-017
72	0.2324	1.9897E-008	1.5785E-008	4.4634E-013	4.7701E-013	-1.0530E-032	1.1188E-008	-5.9087E-017
73	0.2328	1.7372E-008	1.5790E-008	4.1701E-013	4.7416E-013	-1.6481E-032	7.9929E-009	-5.9102E-017
74	0.2336	1.3799E-008	1.5595E-008	3.6637E-013	4.5604E-013	-3.2847E-032	4.2057E-009	-5.9064E-017
75	0.2344	1.1327E-008	1.5222E-008	3.2326E-013	4.3088E-013	-5.3124E-032	2.2847E-009	-5.8885E-017
76	0.2352	9.5380E-009	1.4725E-008	2.8649E-013	4.0309E-013	-7.5956E-032	1.2886E-009	-5.8474E-017

77	0.2359	8.2027E-009	1.4148E-008	2.5517E-013	3.7526E-013	-1.0118E-031	7.5233E-010	-5.7701E-017
78	0.2367	7.1876E-009	1.3526E-008	2.2865E-013	3.4886E-013	-1.2857E-031	4.5391E-010	-5.6398E-017
79	0.2375	6.4066E-009	1.2885E-008	2.0635E-013	3.2471E-013	-1.5714E-031	2.8277E-010	-5.4376E-017
80	0.2383	5.8004E-009	1.2240E-008	1.8768E-013	3.0309E-013	-1.8496E-031	1.8177E-010	-5.1475E-017
81	0.2391	5.3268E-009	1.1604E-008	1.7198E-013	2.8393E-013	-2.0941E-031	1.2048E-010	-4.7637E-017
82	0.2398	4.9548E-009	1.0983E-008	1.5857E-013	2.6682E-013	-2.2781E-031	8.2266E-011	-4.2966E-017
83	0.2406	4.6612E-009	1.0380E-008	1.4667E-013	2.5102E-013	-2.3827E-031	5.7795E-011	-3.7740E-017
84	0.2414	4.4282E-009	9.7997E-009	1.3539E-013	2.3554E-013	-2.4035E-031	4.1718E-011	-3.2344E-017
85	0.2422	4.2421E-009	9.2430E-009	1.2385E-013	2.1919E-013	-2.3504E-031	3.0892E-011	-2.7158E-017
86	0.2430	4.0916E-009	8.7125E-009	1.1125E-013	2.0089E-013	-2.2428E-031	2.3428E-011	-2.2460E-017
87	0.2437	3.9680E-009	8.2109E-009	9.7230E-014	1.8003E-013	-2.1022E-031	1.8165E-011	-1.8398E-017
88	0.2445	3.8640E-009	7.7407E-009	8.2114E-014	1.5686E-013	-1.9475E-031	1.4376E-011	-1.5001E-017
89	0.2453	3.7736E-009	7.3041E-009	6.6901E-014	1.3257E-013	-1.7906E-031	1.1592E-011	-1.2265E-017
90	0.2461	3.6921E-009	6.9032E-009	5.2852E-014	1.0894E-013	-1.6438E-031	9.5094E-012	-1.0026E-017
91	0.2469	3.6158E-009	6.5392E-009	4.0921E-014	8.7632E-014	-1.5102E-031	7.9241E-012	-8.2327E-018
92	0.2484	3.4683E-009	5.9228E-009	2.4339E-014	5.5469E-014	-1.2881E-031	5.7377E-012	-5.6536E-018
93	0.2500	3.3160E-009	5.4480E-009	1.5032E-014	3.5346E-014	-1.1225E-031	4.3405E-012	-3.9748E-018
94	0.2516	3.1557E-009	5.1053E-009	9.9749E-015	2.3631E-014	-1.0042E-031	3.4031E-012	-2.8610E-018
95	0.2531	2.9916E-009	4.8793E-009	7.1575E-015	1.6896E-014	-9.2306E-032	2.7477E-012	-2.1053E-018
96	0.2562	2.6798E-009	4.7034E-009	4.5642E-015	1.0937E-014	-8.3965E-032	1.9234E-012	-1.2117E-018
97	0.2594	2.4081E-009	4.7977E-009	3.5905E-015	8.5184E-015	-8.2301E-032	1.4315E-012	-7.3861E-019
98	0.2625	2.1891E-009	5.0707E-009	3.2623E-015	7.4477E-015	-8.4684E-032	1.1138E-012	-4.7246E-019
99	0.2656	2.0179E-009	5.4556E-009	3.2483E-015	6.9068E-015	-8.9595E-032	8.9605E-013	-3.1502E-019
100	0.2688	1.8841E-009	5.9056E-009	3.4171E-015	6.6236E-015	-9.5983E-032	7.4019E-013	-2.1791E-019
101	0.2750	1.6918E-009	6.8716E-009	4.0816E-015	6.5052E-015	-1.1140E-031	5.3831E-013	-1.1531E-019
102	0.2812	1.5510E-009	7.8646E-009	5.0498E-015	6.7083E-015	-1.2881E-031	4.1235E-013	-6.6513E-020
103	0.2875	1.4355E-009	8.8269E-009	6.2361E-015	7.0412E-015	-1.4731E-031	3.2789E-013	-4.1038E-020
104	0.2938	1.3325E-009	9.7327E-009	7.5768E-015	7.3717E-015	-1.6649E-031	2.6814E-013	-2.6707E-020
105	0.3000	1.2363E-009	1.0571E-008	9.0100E-015	7.6134E-015	-1.8617E-031	2.2408E-013	-1.8150E-020
106	0.3063	1.1446E-009	1.1336E-008	1.0473E-014	7.7160E-015	-2.0627E-031	1.9051E-013	-1.2787E-020
107	0.3125	1.0573E-009	1.2028E-008	1.1907E-014	7.6600E-015	-2.2676E-031	1.6426E-013	-9.2913E-021
108	0.3188	9.7480E-010	1.2647E-008	1.3259E-014	7.4514E-015	-2.4767E-031	1.4331E-013	-6.9358E-021
109	0.3250	8.9789E-010	1.3194E-008	1.4487E-014	7.1141E-015	-2.6902E-031	1.2628E-013	-5.3041E-021
110	0.3313	8.2719E-010	1.3671E-008	1.5564E-014	6.6819E-015	-2.9087E-031	1.1225E-013	-4.1461E-021
111	0.3375	7.6307E-010	1.4082E-008	1.6475E-014	6.1910E-015	-3.1325E-031	1.0055E-013	-3.3069E-021
112	0.3438	7.0562E-010	1.4430E-008	1.7216E-014	5.6743E-015	-3.3620E-031	9.0680E-014	-2.6871E-021
113	0.3500	6.5470E-010	1.4718E-008	1.7794E-014	5.1593E-015	-3.5969E-031	8.2306E-014	-2.2223E-021
114	0.3625	5.7174E-010	1.5120E-008	1.8511E-014	4.2177E-015	-4.0838E-031	6.9143E-014	-1.6036E-021
115	0.3750	5.0720E-010	1.5347E-008	1.8778E-014	3.4119E-015	-4.5929E-031	5.9062E-014	-1.2143E-021
116	0.3875	4.5700E-010	1.5433E-008	1.8715E-014	2.7560E-015	-5.1224E-031	5.1156E-014	-9.5781E-022
117	0.4000	4.1761E-010	1.5408E-008	1.8425E-014	2.2353E-015	-5.6640E-031	4.4832E-014	-7.8047E-022
118	0.4125	3.8627E-010	1.5299E-008	1.7987E-014	1.8265E-015	-6.2138E-031	3.9690E-014	-6.5359E-022
119	0.4250	3.6093E-010	1.5128E-008	1.7460E-014	1.5063E-015	-6.7688E-031	3.5450E-014	-5.5993E-022
120	0.4375	3.4009E-010	1.4914E-008	1.6885E-014	1.2547E-015	-7.3304E-031	3.1914E-014	-4.8903E-022
121	0.4500	3.2266E-010	1.4674E-008	1.6291E-014	1.0560E-015	-7.8578E-031	2.8935E-014	-4.3382E-022
122	0.4625	3.0782E-010	1.4425E-008	1.5699E-014	8.9797E-016	-8.4175E-031	2.6401E-014	-3.9155E-022
123	0.4750	2.9494E-010	1.4185E-008	1.5120E-014	7.7163E-016	-8.8731E-031	2.4228E-014	-3.6091E-022
124	0.4812	2.8903E-010	1.4080E-008	1.4837E-014	7.1818E-016	-9.1155E-031	2.3253E-014	-3.5777E-022
125	0.4875	2.8359E-010	1.3995E-008	1.4571E-014	6.7223E-016	-1.0722E-030	2.2378E-014	-3.4260E-022
126	0.4906	2.8113E-010	1.3964E-008	1.4451E-014	6.5283E-016	-1.0856E-030	2.1995E-014	-3.3237E-022
127	0.4938	2.7904E-010	1.3943E-008	1.4349E-014	6.3722E-016	-9.3877E-031	2.1678E-014	-3.2854E-022
128	0.4969	2.7765E-010	1.3933E-008	1.4283E-014	6.2737E-016	-9.3856E-031	2.1474E-014	-2.9191E-022
129	0.5000	2.7765E-010	1.3933E-008	1.4283E-014	6.2737E-016	-9.3856E-031	2.1474E-014	-2.9191E-022

	X(cm)	MOLE FRACTIONS: KCO3	KO3
1	0.0000	-1.1708E-027	3.3262E-013
2	0.0250	-5.7006E-026	1.5976E-011
3	0.0500	-2.7786E-024	3.3255E-011
4	0.0750	-2.7532E-024	5.0732E-011
5	0.0875	-2.3456E-024	5.9487E-011
6	0.1000	7.7490E-024	6.8253E-011
7	0.1250	7.5039E-022	8.5949E-011
8	0.1500	7.5845E-022	1.0798E-010
9	0.1625	1.3233E-021	1.5948E-010
10	0.1750	2.0328E-020	7.2913E-010
11	0.1875	-1.0937E-019	7.3009E-009
12	0.1938	-1.2230E-019	2.8555E-008
13	0.2000	-2.1204E-020	1.3143E-007
14	0.2031	-3.0549E-021	2.7731E-007
15	0.2047	-5.5205E-022	4.1438E-007
16	0.2063	-6.7583E-023	6.5274E-007
17	0.2078	-7.5278E-024	1.0555E-006
18	0.2086	-3.0509E-024	1.3416E-006
19	0.2094	-2.6094E-024	1.7247E-006
20	0.2102	-3.0376E-024	2.2327E-006
21	0.2105	-3.5676E-024	2.5435E-006
22	0.2109	-4.5061E-024	2.9085E-006
23	0.2113	-6.1503E-024	3.3370E-006
24	0.2117	-9.0273E-024	3.8391E-006

25	0.2121	-1.4064E-023	4.4248E-006
26	0.2125	-2.2895E-023	5.1019E-006
27	0.2129	-3.8474E-023	5.8735E-006
28	0.2133	-6.7554E-023	6.7340E-006
29	0.2137	-1.5383E-022	7.6648E-006
30	0.2141	-1.0945E-021	8.6320E-006
31	0.2145	-2.2409E-020	9.5878E-006
32	0.2148	-6.0504E-019	1.0478E-005
33	0.2152	-7.0156E-020	1.1255E-005
34	0.2156	2.5108E-021	1.1886E-005
35	0.2164	-9.5733E-021	1.2686E-005
36	0.2172	4.2566E-020	1.3088E-005
37	0.2180	-1.9894E-022	1.3277E-005
38	0.2188	-6.0439E-022	1.3370E-005
39	0.2195	-6.4333E-022	1.3416E-005
40	0.2203	-6.8760E-022	1.3433E-005
41	0.2211	-7.4218E-022	1.3430E-005
42	0.2219	-8.1056E-022	1.3409E-005
43	0.2234	-1.0148E-021	1.3315E-005
44	0.2250	-1.4037E-021	1.3130E-005
45	0.2258	-1.7582E-021	1.2945E-005
46	0.2266	-2.3470E-021	1.2595E-005
47	0.2270	-2.7885E-021	1.2304E-005
48	0.2273	-3.3822E-021	1.1883E-005
49	0.2277	-4.1887E-021	1.1286E-005
50	0.2281	-5.2940E-021	1.0467E-005
51	0.2283	-5.9947E-021	9.9610E-006
52	0.2285	-6.8195E-021	9.3806E-006
53	0.2287	-7.7915E-021	8.7251E-006
54	0.2289	-8.9382E-021	7.9979E-006
55	0.2291	-1.0292E-020	7.2076E-006
56	0.2293	-1.1891E-020	6.3685E-006
57	0.2295	-1.3782E-020	5.5008E-006
58	0.2297	-1.6016E-020	4.6301E-006
59	0.2299	-1.8657E-020	3.7853E-006
60	0.2301	-2.1779E-020	2.9962E-006
61	0.2303	-2.5467E-020	2.2899E-006
62	0.2305	-2.9822E-020	1.6867E-006
63	0.2307	-3.4964E-020	1.1972E-006
64	0.2309	-4.1028E-020	8.2120E-007
65	0.2311	-4.8177E-020	5.4815E-007
66	0.2313	-5.6597E-020	3.6040E-007
67	0.2314	-6.6504E-020	2.3726E-007
68	0.2316	-7.8149E-020	1.5904E-007
69	0.2318	-9.1824E-020	1.0979E-007
70	0.2320	-1.0786E-019	7.8202E-008
71	0.2322	-1.2665E-019	5.7143E-008
72	0.2324	-1.4864E-019	4.2437E-008
73	0.2328	-2.0430E-019	2.4235E-008
74	0.2336	-3.8155E-019	8.3191E-009
75	0.2344	-6.9743E-019	2.9895E-009
76	0.2352	-1.2413E-018	1.1282E-009
77	0.2359	-2.1409E-018	4.4759E-010
78	0.2367	-3.5600E-018	1.8702E-010
79	0.2375	-5.6783E-018	8.2420E-011
80	0.2383	-8.6430E-018	3.8331E-011
81	0.2391	-1.2499E-017	1.8804E-011
82	0.2398	-1.7130E-017	9.7172E-012
83	0.2406	-2.2247E-017	5.2791E-012
84	0.2414	-2.7464E-017	3.0072E-012
85	0.2422	-3.2402E-017	1.7907E-012
86	0.2430	-3.6784E-017	1.1110E-012
87	0.2437	-4.0468E-017	7.1571E-013
88	0.2445	-4.3426E-017	4.7711E-013
89	0.2453	-4.5664E-017	3.2802E-013
90	0.2461	-4.7353E-017	2.3186E-013
91	0.2469	-4.8547E-017	1.6802E-013
92	0.2484	-4.9790E-017	9.4152E-014
93	0.2500	-4.9978E-017	5.6340E-014
94	0.2516	-4.9470E-017	3.5548E-014
95	0.2531	-4.8510E-017	2.3453E-014
96	0.2562	-4.5855E-017	1.1490E-014
97	0.2594	-4.2808E-017	6.3201E-015
98	0.2625	-3.9759E-017	3.8455E-015
99	0.2656	-3.6906E-017	2.5546E-015
100	0.2688	-3.4326E-017	1.8299E-015
101	0.2750	-3.0112E-017	1.1261E-015
102	0.2812	-2.6767E-017	8.0964E-016
103	0.2875	-2.4104E-017	6.4200E-016
104	0.2938	-2.1959E-017	5.3965E-016

105	0.3000	-2.0210E-017	4.6882E-016
106	0.3063	-1.8768E-017	4.1450E-016
107	0.3125	-1.7571E-017	3.6959E-016
108	0.3188	-1.6574E-017	3.3070E-016
109	0.3250	-1.5744E-017	2.9616E-016
110	0.3313	-1.5055E-017	2.6519E-016
111	0.3375	-1.4486E-017	2.3738E-016
112	0.3438	-1.4021E-017	2.1251E-016
113	0.3500	-1.3647E-017	1.9042E-016
114	0.3625	-1.3156E-017	1.5419E-016
115	0.3750	-1.2871E-017	1.2575E-016
116	0.3875	-1.2742E-017	1.0354E-016
117	0.4000	-1.2723E-017	8.6178E-017
118	0.4125	-1.2783E-017	7.2536E-017
119	0.4250	-1.2903E-017	6.1736E-017
120	0.4375	-1.3096E-017	5.3109E-017
121	0.4500	-1.3271E-017	4.6152E-017
122	0.4625	-1.3515E-017	4.0488E-017
123	0.4750	-1.3759E-017	3.5836E-017
124	0.4812	-1.4540E-017	3.3818E-017
125	0.4875	-1.5520E-017	3.2048E-017
126	0.4906	-1.6117E-017	3.1287E-017
127	0.4938	-1.3298E-017	3.0664E-017
128	0.4969	-1.4869E-017	3.0266E-017
129	0.5000	-1.4869E-017	3.0266E-017

```
KEYWORD INPUT

!
! problem type definition
!
ENRG   ! Solve Gas Energy Equation
FLUX   ! Flux Balance for Inlet Species
FREE   ! Freely Propagating Flame
MIX   ! Use Mixture-averaged Transport
!
! physical property
!
EQUI 1.1   ! Equivalence Ratio
FLRT 1.0   ! Mass Flow Rate (g/cm2-sec)
PRES 1.0   ! Pressure (atm)
QLOS 0.0   ! Heat Flux Per Unit Length (cal/cm-sec)
TINF 298.0   ! Ambient Temperature (K)
TUNBURNT 673.0   ! Unburnt Gas Temperature (K)
!
! reactor dimension definition
!
CURV 0.5   ! Adaptive Grid Control Based On Solution Curvature
GRAD 0.1   ! Adaptive Grid Control Based On Solution Gradient
NADP 10   ! Number of Adaptive Grid Points
NPTS 6   ! Number of Uniform Grid Points
NTOT 250   ! Maximum Number of Grid Points Allowed
XEND 0.5   ! Ending Axial Position (cm)
XSTR 0.0   ! Starting Axial Position (cm)
!
! species property
!
ADD KO2 1.47E-5   ! Added Species Fraction of Total Reactant Species (mole fraction)
CPROD H2O   ! Complete-Combustion Products
CPROD N2   ! Complete-Combustion Products
FUEL H2 2.0   ! Fuel Fraction of Total Fuel Species (mole fraction)
MOLE   ! Print Mole Fractions
OXID N2 3.76   ! Oxidizer Fraction of Total Oxidizer Species (mole fraction)
OXID O2 1.0   ! Oxidizer Fraction of Total Oxidizer Species (mole fraction)
PRMN 0.0   ! Minimum for Product Estimates (mole fraction)
XIMN 0.0   ! Minimum for Estimated Intermediate Fraction (mole fraction)
!
! solver control
!
!USE_ADVANCED_TECHNIQUE   ! Advanced Solution Technique (Default)
ATIM 1.0E-9   ! Absolute Tolerance for Pseudo Timestepping
ATOL 1.0E-9   ! Absolute Tolerance
DTMN 1.0E-10   ! Minimum Pseudo Time Step (sec)
DTMX 0.01   ! Maximum Pseudo Time Step (sec)
IRET 25   ! Number Time Steps Before Increasing
ISTP 0   ! Number of Initial Pseudo Time Steps
MAXTIME 100   ! Maximum Number of Pseudo Time Stepping Operations Allowed
NDPR 100   ! Output Frequency during Integration
NJAC 20   ! Number of Iterations before Updating Jacobian
RTIM 0.0001   ! Relative Tolerance for Pseudo Timestepping
RTOL 0.0001   ! Relative Tolerance
SFLR -0.001   ! Minimum Bounds on Species Fractions
SPOS 0.0   ! Positive Value to Reset Species Fractions
SSMAXITER 100   ! Maximum Number of Iterations per Steady State Search
TIM1 100.0 1.0E-6   ! Pseudo Time Steps (Fixed Temperature) (none, sec)
TIM2 100.0 1.0E-6   ! Pseudo Time Steps (Energy Equation) (none, sec)
TJAC 20   ! Number of Transient Iterations before Updating Jacobian
TPROF   ! Automatic Estimated Temperature Profile
TRMAXITER 25   ! Maximum Number of Iterations per Pseudo Time Step
WDIF   ! Windward Differencing
!
! output control and other misc. property
!
DFAC 2.0   ! Time Step Decrement Factor
EPSS 0.001   ! Threshold for Species Sensitivity
FLT_NPOINTS 50   ! Flamelet Grid Points
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         GFAC 1.0   ! Gas Reaction Rate Multiplier
         PRNT 1   ! Print Level Control
         SIZE 100000000   ! Solution Data Block Size (bytes)
         UFAC 2.0   ! Time Step Increment Factor
         ! Number of Continuation 0   ! Continuation Count
         END
 FIRST SOLUTION ESTIMATE IS EQUILIBRIUM

 INFO...using default f(Tequilibrium) fixed temperature:   1623.52279795999

 TWOPNT:  DOUBLE PRECISION (TWO POINT BOUNDARY VALUE PROBLEM) SOLVER,
         VERSION 3.30 OF APRIL 1998 BY DR. JOSEPH F. GRCAR.

 TWOPNT:  INITIAL GUESS:

      X(cm)   T(K)            AREA(cm^2)      V(cm/s)         RHO(g/cm^3)     HDOT(cal/s/cm^3)


======
THIS IS THE FIRST CALL TO AREA
======

   1   0.0000  6.7300E+002     1.0000E+000     2.7112E+003     3.6884E-004    -1.8303E-005
   2   0.1000  6.7300E+002     1.0000E+000     2.7112E+003     3.6884E-004    -1.8303E-005
   3   0.2000  1.0791E+003     1.0000E+000     4.2122E+003     2.3740E-004     1.1252E+005
   4   0.2500  1.6235E+003     1.0000E+000     6.0839E+003     1.6437E-004     1.7842E+005
   5   0.3000  2.1679E+003     1.0000E+000     7.8117E+003     1.2801E-004     7.3859E+004
   6   0.4000  2.5740E+003     1.0000E+000     9.0166E+003     1.1091E-004     8.1360E-003
   7   0.5000  2.5740E+003     1.0000E+000     9.0166E+003     1.1091E-004     8.1360E-003

      X(cm)   MOLE FRACTIONS:
              H2              H               O               O2              OH              H2O             HO2
   1   0.0000  3.1609E-001     0.0000E+000     0.0000E+000     1.4368E-001     0.0000E+000     0.0000E+000     0.0000E+000
   2   0.1000  3.1609E-001     0.0000E+000     0.0000E+000     1.4368E-001     0.0000E+000     0.0000E+000     0.0000E+000
   3   0.2000  2.5829E-001     1.5742E-003     2.5181E-004     1.1368E-001     2.3968E-003     6.5944E-002     2.8537E-007
   4   0.2500  1.8081E-001     3.6843E-003     5.8937E-004     7.3469E-002     5.6097E-003     1.5434E-001     6.6791E-007
   5   0.3000  1.0334E-001     5.7945E-003     9.2692E-004     3.3258E-002     8.8225E-003     2.4274E-001     1.0505E-006
   6   0.4000  4.5540E-002     7.3687E-003     1.1787E-003     3.2614E-003     1.1219E-002     3.0868E-001     1.3358E-006
   7   0.5000  4.5540E-002     7.3687E-003     1.1787E-003     3.2614E-003     1.1219E-002     3.0868E-001     1.3358E-006

      X(cm)   MOLE FRACTIONS:
              H2O2            C               CH              CH2             CH2(S)          CH3             CH4
   1   0.0000  0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000
   2   0.1000  0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000
   3   0.2000  3.1185E-008     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000
   4   0.2500  7.2987E-008     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000
   5   0.3000  1.1479E-007     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000
   6   0.4000  1.4597E-007     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000
   7   0.5000  1.4597E-007     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000

      X(cm)   MOLE FRACTIONS:
              CO              CO2             HCO             CH2O            CH2OH           CH3O            CH3OH
   1   0.0000  0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000
   2   0.1000  0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000
   3   0.2000  0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000
   4   0.2500  0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000
   5   0.3000  0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000
   6   0.4000  0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000
   7   0.5000  0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000

      X(cm)   MOLE FRACTIONS:
              C2H             C2H2            C2H3            C2H4            C2H5            C2H6            HCCO
   1   0.0000  0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000
   2   0.1000  0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000
   3   0.2000  0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000
   4   0.2500  0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000
   5   0.3000  0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000
   6   0.4000  0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000
   7   0.5000  0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000     0.0000E+000

      X(cm)   MOLE FRACTIONS:
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		CH2CO	HCCOH	N	NH	NH2	NH3	NNH
1	0.0000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
2	0.1000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
3	0.2000	0.0000E+000	0.0000E+000	9.6140E-008	2.2879E-008	9.4061E-009	1.6321E-008	3.1008E-009
4	0.2500	0.0000E+000	0.0000E+000	2.2501E-007	5.3547E-008	2.2015E-008	3.8199E-008	7.2573E-009
5	0.3000	0.0000E+000	0.0000E+000	3.5389E-007	8.4215E-008	3.4623E-008	6.0078E-008	1.1414E-008
6	0.4000	0.0000E+000	0.0000E+000	4.5003E-007	1.0709E-007	4.4029E-008	7.6399E-008	1.4515E-008
7	0.5000	0.0000E+000	0.0000E+000	4.5003E-007	1.0709E-007	4.4029E-008	7.6399E-008	1.4515E-008

	X(cm)	MOLE FRACTIONS:						
		NO	NO2	N2O	HNO	CN	HCN	H2CN
1	0.0000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
2	0.1000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
3	0.2000	6.1817E-004	6.3835E-008	3.0683E-008	4.4450E-008	0.0000E+000	0.0000E+000	0.0000E+000
4	0.2500	1.4468E-003	1.4940E-007	7.1813E-008	1.0403E-007	0.0000E+000	0.0000E+000	0.0000E+000
5	0.3000	2.2755E-003	2.3497E-007	1.1294E-007	1.6362E-007	0.0000E+000	0.0000E+000	0.0000E+000
6	0.4000	2.8936E-003	2.9881E-007	1.4363E-007	2.0807E-007	0.0000E+000	0.0000E+000	0.0000E+000
7	0.5000	2.8936E-003	2.9881E-007	1.4363E-007	2.0807E-007	0.0000E+000	0.0000E+000	0.0000E+000

	X(cm)	MOLE FRACTIONS:						
		HCNN	HCNO	HOCN	HNCO	NCO	N2	AR
1	0.0000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	5.4022E-001	0.0000E+000
2	0.1000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	5.4022E-001	0.0000E+000
3	0.2000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	5.5723E-001	0.0000E+000
4	0.2500	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	5.8003E-001	0.0000E+000
5	0.3000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	6.0283E-001	0.0000E+000
6	0.4000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	6.1984E-001	0.0000E+000
7	0.5000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	6.1984E-001	0.0000E+000

	X(cm)	MOLE FRACTIONS:						
		C3H7	C3H8	CH2CHO	CH3CHO	K	KO	HKO
1	0.0000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
2	0.1000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
3	0.2000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	2.0556E-006	1.4510E-008	1.5385E-006
4	0.2500	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	4.8111E-006	3.3960E-008	3.6009E-006
5	0.3000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	7.5666E-006	5.3411E-008	5.6633E-006
6	0.4000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	9.6223E-006	6.7921E-008	7.2018E-006
7	0.5000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	9.6223E-006	6.7921E-008	7.2018E-006

	X(cm)	MOLE FRACTIONS:						
		KO2	HK	K2O	K2O2	K2CO3	K2H2O2	KHCO3
1	0.0000	1.4700E-005	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
2	0.1000	1.4700E-005	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000	0.0000E+000
3	0.2000	1.1560E-005	2.9417E-009	1.0429E-015	6.6613E-018	0.0000E+000	9.8467E-016	0.0000E+000
4	0.2500	7.3500E-006	6.8849E-009	2.4409E-015	1.5591E-017	0.0000E+000	2.3046E-015	0.0000E+000
5	0.3000	3.1404E-006	1.0828E-008	3.8390E-015	2.4520E-017	0.0000E+000	3.6245E-015	0.0000E+000
6	0.4000	6.0394E-011	1.3770E-008	4.8819E-015	3.1182E-017	0.0000E+000	4.6092E-015	0.0000E+000
7	0.5000	6.0394E-011	1.3770E-008	4.8819E-015	3.1182E-017	0.0000E+000	4.6092E-015	0.0000E+000

	X(cm)	MOLE FRACTIONS:	
		KCO3	KO3
1	0.0000	0.0000E+000	0.0000E+000
2	0.1000	0.0000E+000	0.0000E+000
3	0.2000	0.0000E+000	2.6266E-019
4	0.2500	0.0000E+000	6.1475E-019
5	0.3000	0.0000E+000	9.6684E-019
6	0.4000	0.0000E+000	1.2295E-018
7	0.5000	0.0000E+000	1.2295E-018

TWOPNT: SOLVE THE PROBLEM.

TASK	LOG10 NORM F	LOG10 COND J	REMARK
START	2.06		
SEARCH	2.00	0.00	DIVERGING
EVOLVE	-6.06	0.00	100 TIME STEPS, 8.0E-06 LAST STRIDE
SEARCH	-6.76	0.00	2 SEARCH STEPS

TWOPNT: FINAL SOLUTION:

	X(cm)	T(K)	AREA(cm^2)	V(cm/s)	RHO(g/cm^3)	HDOT(cal/s/cm^3)
1	0.0000	6.7300E+002	1.0000E+000	2.7111E+003	3.6885E-004	2.4215E-001
2	0.1000	6.7300E+002	1.0000E+000	2.7069E+003	3.6943E-004	1.7531E+001
3	0.2000	1.0791E+003	1.0000E+000	4.1433E+003	2.4135E-004	2.6455E+003
4	0.2500	1.6235E+003	1.0000E+000	6.0855E+003	1.6433E-004	2.8959E+003
5	0.3000	2.1679E+003	1.0000E+000	8.0489E+003	1.2424E-004	9.3481E+002
6	0.4000	2.5740E+003	1.0000E+000	9.4679E+003	1.0562E-004	4.8010E+002
7	0.5000	2.5740E+003	1.0000E+000	9.4679E+003	1.0562E-004	4.8010E+002

	X(cm)	MOLE FRACTIONS:						
		H2	H	O	O2	OH	H2O	HO2
1	0.0000	3.1607E-001	5.7347E-007	2.9306E-009	1.4368E-001	2.7557E-008	4.6598E-006	6.3979E-007
2	0.1000	3.1443E-001	2.6601E-005	4.7691E-007	1.4334E-001	4.5651E-006	9.4214E-004	1.5907E-004
3	0.2000	2.1428E-001	1.3212E-002	1.3778E-003	9.6223E-002	1.0310E-003	1.0709E-001	1.1827E-004
4	0.2500	8.3101E-002	6.1914E-002	1.0109E-002	3.4683E-002	1.0572E-002	2.1906E-001	2.6853E-005
5	0.3000	7.0070E-002	5.2674E-002	1.2785E-002	2.0894E-002	2.3627E-002	2.3381E-001	8.4608E-006
6	0.4000	7.0106E-002	3.9748E-002	1.1285E-002	1.6380E-002	3.0591E-002	2.4023E-001	5.2970E-006
7	0.5000	7.0106E-002	3.9748E-002	1.1285E-002	1.6380E-002	3.0591E-002	2.4023E-001	5.2970E-006

	X(cm)	MOLE FRACTIONS:						
		H2O2	C	CH	CH2	CH2(S)	CH3	CH4
1	0.0000	3.2702E-008	4.2172E-042	4.2680E-042	3.5925E-040	1.1410E-041	7.4766E-037	1.9262E-034
2	0.1000	8.1810E-006	7.3643E-040	6.5228E-040	8.1018E-038	2.5731E-039	1.7217E-034	4.4465E-032
3	0.2000	3.7152E-006	4.0132E-034	7.8612E-034	4.6351E-033	1.1766E-033	2.2161E-031	8.8966E-030
4	0.2500	2.0712E-006	2.3916E-031	5.2801E-032	7.7905E-032	5.6487E-032	1.9821E-030	3.0811E-030
5	0.3000	3.9416E-007	2.6731E-031	7.2809E-032	9.0184E-032	4.5279E-032	9.3542E-031	2.1515E-031
6	0.4000	2.4535E-007	2.5830E-030	5.4446E-031	4.4478E-031	6.1619E-032	9.6437E-031	1.1310E-031
7	0.5000	2.4535E-007	2.5830E-030	5.4446E-031	4.4478E-031	6.1619E-032	9.6437E-031	1.1310E-031

	X(cm)	MOLE FRACTIONS:						
		CO	CO2	HCO	CH2O	CH2OH	CH3O	CH3OH
1	0.0000	1.3077E-028	3.4019E-037	6.0312E-035	2.2728E-033	8.4661E-039	2.1791E-037	2.8224E-036
2	0.1000	3.2833E-026	1.0574E-034	1.7946E-032	6.8141E-031	2.5766E-036	6.6321E-035	8.6307E-034
3	0.2000	3.5189E-022	9.6948E-024	4.0773E-027	1.8733E-028	1.6278E-031	1.0976E-032	6.2189E-032
4	0.2500	2.7250E-020	1.5160E-019	3.5513E-025	1.6996E-027	1.1558E-030	2.1631E-032	3.7663E-032
5	0.3000	2.8366E-019	5.3518E-019	1.6128E-024	4.5792E-027	8.1503E-031	1.2414E-032	1.1814E-032
6	0.4000	5.7763E-019	4.5249E-019	1.7805E-024	1.0270E-026	6.7681E-031	1.1168E-032	1.4078E-032
7	0.5000	5.7763E-019	4.5249E-019	1.7805E-024	1.0270E-026	6.7681E-031	1.1168E-032	1.4078E-032

	X(cm)	MOLE FRACTIONS:						
		C2H	C2H2	C2H3	C2H4	C2H5	C2H6	HCCO
1	0.0000	4.5267E-065	5.8138E-057	6.4921E-061	1.0837E-057	2.5812E-060	4.9893E-059	3.9069E-057
2	0.1000	1.3460E-062	1.7451E-054	1.9661E-058	3.3058E-055	8.5444E-058	1.6640E-056	7.8025E-055
3	0.2000	8.5929E-057	4.6304E-052	1.7950E-053	8.9394E-053	2.7884E-055	4.4879E-054	2.1223E-050
4	0.2500	1.5615E-052	4.8681E-050	6.1263E-052	6.6401E-052	5.2972E-055	8.2871E-055	4.9032E-048
5	0.3000	4.9160E-050	2.2010E-048	1.3133E-051	4.0444E-052	7.3452E-056	1.6554E-056	8.8272E-047
6	0.4000	2.7504E-048	5.9261E-047	7.9535E-051	1.6128E-051	1.1174E-055	4.0000E-057	1.1996E-045
7	0.5000	2.7504E-048	5.9261E-047	7.9535E-051	1.6128E-051	1.1174E-055	4.0000E-057	1.1996E-045

	X(cm)	MOLE FRACTIONS:						
		CH2CO	HCCOH	N	NH	NH2	NH3	NNH
1	0.0000	4.2338E-054	1.9501E-060	3.4786E-014	1.5707E-014	5.3417E-016	1.8101E-015	6.9702E-015
2	0.1000	1.4800E-051	6.8168E-058	6.3739E-012	2.4281E-012	8.4195E-014	3.8613E-013	1.7861E-012
3	0.2000	5.6491E-049	2.4658E-055	5.4629E-009	1.1311E-009	1.9157E-011	4.8742E-011	5.3310E-009
4	0.2500	2.5442E-047	3.6603E-052	7.9036E-008	1.6436E-008	2.0673E-010	9.3263E-011	5.9832E-008
5	0.3000	1.0055E-046	1.5673E-050	8.2468E-008	2.4073E-008	9.1234E-010	3.6648E-010	7.8294E-008
6	0.4000	7.1248E-046	7.2700E-049	3.1853E-007	3.5508E-008	3.1838E-009	1.5514E-009	7.2502E-008
7	0.5000	7.1248E-046	7.2700E-049	3.1853E-007	3.5508E-008	3.1838E-009	1.5514E-009	7.2502E-008

	X(cm)	MOLE FRACTIONS:						
		NO	NO2	N2O	HNO	CN	HCN	H2CN
1	0.0000	5.8858E-012	6.0014E-013	7.3772E-014	7.7194E-015	1.0443E-044	1.7581E-037	1.3700E-039
2	0.1000	1.4879E-009	1.7099E-010	2.3211E-011	1.9272E-012	2.6624E-042	5.3007E-035	4.1658E-037
3	0.2000	3.5989E-007	1.1312E-010	6.3770E-009	2.3173E-010	5.2757E-037	1.3849E-032	8.2309E-035
4	0.2500	5.5717E-006	4.4470E-010	3.6339E-008	1.6114E-009	4.9708E-033	1.0767E-030	4.7401E-034
5	0.3000	1.2330E-005	7.8671E-010	5.1668E-008	2.3272E-009	1.2009E-030	6.0087E-029	2.7018E-033
6	0.4000	4.9070E-005	4.4016E-009	9.9741E-008	5.4549E-009	2.7167E-029	8.5113E-028	1.0572E-032
7	0.5000	4.9070E-005	4.4016E-009	9.9741E-008	5.4549E-009	2.7167E-029	8.5113E-028	1.0572E-032

	X(cm)	MOLE FRACTIONS:						
		HCNN	HCNO	HOCN	HNCO	NCO	N2	AR

1	0.0000	3.2023E-043	1.0582E-042	1.6821E-041	1.5859E-036	4.9818E-039	5.4024E-001	0.0000E+000
2	0.1000	6.3953E-041	3.3162E-040	5.2711E-039	4.9697E-034	1.5545E-036	5.4108E-001	0.0000E+000
3	0.2000	6.3325E-036	9.5003E-038	1.5091E-036	1.3573E-031	1.4071E-033	5.6665E-001	0.0000E+000
4	0.2500	3.4961E-035	4.1949E-036	2.1065E-033	7.9659E-030	5.3918E-031	5.8051E-001	0.0000E+000
5	0.3000	1.3757E-035	2.7573E-035	2.8439E-031	1.3506E-028	3.1312E-029	5.8611E-001	0.0000E+000
6	0.4000	5.1198E-035	2.2718E-033	7.6028E-030	1.2951E-027	3.4210E-028	5.9159E-001	0.0000E+000
7	0.5000	5.1198E-035	2.2718E-033	7.6028E-030	1.2951E-027	3.4210E-028	5.9159E-001	0.0000E+000

	X(cm)	MOLE FRACTIONS:						
		C3H7	C3H8	CH2CHO	CH3CHO	K	KO	HKO
1	0.0000	2.2595E-086	8.6620E-085	2.2612E-055	2.5970E-056	5.8084E-015	1.5213E-015	5.6422E-010
2	0.1000	9.6023E-084	3.6959E-082	7.9382E-053	9.1545E-054	2.3723E-012	5.2446E-013	2.7862E-007
3	0.2000	1.3866E-080	1.3232E-079	3.0137E-050	7.5055E-052	6.7376E-009	1.7123E-009	1.5348E-005
4	0.2500	3.6237E-081	6.0136E-081	1.3267E-049	8.6487E-052	7.2911E-009	2.9558E-009	1.5776E-005
5	0.3000	1.2050E-082	3.8059E-083	5.0990E-050	5.8208E-052	4.3616E-007	1.1764E-007	1.5373E-005
6	0.4000	2.0955E-082	5.2579E-084	7.6787E-050	1.4706E-051	5.1788E-006	3.0734E-007	1.0570E-005
7	0.5000	2.0955E-082	5.2579E-084	7.6787E-050	1.4706E-051	5.1788E-006	3.0734E-007	1.0570E-005

	X(cm)	MOLE FRACTIONS:						
		KO2	HK	K2O	K2O2	K2CO3	K2H2O2	KHCO3
1	0.0000	1.4677E-005	9.7634E-014	2.9498E-017	3.3462E-018	1.3773E-042	7.3829E-012	1.8225E-021
2	0.1000	2.3900E-006	2.5502E-011	1.6233E-014	1.8704E-015	7.8495E-040	4.1338E-009	1.0093E-018
3	0.2000	2.2381E-008	1.6304E-008	7.3357E-013	7.7367E-013	9.2327E-034	5.1297E-009	1.0518E-018
4	0.2500	2.7844E-009	6.5490E-009	1.3969E-014	3.6411E-014	2.1758E-033	3.9696E-012	6.1805E-020
5	0.3000	9.5902E-010	2.2778E-008	1.1044E-014	4.9965E-015	4.5109E-033	1.0831E-013	1.6553E-022
6	0.4000	2.5738E-010	3.9503E-008	1.1889E-014	6.3853E-016	4.9037E-033	9.9287E-015	3.7099E-024
7	0.5000	2.5738E-010	3.9503E-008	1.1889E-014	6.3853E-016	4.9037E-033	9.9287E-015	3.7099E-024

	X(cm)	MOLE FRACTIONS:	
		KCO3	KO3
1	0.0000	5.4409E-024	2.2082E-008
2	0.1000	3.0100E-021	1.2048E-005
3	0.2000	9.0142E-021	1.0965E-008
4	0.2500	8.5453E-019	3.0115E-014
5	0.3000	2.8479E-019	2.3712E-016
6	0.4000	8.2948E-020	2.8060E-017
7	0.5000	8.2948E-020	2.8060E-017

TWOPNT: SUCCESS. PROBLEM SOLVED.

PREMIX: FINISHED FIXED TEMPERATURE CASE,ADDING THE ENERGY EQUATION.

TWOPNT: DOUBLE PRECISION (TWO POINT BOUNDARY VALUE PROBLEM) SOLVER,
VERSION 3.30 OF APRIL 1998 BY DR. JOSEPH F. GRCAR.

TWOPNT: INITIAL GUESS:

	X(cm)	T(K)	AREA(cm^2)	V(cm/s)	RHO(g/cm^3)	HDOT(cal/s/cm^3)
1	0.0000	6.7300E+002	1.0000E+000	2.7111E+003	3.6885E-004	2.4215E-001
2	0.1000	6.7300E+002	1.0000E+000	2.7069E+003	3.6943E-004	1.7531E+001
3	0.2000	1.0791E+003	1.0000E+000	4.1433E+003	2.4135E-004	2.6455E+003
4	0.2500	1.6235E+003	1.0000E+000	6.0855E+003	1.6433E-004	2.8959E+003
5	0.3000	2.1679E+003	1.0000E+000	8.0489E+003	1.2424E-004	9.3481E+002
6	0.4000	2.5740E+003	1.0000E+000	9.4679E+003	1.0562E-004	4.8010E+002
7	0.5000	2.5740E+003	1.0000E+000	9.4679E+003	1.0562E-004	4.8010E+002

	X(cm)	MOLE FRACTIONS:						
		H2	H	O	O2	OH	H2O	HO2
1	0.0000	3.1607E-001	5.7347E-007	2.9306E-009	1.4368E-001	2.7557E-008	4.6598E-006	6.3979E-007
2	0.1000	3.1443E-001	2.6601E-005	4.7691E-007	1.4334E-001	4.5651E-006	9.4214E-004	1.5907E-004
3	0.2000	2.1428E-001	1.3212E-002	1.3778E-003	9.6223E-002	1.0310E-003	1.0709E-001	1.1827E-004
4	0.2500	8.3101E-002	6.1914E-002	1.0109E-002	3.4683E-002	1.0572E-002	2.1906E-001	2.6853E-005
5	0.3000	7.0070E-002	5.2674E-002	1.2785E-002	2.0894E-002	2.3627E-002	2.3381E-001	8.4608E-006
6	0.4000	7.0106E-002	3.9748E-002	1.1285E-002	1.6380E-002	3.0591E-002	2.4023E-001	5.2970E-006
7	0.5000	7.0106E-002	3.9748E-002	1.1285E-002	1.6380E-002	3.0591E-002	2.4023E-001	5.2970E-006

	X(cm)	MOLE FRACTIONS:						
		H2O2	C	CH	CH2	CH2(S)	CH3	CH4
1	0.0000	3.2702E-008	4.2172E-042	4.2680E-042	3.5925E-040	1.1410E-041	7.4766E-037	1.9262E-034
2	0.1000	8.1810E-006	7.3643E-040	6.5228E-040	8.1018E-038	2.5731E-039	1.7217E-034	4.4465E-032
3	0.2000	3.7152E-006	4.0132E-034	7.8612E-034	4.6351E-033	1.1766E-033	2.2161E-031	8.8966E-030

4	0.2500	2.0712E-006	2.3916E-031	5.2801E-032	7.7905E-032	5.6487E-032	1.9821E-030	3.0811E-030
5	0.3000	3.9416E-007	2.6731E-031	7.2809E-032	9.0184E-032	4.5279E-032	9.3542E-031	2.1515E-031
6	0.4000	2.4535E-007	2.5830E-030	5.4446E-031	4.4478E-031	6.1619E-032	9.6437E-031	1.1310E-031
7	0.5000	2.4535E-007	2.5830E-030	5.4446E-031	4.4478E-031	6.1619E-032	9.6437E-031	1.1310E-031

	X(cm)	MOLE FRACTIONS:						
		CO	CO2	HCO	CH2O	CH2OH	CH3O	CH3OH
1	0.0000	1.3077E-028	3.4019E-037	6.0312E-035	2.2728E-033	8.4661E-039	2.1791E-037	2.8224E-036
2	0.1000	3.2833E-026	1.0574E-034	1.7946E-032	6.8141E-031	2.5766E-036	6.6321E-035	8.6307E-034
3	0.2000	3.5189E-022	9.6948E-024	4.0773E-027	1.8733E-028	1.6278E-031	1.0976E-032	6.2189E-032
4	0.2500	2.7250E-020	1.5160E-019	3.5513E-025	1.6996E-027	1.1558E-030	2.1631E-032	3.7663E-032
5	0.3000	2.8366E-019	5.3518E-019	1.6128E-024	4.5792E-027	8.1503E-031	1.2414E-032	1.1814E-032
6	0.4000	5.7763E-019	4.5249E-019	1.7805E-024	1.0270E-026	6.7681E-031	1.1168E-032	1.4078E-032
7	0.5000	5.7763E-019	4.5249E-019	1.7805E-024	1.0270E-026	6.7681E-031	1.1168E-032	1.4078E-032

	X(cm)	MOLE FRACTIONS:						
		C2H	C2H2	C2H3	C2H4	C2H5	C2H6	HCCO
1	0.0000	4.5267E-065	5.8138E-057	6.4921E-061	1.0837E-057	2.5812E-060	4.9893E-059	3.9069E-057
2	0.1000	1.3460E-062	1.7451E-054	1.9661E-058	3.3058E-055	8.5444E-058	1.6640E-056	7.8025E-055
3	0.2000	8.5929E-057	4.6304E-052	1.7950E-053	8.9394E-053	2.7884E-055	4.4879E-054	2.1223E-050
4	0.2500	1.5615E-052	4.8681E-050	6.1263E-052	6.6401E-052	5.2972E-055	8.2871E-055	4.9032E-048
5	0.3000	4.9160E-050	2.2010E-048	1.3133E-051	4.0444E-052	7.3452E-056	1.6554E-056	8.8272E-047
6	0.4000	2.7504E-048	5.9261E-047	7.9535E-051	1.6128E-051	1.1174E-055	4.0000E-057	1.1996E-045
7	0.5000	2.7504E-048	5.9261E-047	7.9535E-051	1.6128E-051	1.1174E-055	4.0000E-057	1.1996E-045

	X(cm)	MOLE FRACTIONS:						
		CH2CO	HCCOH	N	NH	NH2	NH3	NNH
1	0.0000	4.2338E-054	1.9501E-060	3.4786E-014	1.5707E-014	5.3417E-016	1.8101E-015	6.9702E-015
2	0.1000	1.4800E-051	6.8168E-058	6.3739E-012	2.4281E-012	8.4195E-014	3.8613E-013	1.7861E-012
3	0.2000	5.6491E-049	2.4658E-055	5.4629E-009	1.1311E-009	1.9157E-011	4.8742E-011	5.3310E-009
4	0.2500	2.5442E-047	3.6603E-052	7.9036E-008	1.6436E-008	2.0673E-010	9.3263E-011	5.9832E-008
5	0.3000	1.0055E-046	1.5673E-050	8.2468E-008	2.4073E-008	9.1234E-010	3.6648E-010	7.8294E-008
6	0.4000	7.1248E-046	7.2700E-049	3.1853E-007	3.5508E-008	3.1838E-009	1.5514E-009	7.2502E-008
7	0.5000	7.1248E-046	7.2700E-049	3.1853E-007	3.5508E-008	3.1838E-009	1.5514E-009	7.2502E-008

	X(cm)	MOLE FRACTIONS:						
		NO	NO2	N2O	HNO	CN	HCN	H2CN
1	0.0000	5.8858E-012	6.0014E-013	7.3772E-014	7.7194E-015	1.0443E-044	1.7581E-037	1.3700E-039
2	0.1000	1.4879E-009	1.7099E-010	2.3211E-011	1.9272E-012	2.6624E-042	5.3007E-035	4.1658E-037
3	0.2000	3.5989E-007	1.1312E-010	6.3770E-009	2.3173E-010	5.2757E-037	1.3849E-032	8.2309E-035
4	0.2500	5.5717E-006	4.4470E-010	3.6339E-008	1.6114E-009	4.9708E-033	1.0767E-030	4.7401E-034
5	0.3000	1.2330E-005	7.8671E-010	5.1668E-008	2.3272E-009	1.2009E-030	6.0087E-029	2.7018E-033
6	0.4000	4.9070E-005	4.4016E-009	9.9741E-008	5.4549E-009	2.7167E-029	8.5113E-028	1.0572E-032
7	0.5000	4.9070E-005	4.4016E-009	9.9741E-008	5.4549E-009	2.7167E-029	8.5113E-028	1.0572E-032

	X(cm)	MOLE FRACTIONS:						
		HCNN	HCNO	HOCN	HNCO	NCO	N2	AR
1	0.0000	3.2023E-043	1.0582E-042	1.6821E-041	1.5859E-036	4.9818E-039	5.4024E-001	0.0000E+000
2	0.1000	6.3953E-041	3.3162E-040	5.2711E-039	4.9697E-034	1.5545E-036	5.4108E-001	0.0000E+000
3	0.2000	6.3325E-036	9.5003E-038	1.5091E-036	1.3573E-031	1.4071E-033	5.6665E-001	0.0000E+000
4	0.2500	3.4961E-035	4.1949E-036	2.1065E-033	7.9659E-030	5.3918E-031	5.8051E-001	0.0000E+000
5	0.3000	1.3757E-035	2.7573E-035	2.8439E-031	1.3506E-028	3.1312E-029	5.8611E-001	0.0000E+000
6	0.4000	5.1198E-035	2.2718E-033	7.6028E-030	1.2951E-027	3.4210E-028	5.9159E-001	0.0000E+000
7	0.5000	5.1198E-035	2.2718E-033	7.6028E-030	1.2951E-027	3.4210E-028	5.9159E-001	0.0000E+000

	X(cm)	MOLE FRACTIONS:						
		C3H7	C3H8	CH2CHO	CH3CHO	K	KO	HKO
1	0.0000	2.2595E-086	8.6620E-085	2.2612E-055	2.5970E-056	5.8084E-015	1.5213E-015	5.6422E-010
2	0.1000	9.6023E-084	3.6959E-082	7.9382E-053	9.1545E-054	2.3723E-012	5.2446E-013	2.7862E-007
3	0.2000	1.3866E-080	1.3232E-079	3.0137E-050	7.5055E-052	6.7376E-009	1.7123E-009	1.5348E-005
4	0.2500	3.6237E-081	6.0136E-081	1.3267E-049	8.6487E-052	7.2911E-009	2.9558E-009	1.5776E-005
5	0.3000	1.2050E-082	3.8059E-083	5.0990E-050	5.8208E-052	4.3616E-007	1.1764E-007	1.5373E-005
6	0.4000	2.0955E-082	5.2579E-084	7.6787E-050	1.4706E-051	5.1788E-006	3.0734E-007	1.0570E-005
7	0.5000	2.0955E-082	5.2579E-084	7.6787E-050	1.4706E-051	5.1788E-006	3.0734E-007	1.0570E-005

	X(cm)	MOLE FRACTIONS:						
		KO2	HK	K2O	K2O2	K2CO3	K2H2O2	KHCO3
1	0.0000	1.4677E-005	9.7634E-014	2.9498E-017	3.3462E-018	1.3773E-042	7.3829E-012	1.8225E-021
2	0.1000	2.3900E-006	2.5502E-011	1.6233E-014	1.8704E-015	7.8495E-040	4.1338E-009	1.0093E-018
3	0.2000	2.2381E-008	1.6304E-008	7.3357E-013	7.7367E-013	9.2327E-034	5.1297E-009	1.0518E-018
4	0.2500	2.7844E-009	6.5490E-009	1.3969E-014	3.6411E-014	2.1758E-033	3.9696E-012	6.1805E-020

5	0.3000	9.5902E-010	2.2778E-008	1.1044E-014	4.9965E-015	4.5109E-033	1.0831E-013	1.6553E-022
6	0.4000	2.5738E-010	3.9503E-008	1.1889E-014	6.3853E-016	4.9037E-033	9.9287E-015	3.7099E-024
7	0.5000	2.5738E-010	3.9503E-008	1.1889E-014	6.3853E-016	4.9037E-033	9.9287E-015	3.7099E-024

	X(cm)	MOLE FRACTIONS: KCO3	KO3
1	0.0000	5.4409E-024	2.2082E-008
2	0.1000	3.0100E-021	1.2048E-005
3	0.2000	9.0142E-021	1.0965E-008
4	0.2500	8.5453E-019	3.0115E-014
5	0.3000	2.8479E-019	2.3712E-016
6	0.4000	8.2948E-020	2.8060E-017
7	0.5000	8.2948E-020	2.8060E-017

TWOPNT: SOLVE THE PROBLEM.

TASK	LOG10 NORM F	LOG10 COND J	REMARK
START	3.94		7 GRID POINTS
SEARCH	4.85	0.00	DIVERGING
EVOLVE	-4.95	0.00	100 TIME STEPS, 8.0E-06 LAST STRIDE
SEARCH	-6.25	0.00	1 SEARCH STEP
REFINE	-6.25		1.00 AND 1.00 RATIOS, 13 GRID POINTS
SEARCH	3.76	0.00	GOING OUT OF BOUNDS
EVOLVE	-5.19	0.00	100 TIME STEPS, 8.0E-06 LAST STRIDE
SEARCH	-6.57	0.00	1 SEARCH STEP
REFINE	-6.57		1.00 AND 1.00 RATIOS, 23 GRID POINTS
SEARCH	-3.33	0.00	21 SEARCH STEPS
REFINE	-3.33		1.00 AND 1.00 RATIOS, 33 GRID POINTS
SEARCH	2.93	0.00	DIVERGING
EVOLVE	2.13	0.00	100 TIME STEPS, 2.0E-06 LAST STRIDE
SEARCH	-3.18	0.00	35 SEARCH STEPS
REFINE	-3.18		1.00 AND 1.00 RATIOS, 43 GRID POINTS
SEARCH	-4.85	0.00	17 SEARCH STEPS
REFINE	-4.85		1.00 AND 0.98 RATIOS, 53 GRID POINTS
SEARCH	-5.14	0.00	25 SEARCH STEPS
REFINE	-5.14		1.00 AND 1.00 RATIOS, 63 GRID POINTS
SEARCH	-3.29	0.00	12 SEARCH STEPS
REFINE	-3.29		1.00 AND 1.00 RATIOS, 73 GRID POINTS
SEARCH	1.86	0.00	DIVERGING
EVOLVE	1.39	0.00	100 TIME STEPS, 1.0E-06 LAST STRIDE
SEARCH	-5.84	0.00	21 SEARCH STEPS
REFINE	-5.84		0.30 AND 0.92 RATIOS, 83 GRID POINTS
SEARCH	-3.46	0.00	9 SEARCH STEPS
REFINE	-3.46		0.28 AND 0.92 RATIOS, 93 GRID POINTS
SEARCH	-3.66	0.00	9 SEARCH STEPS
REFINE	-3.66		0.31 AND 0.92 RATIOS, 103 GRID POINTS
SEARCH	-3.23	0.00	8 SEARCH STEPS
REFINE	-3.23		0.20 AND 0.92 RATIOS, 113 GRID POINTS
SEARCH	-2.99	0.00	8 SEARCH STEPS
REFINE	-2.99		0.20 AND 0.92 RATIOS, 123 GRID POINTS
SEARCH	-3.03	0.00	8 SEARCH STEPS
REFINE	-3.03		0.19 AND 0.92 RATIOS, 133 GRID POINTS
SEARCH	-2.65	0.00	6 SEARCH STEPS
REFINE	-2.65		0.13 AND 0.76 RATIOS, 135 GRID POINTS
SEARCH	-3.54	0.00	4 SEARCH STEPS

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          REFINE    -3.54          0.10 AND 0.64 RATIOS, 137 GRID POINTS
          SEARCH    -5.29    0.00  4 SEARCH STEPS

          REFINE    -5.29          0.10 AND 0.50 RATIOS, 139 GRID POINTS
          SEARCH    -4.42    0.00  3 SEARCH STEPS

          REFINE    -4.42          0.10 AND 0.35 RATIOS

TWOPNT:  FINAL SOLUTION:
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	X(cm)	T(K)	AREA(cm^2)	V(cm/s)	RHO(g/cm^3)	HDOT(cal/s/cm^3)
1	0.0000	6.7300E+002	1.0000E+000	9.7192E+002	3.6884E-004	-1.2776E-005
2	0.0500	6.7300E+002	1.0000E+000	9.7192E+002	3.6884E-004	4.3248E-005
3	0.0750	6.7300E+002	1.0000E+000	9.7192E+002	3.6884E-004	4.6038E-005
4	0.1000	6.7300E+002	1.0000E+000	9.7192E+002	3.6884E-004	4.6443E-005
5	0.1125	6.7300E+002	1.0000E+000	9.7192E+002	3.6884E-004	4.6537E-005
6	0.1250	6.7300E+002	1.0000E+000	9.7192E+002	3.6884E-004	4.6611E-005
7	0.1313	6.7300E+002	1.0000E+000	9.7192E+002	3.6884E-004	4.6654E-005
8	0.1344	6.7300E+002	1.0000E+000	9.7192E+002	3.6884E-004	4.6686E-005
9	0.1375	6.7300E+002	1.0000E+000	9.7192E+002	3.6884E-004	4.6741E-005
10	0.1383	6.7300E+002	1.0000E+000	9.7192E+002	3.6884E-004	4.6764E-005
11	0.1391	6.7300E+002	1.0000E+000	9.7192E+002	3.6884E-004	4.6793E-005
12	0.1398	6.7300E+002	1.0000E+000	9.7192E+002	3.6884E-004	4.6830E-005
13	0.1406	6.7300E+002	1.0000E+000	9.7192E+002	3.6884E-004	4.6876E-005
14	0.1414	6.7300E+002	1.0000E+000	9.7192E+002	3.6884E-004	4.6934E-005
15	0.1422	6.7300E+002	1.0000E+000	9.7192E+002	3.6884E-004	4.7010E-005
16	0.1438	6.7300E+002	1.0000E+000	9.7192E+002	3.6884E-004	4.7225E-005
17	0.1469	6.7300E+002	1.0000E+000	9.7192E+002	3.6884E-004	4.8069E-005
18	0.1500	6.7300E+002	1.0000E+000	9.7192E+002	3.6884E-004	5.0221E-005
19	0.1625	6.7300E+002	1.0000E+000	9.7192E+002	3.6884E-004	9.2781E-005
20	0.1656	6.7300E+002	1.0000E+000	9.7192E+002	3.6884E-004	1.9328E-004
21	0.1688	6.7300E+002	1.0000E+000	9.7192E+002	3.6884E-004	4.4233E-004
22	0.1750	6.7300E+002	1.0000E+000	9.7192E+002	3.6884E-004	2.1104E-003
23	0.1875	6.7302E+002	1.0000E+000	9.7192E+002	3.6884E-004	2.7104E-002
24	0.1938	6.7306E+002	1.0000E+000	9.7195E+002	3.6883E-004	1.6813E-001
25	0.2000	6.7323E+002	1.0000E+000	9.7208E+002	3.6878E-004	9.2938E-001
26	0.2031	6.7345E+002	1.0000E+000	9.7230E+002	3.6870E-004	2.6094E+000
27	0.2047	6.7367E+002	1.0000E+000	9.7251E+002	3.6862E-004	4.5194E+000
28	0.2063	6.7401E+002	1.0000E+000	9.7287E+002	3.6848E-004	7.8798E+000
29	0.2078	6.7455E+002	1.0000E+000	9.7346E+002	3.6826E-004	1.3862E+001
30	0.2086	6.7493E+002	1.0000E+000	9.7390E+002	3.6809E-004	1.8561E+001
31	0.2094	6.7542E+002	1.0000E+000	9.7447E+002	3.6788E-004	2.4950E+001
32	0.2102	6.7606E+002	1.0000E+000	9.7521E+002	3.6760E-004	3.3624E+001
33	0.2109	6.7687E+002	1.0000E+000	9.7617E+002	3.6723E-004	4.5358E+001
34	0.2113	6.7735E+002	1.0000E+000	9.7676E+002	3.6701E-004	5.2725E+001
35	0.2117	6.7790E+002	1.0000E+000	9.7743E+002	3.6676E-004	6.1300E+001
36	0.2121	6.7853E+002	1.0000E+000	9.7819E+002	3.6648E-004	7.1258E+001
37	0.2125	6.7923E+002	1.0000E+000	9.7906E+002	3.6615E-004	8.2789E+001
38	0.2129	6.8003E+002	1.0000E+000	9.8006E+002	3.6578E-004	9.6096E+001
39	0.2133	6.8094E+002	1.0000E+000	9.8118E+002	3.6536E-004	1.1138E+002
40	0.2137	6.8195E+002	1.0000E+000	9.8246E+002	3.6489E-004	1.2884E+002
41	0.2141	6.8309E+002	1.0000E+000	9.8390E+002	3.6435E-004	1.4866E+002
42	0.2145	6.8437E+002	1.0000E+000	9.8552E+002	3.6375E-004	1.7100E+002
43	0.2148	6.8581E+002	1.0000E+000	9.8735E+002	3.6308E-004	1.9606E+002
44	0.2156	6.8917E+002	1.0000E+000	9.9167E+002	3.6149E-004	2.5483E+002
45	0.2164	6.9326E+002	1.0000E+000	9.9695E+002	3.5958E-004	3.2677E+002
46	0.2172	6.9818E+002	1.0000E+000	1.0033E+003	3.5729E-004	4.1384E+002
47	0.2180	7.0404E+002	1.0000E+000	1.0110E+003	3.5459E-004	5.1740E+002
48	0.2188	7.1094E+002	1.0000E+000	1.0200E+003	3.5145E-004	6.3828E+002
49	0.2195	7.1901E+002	1.0000E+000	1.0306E+003	3.4785E-004	7.7695E+002
50	0.2203	7.2833E+002	1.0000E+000	1.0428E+003	3.4377E-004	9.3350E+002
51	0.2211	7.3902E+002	1.0000E+000	1.0568E+003	3.3920E-004	1.1075E+003
52	0.2219	7.5115E+002	1.0000E+000	1.0728E+003	3.3417E-004	1.2980E+003
53	0.2234	7.7994E+002	1.0000E+000	1.1105E+003	3.2280E-004	1.7140E+003
54	0.2250	8.1415E+002	1.0000E+000	1.1552E+003	3.1033E-004	2.1658E+003
55	0.2258	8.3320E+002	1.0000E+000	1.1799E+003	3.0383E-004	2.4031E+003
56	0.2266	8.5370E+002	1.0000E+000	1.2064E+003	2.9716E-004	2.6447E+003
57	0.2270	8.6447E+002	1.0000E+000	1.2202E+003	2.9378E-004	2.7674E+003
58	0.2273	8.7563E+002	1.0000E+000	1.2346E+003	2.9037E-004	2.8915E+003
59	0.2277	8.8715E+002	1.0000E+000	1.2493E+003	2.8694E-004	3.0173E+003

60	0.2279	8.9305E+002	1.0000E+000	1.2569E+003	2.8522E-004	3.0811E+003
61	0.2281	8.9904E+002	1.0000E+000	1.2645E+003	2.8349E-004	3.1457E+003
62	0.2283	9.0513E+002	1.0000E+000	1.2723E+003	2.8176E-004	3.2111E+003
63	0.2285	9.1131E+002	1.0000E+000	1.2802E+003	2.8002E-004	3.2774E+003
64	0.2287	9.1758E+002	1.0000E+000	1.2882E+003	2.7828E-004	3.3446E+003
65	0.2289	9.2394E+002	1.0000E+000	1.2963E+003	2.7654E-004	3.4129E+003
66	0.2291	9.3039E+002	1.0000E+000	1.3045E+003	2.7480E-004	3.4820E+003
67	0.2293	9.3693E+002	1.0000E+000	1.3128E+003	2.7306E-004	3.5518E+003
68	0.2295	9.4355E+002	1.0000E+000	1.3213E+003	2.7132E-004	3.6220E+003
69	0.2297	9.5026E+002	1.0000E+000	1.3298E+003	2.6958E-004	3.6923E+003
70	0.2299	9.5705E+002	1.0000E+000	1.3384E+003	2.6785E-004	3.7623E+003
71	0.2301	9.6391E+002	1.0000E+000	1.3471E+003	2.6612E-004	3.8314E+003
72	0.2303	9.7086E+002	1.0000E+000	1.3559E+003	2.6439E-004	3.8992E+003
73	0.2305	9.7788E+002	1.0000E+000	1.3648E+003	2.6267E-004	3.9655E+003
74	0.2307	9.8496E+002	1.0000E+000	1.3737E+003	2.6096E-004	4.0300E+003
75	0.2309	9.9212E+002	1.0000E+000	1.3828E+003	2.5925E-004	4.0929E+003
76	0.2311	9.9935E+002	1.0000E+000	1.3919E+003	2.5755E-004	4.1544E+003
77	0.2313	1.0066E+003	1.0000E+000	1.4011E+003	2.5586E-004	4.2146E+003
78	0.2314	1.0140E+003	1.0000E+000	1.4104E+003	2.5417E-004	4.2740E+003
79	0.2316	1.0214E+003	1.0000E+000	1.4197E+003	2.5250E-004	4.3327E+003
80	0.2318	1.0289E+003	1.0000E+000	1.4292E+003	2.5084E-004	4.3909E+003
81	0.2320	1.0364E+003	1.0000E+000	1.4386E+003	2.4918E-004	4.4487E+003
82	0.2324	1.0516E+003	1.0000E+000	1.4578E+003	2.4590E-004	4.5629E+003
83	0.2328	1.0670E+003	1.0000E+000	1.4772E+003	2.4268E-004	4.6749E+003
84	0.2336	1.0983E+003	1.0000E+000	1.5166E+003	2.3637E-004	4.8903E+003
85	0.2344	1.1300E+003	1.0000E+000	1.5566E+003	2.3031E-004	5.0891E+003
86	0.2352	1.1619E+003	1.0000E+000	1.5968E+003	2.2450E-004	5.2668E+003
87	0.2359	1.1939E+003	1.0000E+000	1.6371E+003	2.1898E-004	5.4183E+003
88	0.2367	1.2257E+003	1.0000E+000	1.6772E+003	2.1375E-004	5.5383E+003
89	0.2375	1.2571E+003	1.0000E+000	1.7168E+003	2.0881E-004	5.6224E+003
90	0.2383	1.2879E+003	1.0000E+000	1.7558E+003	2.0417E-004	5.6671E+003
91	0.2391	1.3180E+003	1.0000E+000	1.7938E+003	1.9984E-004	5.6704E+003
92	0.2398	1.3471E+003	1.0000E+000	1.8308E+003	1.9581E-004	5.6324E+003
93	0.2406	1.3753E+003	1.0000E+000	1.8665E+003	1.9206E-004	5.5549E+003
94	0.2414	1.4023E+003	1.0000E+000	1.9008E+003	1.8860E-004	5.4414E+003
95	0.2422	1.4282E+003	1.0000E+000	1.9336E+003	1.8540E-004	5.2967E+003
96	0.2430	1.4528E+003	1.0000E+000	1.9649E+003	1.8245E-004	5.1266E+003
97	0.2437	1.4763E+003	1.0000E+000	1.9945E+003	1.7973E-004	4.9372E+003
98	0.2445	1.4985E+003	1.0000E+000	2.0226E+003	1.7724E-004	4.7345E+003
99	0.2453	1.5195E+003	1.0000E+000	2.0492E+003	1.7494E-004	4.5244E+003
100	0.2461	1.5394E+003	1.0000E+000	2.0742E+003	1.7283E-004	4.3120E+003
101	0.2469	1.5582E+003	1.0000E+000	2.0977E+003	1.7089E-004	4.1015E+003
102	0.2484	1.5926E+003	1.0000E+000	2.1406E+003	1.6747E-004	3.7017E+003
103	0.2500	1.6235E+003	1.0000E+000	2.1790E+003	1.6452E-004	3.3373E+003
104	0.2516	1.6515E+003	1.0000E+000	2.2135E+003	1.6195E-004	3.0159E+003
105	0.2531	1.6770E+003	1.0000E+000	2.2447E+003	1.5971E-004	2.7383E+003
106	0.2562	1.7214E+003	1.0000E+000	2.2983E+003	1.5598E-004	2.3109E+003
107	0.2594	1.7601E+003	1.0000E+000	2.3445E+003	1.5290E-004	1.9968E+003
108	0.2625	1.7945E+003	1.0000E+000	2.3852E+003	1.5029E-004	1.7623E+003
109	0.2656	1.8255E+003	1.0000E+000	2.4216E+003	1.4803E-004	1.5823E+003
110	0.2688	1.8537E+003	1.0000E+000	2.4545E+003	1.4605E-004	1.4399E+003
111	0.2750	1.9029E+003	1.0000E+000	2.5110E+003	1.4276E-004	1.2309E+003
112	0.2812	1.9461E+003	1.0000E+000	2.5603E+003	1.4002E-004	1.0792E+003
113	0.2875	1.9848E+003	1.0000E+000	2.6039E+003	1.3767E-004	9.6379E+002
114	0.2938	2.0200E+003	1.0000E+000	2.6432E+003	1.3562E-004	8.7288E+002
115	0.3000	2.0521E+003	1.0000E+000	2.6790E+003	1.3381E-004	7.9912E+002
116	0.3063	2.0818E+003	1.0000E+000	2.7118E+003	1.3219E-004	7.3758E+002
117	0.3125	2.1094E+003	1.0000E+000	2.7421E+003	1.3073E-004	6.8484E+002
118	0.3188	2.1350E+003	1.0000E+000	2.7702E+003	1.2941E-004	6.3850E+002
119	0.3250	2.1590E+003	1.0000E+000	2.7963E+003	1.2820E-004	5.9693E+002
120	0.3313	2.1814E+003	1.0000E+000	2.8206E+003	1.2710E-004	5.5901E+002
121	0.3375	2.2024E+003	1.0000E+000	2.8433E+003	1.2608E-004	5.2403E+002
122	0.3438	2.2220E+003	1.0000E+000	2.8644E+003	1.2515E-004	4.9156E+002
123	0.3500	2.2404E+003	1.0000E+000	2.8841E+003	1.2430E-004	4.6136E+002
124	0.3625	2.2729E+003	1.0000E+000	2.9189E+003	1.2282E-004	4.0755E+002
125	0.3750	2.3017E+003	1.0000E+000	2.9494E+003	1.2155E-004	3.6058E+002
126	0.3875	2.3272E+003	1.0000E+000	2.9763E+003	1.2045E-004	3.1960E+002
127	0.4000	2.3498E+003	1.0000E+000	3.0001E+003	1.1949E-004	2.8395E+002
128	0.4125	2.3700E+003	1.0000E+000	3.0211E+003	1.1866E-004	2.5298E+002
129	0.4250	2.3880E+003	1.0000E+000	3.0399E+003	1.1793E-004	2.2609E+002
130	0.4375	2.4041E+003	1.0000E+000	3.0567E+003	1.1728E-004	2.0271E+002

131	0.4500	2.4186E+003	1.0000E+000	3.0718E+003	1.1670E-004	1.8235E+002
132	0.4625	2.4317E+003	1.0000E+000	3.0855E+003	1.1618E-004	1.6462E+002
133	0.4750	2.4436E+003	1.0000E+000	3.0981E+003	1.1571E-004	1.4921E+002
134	0.4812	2.4492E+003	1.0000E+000	3.1042E+003	1.1548E-004	1.4220E+002
135	0.4875	2.4543E+003	1.0000E+000	3.1099E+003	1.1527E-004	1.3588E+002
136	0.4906	2.4566E+003	1.0000E+000	3.1126E+003	1.1517E-004	1.3285E+002
137	0.4938	2.4585E+003	1.0000E+000	3.1148E+003	1.1509E-004	1.3022E+002
138	0.4969	2.4597E+003	1.0000E+000	3.1163E+003	1.1503E-004	1.2821E+002
139	0.5000	2.4597E+003	1.0000E+000	3.1163E+003	1.1503E-004	1.2821E+002

	X(cm)	MOLE FRACTIONS:						
		H2	H	O	O2	OH	H2O	HO2
1	0.0000	3.1609E-001	1.3715E-011	3.7390E-015	1.4368E-001	9.9553E-013	7.6861E-011	5.8892E-011
2	0.0500	3.1609E-001	1.2524E-010	1.1203E-013	1.4368E-001	3.0350E-011	2.8457E-009	2.6695E-009
3	0.0750	3.1609E-001	1.3218E-010	1.1862E-013	1.4368E-001	3.0739E-011	4.2474E-009	4.0453E-009
4	0.1000	3.1609E-001	1.3314E-010	1.1955E-013	1.4368E-001	3.0801E-011	5.6519E-009	5.4308E-009
5	0.1125	3.1609E-001	1.3333E-010	1.1974E-013	1.4368E-001	3.0828E-011	6.3548E-009	6.1244E-009
6	0.1250	3.1609E-001	1.3346E-010	1.1988E-013	1.4368E-001	3.0854E-011	7.0583E-009	6.8188E-009
7	0.1313	3.1609E-001	1.3354E-010	1.1996E-013	1.4368E-001	3.0868E-011	7.4101E-009	7.1662E-009
8	0.1344	3.1609E-001	1.3361E-010	1.2002E-013	1.4368E-001	3.0874E-011	7.5861E-009	7.3400E-009
9	0.1375	3.1609E-001	1.3374E-010	1.2014E-013	1.4368E-001	3.0881E-011	7.7622E-009	7.5142E-009
10	0.1383	3.1609E-001	1.3380E-010	1.2019E-013	1.4368E-001	3.0883E-011	7.8062E-009	7.5578E-009
11	0.1391	3.1609E-001	1.3387E-010	1.2026E-013	1.4368E-001	3.0884E-011	7.8502E-009	7.6014E-009
12	0.1398	3.1609E-001	1.3396E-010	1.2034E-013	1.4368E-001	3.0886E-011	7.8943E-009	7.6452E-009
13	0.1406	3.1609E-001	1.3408E-010	1.2045E-013	1.4368E-001	3.0888E-011	7.9383E-009	7.6891E-009
14	0.1414	3.1609E-001	1.3424E-010	1.2059E-013	1.4368E-001	3.0890E-011	7.9824E-009	7.7333E-009
15	0.1422	3.1609E-001	1.3443E-010	1.2076E-013	1.4368E-001	3.0892E-011	8.0265E-009	7.7778E-009
16	0.1438	3.1609E-001	1.3500E-010	1.2127E-013	1.4368E-001	3.0896E-011	8.1150E-009	7.8686E-009
17	0.1469	3.1609E-001	1.3725E-010	1.2329E-013	1.4368E-001	3.0906E-011	8.2933E-009	8.0625E-009
18	0.1500	3.1609E-001	1.4300E-010	1.2844E-013	1.4368E-001	3.0921E-011	8.4766E-009	8.2989E-009
19	0.1625	3.1609E-001	2.5707E-010	2.3199E-013	1.4368E-001	3.1129E-011	9.3669E-009	1.0644E-008
20	0.1656	3.1609E-001	5.2672E-010	4.7071E-013	1.4368E-001	3.1537E-011	9.8437E-009	1.2975E-008
21	0.1688	3.1609E-001	1.1948E-009	1.0685E-012	1.4368E-001	3.2594E-011	1.0989E-008	1.9868E-008
22	0.1750	3.1608E-001	5.6665E-009	5.1110E-012	1.4368E-001	4.0649E-011	1.9763E-008	7.8028E-008
23	0.1875	3.1607E-001	7.2375E-008	6.6219E-011	1.4368E-001	2.4268E-010	1.4957E-007	9.1620E-007
24	0.1938	3.1604E-001	4.4398E-007	4.1269E-010	1.4368E-001	2.8282E-009	6.3400E-007	3.2595E-006
25	0.2000	3.1596E-001	2.3619E-006	2.3744E-009	1.4369E-001	3.9159E-008	3.1521E-006	1.2266E-005
26	0.2031	3.1586E-001	6.3458E-006	6.9372E-009	1.4370E-001	1.8150E-007	7.8899E-006	2.3294E-005
27	0.2047	3.1578E-001	1.0610E-005	1.2442E-008	1.4370E-001	4.0996E-007	1.3358E-005	3.2417E-005
28	0.2063	3.1567E-001	1.7616E-005	2.2938E-008	1.4371E-001	9.2714E-007	2.3618E-005	4.5743E-005
29	0.2078	3.1550E-001	2.9099E-005	4.3508E-008	1.4371E-001	2.0544E-006	4.2327E-005	6.4290E-005
30	0.2086	3.1539E-001	3.7565E-005	6.1247E-008	1.4371E-001	3.0557E-006	5.6985E-005	7.5664E-005
31	0.2094	3.1526E-001	4.8490E-005	8.7784E-008	1.4372E-001	4.5373E-006	7.7304E-005	8.8787E-005
32	0.2102	3.1510E-001	6.2557E-005	1.2847E-007	1.4372E-001	6.6910E-006	1.0519E-004	1.0362E-004
33	0.2109	3.1491E-001	8.0634E-005	1.9299E-007	1.4372E-001	9.7614E-006	1.4304E-004	1.1998E-004
34	0.2113	3.1480E-001	9.1588E-005	2.4105E-007	1.4372E-001	1.1748E-005	1.6679E-004	1.2861E-004
35	0.2117	3.1467E-001	1.0403E-004	3.0540E-007	1.4371E-001	1.4114E-005	1.9468E-004	1.3752E-004
36	0.2121	3.1454E-001	1.1815E-004	3.9318E-007	1.4371E-001	1.6914E-005	2.2732E-004	1.4664E-004
37	0.2125	3.1439E-001	1.3416E-004	5.1490E-007	1.4371E-001	2.0208E-005	2.6545E-004	1.5588E-004
38	0.2129	3.1422E-001	1.5231E-004	6.8569E-007	1.4371E-001	2.4059E-005	3.0985E-004	1.6515E-004
39	0.2133	3.1404E-001	1.7286E-004	9.2646E-007	1.4370E-001	2.8535E-005	3.6141E-004	1.7434E-004
40	0.2137	3.1384E-001	1.9613E-004	1.2646E-006	1.4370E-001	3.3704E-005	4.2111E-004	1.8334E-004
41	0.2141	3.1363E-001	2.2243E-004	1.7335E-006	1.4369E-001	3.9637E-005	4.9004E-004	1.9202E-004
42	0.2145	3.1339E-001	2.5216E-004	2.3703E-006	1.4368E-001	4.6403E-005	5.6941E-004	2.0026E-004
43	0.2148	3.1313E-001	2.8572E-004	3.2119E-006	1.4366E-001	5.4068E-005	6.6055E-004	2.0795E-004
44	0.2156	3.1253E-001	3.6571E-004	5.6078E-006	1.4363E-001	7.2300E-005	8.8251E-004	2.2125E-004
45	0.2164	3.1183E-001	4.6646E-004	9.0175E-006	1.4358E-001	9.4498E-005	1.1622E-003	2.3151E-004
46	0.2172	3.1100E-001	5.9287E-004	1.3509E-005	1.4351E-001	1.2091E-004	1.5100E-003	2.3842E-004
47	0.2180	3.1003E-001	7.5079E-004	1.9207E-005	1.4342E-001	1.5164E-004	1.9373E-003	2.4199E-004
48	0.2188	3.0891E-001	9.4710E-004	2.6361E-005	1.4330E-001	1.8662E-004	2.4565E-003	2.4250E-004
49	0.2195	3.0760E-001	1.1898E-003	3.5366E-005	1.4315E-001	2.2567E-004	3.0807E-003	2.4038E-004
50	0.2203	3.0610E-001	1.4880E-003	4.6786E-005	1.4296E-001	2.6846E-004	3.8246E-003	2.3617E-004
51	0.2211	3.0437E-001	1.8520E-003	6.1404E-005	1.4273E-001	3.1455E-004	4.7041E-003	2.3037E-004
52	0.2219	3.0240E-001	2.2932E-003	8.0290E-005	1.4244E-001	3.6338E-004	5.7368E-003	2.2343E-004
53	0.2234	2.9764E-001	3.4413E-003	1.3512E-004	1.4168E-001	4.6694E-004	8.3179E-003	2.0725E-004
54	0.2250	2.9169E-001	5.0265E-003	2.2291E-004	1.4067E-001	5.7686E-004	1.1589E-002	1.9006E-004
55	0.2258	2.8820E-001	6.0231E-003	2.8593E-004	1.4007E-001	6.3533E-004	1.3517E-002	1.8145E-004
56	0.2266	2.8430E-001	7.1746E-003	3.6709E-004	1.3937E-001	6.9707E-004	1.5690E-002	1.7293E-004
57	0.2270	2.8219E-001	7.8137E-003	4.1603E-004	1.3898E-001	7.2954E-004	1.6878E-002	1.6872E-004
58	0.2273	2.7997E-001	8.4972E-003	4.7165E-004	1.3856E-001	7.6332E-004	1.8146E-002	1.6457E-004
59	0.2277	2.7763E-001	9.2268E-003	5.3462E-004	1.3811E-001	7.9861E-004	1.9496E-002	1.6047E-004

60	0.2279	2.7641E-001	9.6094E-003	5.6913E-004	1.3786E-001	8.1693E-004	2.0205E-002	1.5844E-004
61	0.2281	2.7517E-001	1.0004E-002	6.0584E-004	1.3761E-001	8.3575E-004	2.0938E-002	1.5643E-004
62	0.2283	2.7389E-001	1.0411E-002	6.4484E-004	1.3735E-001	8.5512E-004	2.1696E-002	1.5444E-004
63	0.2285	2.7258E-001	1.0831E-002	6.8623E-004	1.3707E-001	8.7511E-004	2.2480E-002	1.5247E-004
64	0.2287	2.7123E-001	1.1263E-002	7.3010E-004	1.3678E-001	8.9577E-004	2.3290E-002	1.5051E-004
65	0.2289	2.6986E-001	1.1708E-002	7.7654E-004	1.3648E-001	9.1718E-004	2.4128E-002	1.4858E-004
66	0.2291	2.6845E-001	1.2166E-002	8.2563E-004	1.3617E-001	9.3943E-004	2.4995E-002	1.4667E-004
67	0.2293	2.6700E-001	1.2637E-002	8.7747E-004	1.3584E-001	9.6263E-004	2.5891E-002	1.4478E-004
68	0.2295	2.6553E-001	1.3121E-002	9.3213E-004	1.3549E-001	9.8689E-004	2.6818E-002	1.4292E-004
69	0.2297	2.6402E-001	1.3618E-002	9.8968E-004	1.3513E-001	1.0123E-003	2.7776E-002	1.4108E-004
70	0.2299	2.6247E-001	1.4128E-002	1.0502E-003	1.3476E-001	1.0390E-003	2.8767E-002	1.3926E-004
71	0.2301	2.6089E-001	1.4652E-002	1.1137E-003	1.3436E-001	1.0672E-003	2.9790E-002	1.3746E-004
72	0.2303	2.5927E-001	1.5189E-002	1.1804E-003	1.3395E-001	1.0969E-003	3.0848E-002	1.3570E-004
73	0.2305	2.5763E-001	1.5739E-002	1.2502E-003	1.3352E-001	1.1283E-003	3.1941E-002	1.3396E-004
74	0.2307	2.5594E-001	1.6303E-002	1.3232E-003	1.3307E-001	1.1616E-003	3.3070E-002	1.3224E-004
75	0.2309	2.5422E-001	1.6880E-002	1.3995E-003	1.3260E-001	1.1967E-003	3.4236E-002	1.3055E-004
76	0.2311	2.5247E-001	1.7470E-002	1.4792E-003	1.3211E-001	1.2338E-003	3.5439E-002	1.2888E-004
77	0.2313	2.5068E-001	1.8073E-002	1.5623E-003	1.3160E-001	1.2730E-003	3.6682E-002	1.2724E-004
78	0.2314	2.4885E-001	1.8689E-002	1.6488E-003	1.3106E-001	1.3144E-003	3.7965E-002	1.2563E-004
79	0.2316	2.4700E-001	1.9318E-002	1.7389E-003	1.3050E-001	1.3581E-003	3.9288E-002	1.2404E-004
80	0.2318	2.4510E-001	1.9960E-002	1.8325E-003	1.2992E-001	1.4041E-003	4.0652E-002	1.2248E-004
81	0.2320	2.4318E-001	2.0613E-002	1.9297E-003	1.2931E-001	1.4524E-003	4.2059E-002	1.2094E-004
82	0.2324	2.3923E-001	2.1957E-002	2.1351E-003	1.2801E-001	1.5567E-003	4.5001E-002	1.1793E-004
83	0.2328	2.3515E-001	2.3346E-002	2.3548E-003	1.2662E-001	1.6710E-003	4.8111E-002	1.1500E-004
84	0.2336	2.2663E-001	2.6250E-002	2.8368E-003	1.2351E-001	1.9319E-003	5.4844E-002	1.0939E-004
85	0.2344	2.1769E-001	2.9292E-002	3.3706E-003	1.1999E-001	2.2361E-003	6.2204E-002	1.0404E-004
86	0.2352	2.0841E-001	3.2439E-002	3.9514E-003	1.1609E-001	2.5852E-003	7.0156E-002	9.8896E-005
87	0.2359	1.9887E-001	3.5651E-002	4.5722E-003	1.1181E-001	2.9784E-003	7.8640E-002	9.3906E-005
88	0.2367	1.8917E-001	3.8884E-002	5.2237E-003	1.0721E-001	3.4134E-003	8.7570E-002	8.9024E-005
89	0.2375	1.7942E-001	4.2094E-002	5.8950E-003	1.0234E-001	3.8857E-003	9.6842E-002	8.4220E-005
90	0.2383	1.6973E-001	4.5235E-002	6.5742E-003	9.7259E-002	4.3897E-003	1.0633E-001	7.9478E-005
91	0.2391	1.6021E-001	4.8264E-002	7.2494E-003	9.2056E-002	4.9183E-003	1.1592E-001	7.4799E-005
92	0.2398	1.5096E-001	5.1143E-002	7.9091E-003	8.6808E-002	5.4644E-003	1.2547E-001	7.0199E-005
93	0.2406	1.4208E-001	5.3838E-002	8.5428E-003	8.1594E-002	6.0207E-003	1.3485E-001	6.5701E-005
94	0.2414	1.3364E-001	5.6323E-002	9.1421E-003	7.6486E-002	6.5803E-003	1.4397E-001	6.1338E-005
95	0.2422	1.2571E-001	5.8577E-002	9.7002E-003	7.1549E-002	7.1372E-003	1.5271E-001	5.7142E-005
96	0.2430	1.1833E-001	6.0591E-002	1.0212E-002	6.6836E-002	7.6864E-003	1.6101E-001	5.3144E-005
97	0.2437	1.1153E-001	6.2356E-002	1.0676E-002	6.2388E-002	8.2236E-003	1.6879E-001	4.9370E-005
98	0.2445	1.0532E-001	6.3876E-002	1.1090E-002	5.8234E-002	8.7457E-003	1.7604E-001	4.5842E-005
99	0.2453	9.9691E-002	6.5156E-002	1.1456E-002	5.4395E-002	9.2504E-003	1.8271E-001	4.2574E-005
100	0.2461	9.4637E-002	6.6207E-002	1.1775E-002	5.0878E-002	9.7358E-003	1.8881E-001	3.9574E-005
101	0.2469	9.0132E-002	6.7042E-002	1.2050E-002	4.7688E-002	1.0201E-002	1.9434E-001	3.6844E-005
102	0.2484	8.2675E-002	6.8114E-002	1.2477E-002	4.2278E-002	1.1066E-002	2.0373E-001	3.2185E-005
103	0.2500	7.6914E-002	6.8547E-002	1.2776E-002	3.7903E-002	1.1852E-002	2.1132E-001	2.8396E-005
104	0.2516	7.2548E-002	6.8477E-002	1.2969E-002	3.4417E-002	1.2560E-002	2.1739E-001	2.5354E-005
105	0.2531	6.9294E-002	6.8029E-002	1.3079E-002	3.1670E-002	1.3195E-002	2.2221E-001	2.2930E-005
106	0.2562	6.5353E-002	6.6320E-002	1.3106E-002	2.7989E-002	1.4249E-002	2.2886E-001	1.9560E-005
107	0.2594	6.3272E-002	6.4129E-002	1.2981E-002	2.5600E-002	1.5100E-002	2.3337E-001	1.7280E-005
108	0.2625	6.2218E-002	6.1777E-002	1.2763E-002	2.3996E-002	1.5791E-002	2.3661E-001	1.5665E-005
109	0.2656	6.1704E-002	5.9439E-002	1.2494E-002	2.2860E-002	1.6357E-002	2.3911E-001	1.4456E-005
110	0.2688	6.1453E-002	5.7199E-002	1.2200E-002	2.2002E-002	1.6828E-002	2.4117E-001	1.3504E-005
111	0.2750	6.1274E-002	5.3126E-002	1.1590E-002	2.0774E-002	1.7539E-002	2.4453E-001	1.2081E-005
112	0.2812	6.1135E-002	4.9540E-002	1.0993E-002	1.9791E-002	1.8072E-002	2.4748E-001	1.0967E-005
113	0.2875	6.0947E-002	4.6370E-002	1.0425E-002	1.8940E-002	1.8475E-002	2.5020E-001	1.0049E-005
114	0.2938	6.0698E-002	4.3544E-002	9.8900E-003	1.8173E-002	1.8779E-002	2.5275E-001	9.2679E-006
115	0.3000	6.0394E-002	4.1002E-002	9.3871E-003	1.7469E-002	1.9005E-002	2.5517E-001	8.5911E-006
116	0.3063	6.0047E-002	3.8700E-002	8.9148E-003	1.6815E-002	1.9166E-002	2.5747E-001	7.9972E-006
117	0.3125	5.9667E-002	3.6604E-002	8.4716E-003	1.6202E-002	1.9273E-002	2.5967E-001	7.4716E-006
118	0.3188	5.9263E-002	3.4689E-002	8.0559E-003	1.5626E-002	1.9334E-002	2.6177E-001	7.0036E-006
119	0.3250	5.8840E-002	3.2935E-002	7.6665E-003	1.5082E-002	1.9358E-002	2.6378E-001	6.5853E-006
120	0.3313	5.8407E-002	3.1324E-002	7.3022E-003	1.4569E-002	1.9348E-002	2.6571E-001	6.2103E-006
121	0.3375	5.7968E-002	2.9845E-002	6.9619E-003	1.4085E-002	1.9311E-002	2.6754E-001	5.8734E-006
122	0.3438	5.7527E-002	2.8486E-002	6.6446E-003	1.3627E-002	1.9251E-002	2.6929E-001	5.5705E-006
123	0.3500	5.7089E-002	2.7237E-002	6.3497E-003	1.3195E-002	1.9173E-002	2.7096E-001	5.2984E-006
124	0.3625	5.6226E-002	2.5053E-002	5.8264E-003	1.2418E-002	1.8972E-002	2.7402E-001	4.8395E-006
125	0.3750	5.5389E-002	2.3178E-002	5.3694E-003	1.1719E-002	1.8733E-002	2.7680E-001	4.4606E-006
126	0.3875	5.4589E-002	2.1560E-002	4.9701E-003	1.1092E-002	1.8468E-002	2.7933E-001	4.1454E-006
127	0.4000	5.3830E-002	2.0159E-002	4.6205E-003	1.0527E-002	1.8191E-002	2.8163E-001	3.8811E-006
128	0.4125	5.3116E-002	1.8938E-002	4.3136E-003	1.0018E-002	1.7909E-002	2.8373E-001	3.6576E-006
129	0.4250	5.2449E-002	1.7870E-002	4.0434E-003	9.5582E-003	1.7629E-002	2.8563E-001	3.4668E-006
130	0.4375	5.1828E-002	1.6933E-002	3.8049E-003	9.1418E-003	1.7354E-002	2.8737E-001	3.3026E-006

131	0.4500	5.1259E-002	1.6110E-002	3.5939E-003	8.7637E-003	1.7088E-002	2.8895E-001	3.1600E-006
132	0.4625	5.0749E-002	1.5388E-002	3.4075E-003	8.4194E-003	1.6835E-002	2.9038E-001	3.0353E-006
133	0.4750	5.0318E-002	1.4767E-002	3.2444E-003	8.1053E-003	1.6601E-002	2.9165E-001	2.9260E-006
134	0.4812	5.0147E-002	1.4500E-002	3.1725E-003	7.9582E-003	1.6495E-002	2.9222E-001	2.8767E-006
135	0.4875	5.0020E-002	1.4276E-002	3.1108E-003	7.8226E-003	1.6406E-002	2.9270E-001	2.8328E-006
136	0.4906	4.9977E-002	1.4188E-002	3.0855E-003	7.7615E-003	1.6371E-002	2.9290E-001	2.8137E-006
137	0.4938	4.9949E-002	1.4122E-002	3.0659E-003	7.7099E-003	1.6345E-002	2.9306E-001	2.7981E-006
138	0.4969	4.9936E-002	1.4084E-002	3.0543E-003	7.6755E-003	1.6331E-002	2.9315E-001	2.7881E-006
139	0.5000	4.9936E-002	1.4084E-002	3.0543E-003	7.6755E-003	1.6331E-002	2.9315E-001	2.7881E-006

	X(cm)	MOLE FRACTIONS:						
		H2O2	C	CH	CH2	CH2(S)	CH3	CH4
1	0.0000	2.3862E-015	-1.0602E-083	-3.1632E-075	-1.2622E-066	-1.5063E-067	-4.4292E-057	-4.0053E-056
2	0.0500	1.0882E-013	-3.4021E-082	-8.9166E-074	-5.2001E-065	-6.2056E-066	-1.8624E-055	-1.6882E-054
3	0.0750	1.9075E-013	-7.9165E-081	-1.9658E-072	-1.0863E-063	-1.2963E-064	-3.8410E-054	-2.7415E-053
4	0.1000	3.0164E-013	-1.9492E-079	-4.8054E-071	-2.6362E-062	-3.1460E-063	-9.3029E-053	-5.7519E-052
5	0.1125	3.6480E-013	-1.9344E-078	-4.7618E-070	-2.6085E-061	-3.1127E-062	-9.1965E-052	-5.0093E-051
6	0.1250	4.3538E-013	-2.2906E-077	-5.6332E-069	-3.0828E-060	-3.6786E-061	-1.0859E-050	-5.4622E-050
7	0.1313	4.7262E-013	-1.2020E-076	-2.9537E-068	-1.6153E-059	-1.9273E-060	-5.6868E-050	-2.6889E-049
8	0.1344	4.9177E-013	-3.6433E-076	-8.9458E-068	-4.8889E-059	-5.8323E-060	-1.7205E-049	-7.8681E-049
9	0.1375	5.1137E-013	-1.2525E-075	-3.0721E-067	-1.6773E-058	-2.0008E-059	-5.9011E-049	-2.6317E-048
10	0.1383	5.1632E-013	-1.8422E-075	-4.5142E-067	-2.4627E-058	-2.9369E-059	-8.6616E-049	-3.8315E-048
11	0.1391	5.2132E-013	-2.8149E-075	-6.8930E-067	-3.7581E-058	-4.4814E-059	-1.3216E-048	-5.8012E-048
12	0.1398	5.2637E-013	-4.4217E-075	-1.0819E-066	-5.8944E-058	-7.0286E-059	-2.0726E-048	-9.0349E-048
13	0.1406	5.3148E-013	-7.0773E-075	-1.7301E-066	-9.4168E-058	-1.1229E-058	-3.3109E-048	-1.4344E-047
14	0.1414	5.3668E-013	-1.1469E-074	-2.8003E-066	-1.5224E-057	-1.8153E-058	-5.3523E-048	-2.3060E-047
15	0.1422	5.4199E-013	-1.8737E-074	-4.5679E-066	-2.4797E-057	-2.9567E-058	-8.7173E-048	-3.7371E-047
16	0.1438	5.5316E-013	-4.7653E-074	-1.1570E-065	-6.2555E-057	-7.4603E-058	-2.1992E-047	-9.3549E-047
17	0.1469	5.7944E-013	-2.2469E-073	-5.3658E-065	-2.8542E-056	-3.4047E-057	-1.0033E-046	-4.2214E-046
18	0.1500	6.2040E-013	-9.7761E-073	-2.1436E-064	-1.0931E-055	-1.3036E-056	-3.8395E-046	-1.5929E-045
19	0.1625	1.3214E-012	-2.8789E-070	-9.0765E-063	-2.5761E-054	-3.0640E-055	-8.9592E-045	-3.6271E-044
20	0.1656	2.5192E-012	-3.3291E-067	-7.0351E-062	-9.3180E-054	-8.9696E-055	-2.5812E-044	-1.0002E-043
21	0.1688	6.9569E-012	-2.0465E-064	-5.1160E-060	-1.9704E-052	-3.1784E-054	-8.7009E-044	-3.2695E-043
22	0.1750	5.2459E-011	-3.7773E-061	-8.3434E-057	-4.8454E-050	-4.0034E-053	-6.9160E-043	-2.5240E-042
23	0.1875	8.9255E-010	-2.7729E-057	-7.9563E-053	-5.3353E-047	-1.1427E-050	-1.1567E-041	-4.0575E-041
24	0.1938	4.3863E-009	-9.5636E-054	-2.3666E-049	-2.9325E-044	-3.4098E-048	-6.2265E-041	-2.0425E-040
25	0.2000	2.3873E-008	-1.5677E-050	-3.4905E-046	-1.0979E-041	-1.1187E-045	-3.9001E-040	-1.2006E-039
26	0.2031	5.6192E-008	8.6079E-048	-2.0746E-045	-1.5345E-039	-4.8652E-044	-1.2647E-039	-3.5809E-039
27	0.2047	8.9819E-008	5.6463E-047	-1.4582E-044	-8.8147E-040	1.2186E-044	-2.7063E-039	-7.0046E-039
28	0.2063	1.4928E-007	9.4255E-046	-6.2423E-043	-2.3563E-039	5.3509E-044	-6.3104E-039	-1.4688E-038
29	0.2078	2.4978E-007	2.3529E-044	1.5400E-041	4.3554E-038	3.8290E-042	-1.4994E-038	-3.1800E-038
30	0.2086	3.2166E-007	1.0461E-045	1.2555E-042	3.4842E-038	5.6896E-042	-2.6534E-038	-4.7958E-038
31	0.2094	4.1510E-007	-1.2332E-044	6.2954E-042	1.9782E-038	-3.4487E-042	-4.7282E-038	-7.3530E-038
32	0.2102	5.3445E-007	-4.2825E-043	2.5757E-041	-3.3090E-037	-2.0432E-041	-8.2897E-038	-1.1314E-037
33	0.2109	6.8363E-007	-6.6519E-043	-2.6031E-040	-8.8436E-037	-5.2874E-041	-1.5028E-037	-1.7334E-037
34	0.2113	7.7043E-007	-1.4715E-042	-1.7094E-039	-7.7751E-037	-1.8354E-041	-1.9966E-037	-2.1424E-037
35	0.2117	8.6699E-007	-9.2231E-042	-4.2379E-039	-3.5893E-037	-1.3358E-040	-2.5739E-037	-2.6459E-037
36	0.2121	9.7377E-007	-1.6058E-041	-8.7393E-039	-4.6070E-036	-2.9093E-040	-3.1419E-037	-3.2418E-037
37	0.2125	1.0912E-006	-2.6299E-041	-1.1650E-039	-5.2612E-036	-5.6087E-040	-3.6683E-037	-3.9787E-037
38	0.2129	1.2194E-006	-1.8308E-041	-3.9162E-039	-2.0400E-036	-2.3215E-040	-3.5471E-037	-4.8312E-037
39	0.2133	1.3586E-006	-1.0542E-041	-1.9095E-039	-7.9638E-037	-1.0170E-040	-3.2598E-037	-5.8319E-037
40	0.2137	1.5088E-006	-5.9844E-042	-9.1609E-040	-3.3210E-037	-5.3262E-041	-2.9247E-037	-7.0231E-037
41	0.2141	1.6698E-006	-5.4091E-042	-6.7273E-040	-2.1137E-037	-4.1375E-041	-2.5958E-037	-8.4638E-037
42	0.2145	1.8414E-006	-1.2879E-041	-1.3220E-039	-3.6453E-037	-5.9946E-041	-2.2890E-037	-1.0233E-036
43	0.2148	2.0231E-006	-5.4361E-041	-4.4444E-039	-1.1407E-036	-1.5984E-040	-2.7773E-037	-1.2727E-036
44	0.2156	2.4157E-006	-6.0820E-040	-1.8482E-038	-8.4974E-036	-2.1776E-039	-4.0930E-037	-1.9557E-036
45	0.2164	2.8379E-006	-1.5515E-040	-9.9751E-039	-1.5975E-036	-2.5521E-040	-3.6112E-037	-3.1093E-036
46	0.2172	3.2838E-006	-4.7304E-041	-2.4638E-039	-2.9875E-037	-8.9004E-041	-2.5188E-037	-4.8468E-036
47	0.2180	3.7474E-006	-1.4052E-041	-5.7555E-040	-5.5224E-038	-5.4876E-041	-1.6411E-037	-7.5441E-036
48	0.2188	4.2230E-006	-4.1506E-042	-1.3483E-040	-1.0280E-038	-5.1298E-041	-1.1132E-037	-1.1810E-035
49	0.2195	4.7039E-006	-1.3997E-042	-3.6492E-041	-2.2275E-039	-6.9494E-041	-9.1973E-038	-1.8607E-035
50	0.2203	5.1817E-006	-1.0625E-042	-2.2805E-041	-1.1301E-039	-1.2856E-040	-1.0687E-037	-2.9443E-035
51	0.2211	5.6452E-006	-2.4820E-042	-4.3421E-041	-1.7472E-039	-2.7977E-040	-1.6596E-037	-4.6668E-035
52	0.2219	6.0792E-006	-8.1241E-042	-1.1329E-040	-3.6970E-039	-6.4453E-040	-2.9676E-037	-7.3908E-035
53	0.2234	6.8011E-006	-7.2679E-041	-6.9568E-040	-1.5452E-038	-3.1495E-039	-9.5382E-037	-1.7473E-034
54	0.2250	7.2496E-006	-5.4463E-040	-3.6673E-039	-5.7193E-038	-1.3711E-038	-2.9361E-036	-3.8397E-034
55	0.2258	7.3512E-006	-1.4830E-039	-8.3342E-039	-1.0976E-037	-2.8457E-038	-5.2609E-036	-5.6774E-034
56	0.2266	7.3504E-006	-3.8973E-039	-1.8552E-038	-2.0823E-037	-5.8689E-038	-9.4434E-036	-8.4147E-034
57	0.2270	7.3128E-006	-6.3275E-039	-2.7655E-038	-2.8701E-037	-8.4243E-038	-1.2722E-035	-1.0265E-033
58	0.2273	7.2484E-006	-1.0200E-038	-4.1074E-038	-3.9506E-037	-1.2086E-037	-1.7168E-035	-1.2543E-033
59	0.2277	7.1583E-006	-1.6314E-038	-6.0675E-038	-5.4199E-037	-1.7288E-037	-2.3158E-035	-1.5334E-033

60	0.2279	7.1044E-006	-2.0631E-038	-7.3692E-038	-6.3456E-037	-2.0661E-037	-2.6912E-035	-1.6959E-033
61	0.2281	7.0444E-006	-2.6046E-038	-8.9406E-038	-7.4259E-037	-2.4681E-037	-3.1281E-035	-1.8761E-033
62	0.2283	6.9788E-006	-3.2829E-038	-1.0834E-037	-8.6838E-037	-2.9463E-037	-3.6357E-035	-2.0757E-033
63	0.2285	6.9078E-006	-4.1304E-038	-1.3110E-037	-1.0145E-036	-3.5137E-037	-4.2242E-035	-2.2964E-033
64	0.2287	6.8319E-006	-5.1867E-038	-1.5840E-037	-1.1839E-036	-4.1853E-037	-4.9053E-035	-2.5401E-033
65	0.2289	6.7514E-006	-6.4995E-038	-1.9103E-037	-1.3797E-036	-4.9784E-037	-5.6920E-035	-2.8087E-033
66	0.2291	6.6668E-006	-8.1265E-038	-2.2995E-037	-1.6055E-036	-5.9125E-037	-6.5988E-035	-3.1043E-033
67	0.2293	6.5786E-006	-1.0137E-037	-2.7624E-037	-1.8652E-036	-7.0098E-037	-7.6420E-035	-3.4290E-033
68	0.2295	6.4872E-006	-1.2614E-037	-3.3113E-037	-2.1633E-036	-8.2957E-037	-8.8397E-035	-3.7853E-033
69	0.2297	6.3933E-006	-1.5656E-037	-3.9605E-037	-2.5045E-036	-9.7985E-037	-1.0212E-034	-4.1753E-033
70	0.2299	6.2973E-006	-1.9383E-037	-4.7261E-037	-2.8940E-036	-1.1550E-036	-1.1780E-034	-4.6016E-033
71	0.2301	6.1998E-006	-2.3935E-037	-5.6266E-037	-3.3377E-036	-1.3587E-036	-1.3570E-034	-5.0668E-033
72	0.2303	6.1014E-006	-2.9477E-037	-6.6828E-037	-3.8420E-036	-1.5949E-036	-1.5607E-034	-5.5733E-033
73	0.2305	6.0025E-006	-3.6206E-037	-7.9182E-037	-4.4136E-036	-1.8681E-036	-1.7922E-034	-6.1239E-033
74	0.2307	5.9037E-006	-4.4354E-037	-9.3596E-037	-5.0601E-036	-2.1834E-036	-2.0546E-034	-6.7212E-033
75	0.2309	5.8056E-006	-5.4192E-037	-1.1037E-036	-5.7898E-036	-2.5462E-036	-2.3516E-034	-7.3680E-033
76	0.2311	5.7087E-006	-6.6039E-037	-1.2983E-036	-6.6115E-036	-2.9628E-036	-2.6869E-034	-8.0671E-033
77	0.2313	5.6133E-006	-8.0268E-037	-1.5237E-036	-7.5349E-036	-3.4399E-036	-3.0648E-034	-8.8210E-033
78	0.2314	5.5200E-006	-9.7317E-037	-1.7841E-036	-8.5706E-036	-3.9852E-036	-3.4899E-034	-9.6326E-033
79	0.2316	5.4293E-006	-1.1770E-036	-2.0841E-036	-9.7300E-036	-4.6069E-036	-3.9671E-034	-1.0504E-032
80	0.2318	5.3414E-006	-1.4202E-036	-2.4291E-036	-1.1026E-035	-5.3143E-036	-4.5021E-034	-1.1439E-032
81	0.2320	5.2569E-006	-1.7102E-036	-2.8252E-036	-1.2472E-035	-6.1176E-036	-5.1007E-034	-1.2439E-032
82	0.2324	5.0987E-006	-2.4567E-036	-3.7924E-036	-1.5857E-035	-8.0508E-036	-6.5084E-034	-1.4641E-032
83	0.2328	4.9561E-006	-3.4962E-036	-5.0414E-036	-1.9991E-035	-1.0492E-035	-8.2364E-034	-1.7114E-032
84	0.2336	4.7226E-006	-6.8059E-036	-8.6247E-036	-3.0927E-035	-1.7296E-035	-1.2836E-033	-2.2896E-032
85	0.2344	4.5537E-006	-1.2698E-035	-1.4178E-035	-4.6251E-035	-2.7422E-035	-1.9307E-033	-2.9705E-032
86	0.2352	4.4434E-006	-2.2882E-035	-2.2585E-035	-6.7424E-035	-4.2172E-035	-2.8202E-033	-3.7471E-032
87	0.2359	4.3788E-006	-4.0057E-035	-3.5067E-035	-9.6374E-035	-6.3285E-035	-4.0163E-033	-4.6065E-032
88	0.2367	4.3427E-006	-6.8378E-035	-5.3283E-035	-1.3558E-034	-9.3026E-035	-5.5910E-033	-5.5309E-032
89	0.2375	4.3167E-006	-1.1406E-034	-7.9406E-035	-1.8813E-034	-1.3426E-034	-7.6216E-033	-6.4991E-032
90	0.2383	4.2836E-006	-1.8604E-034	-1.1618E-034	-2.5769E-034	-1.9043E-034	-1.0187E-032	-7.4887E-032
91	0.2391	4.2307E-006	-2.9674E-034	-1.6690E-034	-3.4841E-034	-2.6551E-034	-1.3363E-032	-8.4778E-032
92	0.2398	4.1507E-006	-4.6254E-034	-2.3534E-034	-4.6474E-034	-3.6376E-034	-1.7217E-032	-9.4469E-032
93	0.2406	4.0419E-006	-7.0404E-034	-3.2551E-034	-6.1112E-034	-4.8946E-034	-2.1804E-032	-1.0379E-031
94	0.2414	3.9076E-006	-1.0458E-033	-4.4148E-034	-7.9170E-034	-6.4654E-034	-2.7158E-032	-1.1263E-031
95	0.2422	3.7540E-006	-1.5153E-033	-5.8697E-034	-1.0100E-033	-8.3823E-034	-3.3296E-032	-1.2088E-031
96	0.2430	3.5883E-006	-2.1417E-033	-7.6514E-034	-1.2689E-033	-1.0668E-033	-4.0210E-032	-1.2849E-031
97	0.2437	3.4176E-006	-2.9536E-033	-9.7834E-034	-1.5700E-033	-1.3333E-033	-4.7874E-032	-1.3542E-031
98	0.2445	3.2478E-006	-3.9765E-033	-1.2279E-033	-1.9143E-033	-1.6377E-033	-5.6244E-032	-1.4167E-031
99	0.2453	3.0831E-006	-5.2304E-033	-1.5143E-033	-2.3015E-033	-1.9787E-033	-6.5260E-032	-1.4725E-031
100	0.2461	2.9262E-006	-6.7273E-033	-1.8366E-033	-2.7308E-033	-2.3541E-033	-7.4847E-032	-1.5215E-031
101	0.2469	2.7788E-006	-8.4677E-033	-2.1928E-033	-3.1997E-033	-2.7603E-033	-8.4913E-032	-1.5639E-031
102	0.2484	2.5148E-006	-1.2636E-032	-2.9940E-033	-4.2439E-033	-3.6466E-033	-1.0609E-031	-1.6284E-031
103	0.2500	2.2861E-006	-1.7470E-032	-3.8639E-033	-5.3688E-033	-4.5669E-033	-1.2732E-031	-1.6655E-031
104	0.2516	2.0886E-006	-2.2677E-032	-4.7652E-033	-6.5376E-033	-5.4803E-033	-1.4782E-031	-1.6769E-031
105	0.2531	1.9177E-006	-2.7941E-032	-5.6676E-033	-7.7223E-033	-6.3578E-033	-1.6716E-031	-1.6674E-031
106	0.2562	1.6409E-006	-3.7560E-032	-7.3860E-033	-1.0061E-032	-7.9328E-033	-2.0147E-031	-1.6034E-031
107	0.2594	1.4236E-006	-4.4921E-032	-8.8199E-033	-1.2119E-032	-9.1045E-033	-2.2704E-031	-1.4969E-031
108	0.2625	1.2507E-006	-4.9889E-032	-9.9554E-033	-1.3860E-032	-9.9054E-033	-2.4478E-031	-1.3720E-031
109	0.2656	1.1115E-006	-5.2897E-032	-1.0834E-032	-1.5307E-032	-1.0410E-032	-2.5638E-031	-1.2467E-031
110	0.2688	9.9830E-007	-5.4492E-032	-1.1509E-032	-1.6503E-032	-1.0693E-032	-2.6340E-031	-1.1307E-031
111	0.2750	8.2948E-007	-5.5139E-032	-1.2445E-032	-1.8335E-032	-1.0843E-032	-2.6896E-031	-9.4126E-032
112	0.2812	7.0816E-007	-5.3984E-032	-1.2986E-032	-1.9543E-032	-1.0602E-032	-2.6611E-031	-7.9189E-032
113	0.2875	6.1785E-007	-5.2094E-032	-1.3306E-032	-2.0328E-032	-1.0159E-032	-2.5859E-031	-6.7577E-032
114	0.2938	5.4856E-007	-5.0019E-032	-1.3512E-032	-2.0833E-032	-9.6202E-033	-2.4863E-031	-5.8546E-032
115	0.3000	4.9405E-007	-4.8023E-032	-1.3665E-032	-2.1152E-032	-9.0428E-033	-2.3748E-031	-5.1454E-032
116	0.3063	4.5028E-007	-4.6227E-032	-1.3804E-032	-2.1351E-032	-8.4612E-033	-2.2588E-031	-4.5817E-032
117	0.3125	4.1455E-007	-4.4684E-032	-1.3951E-032	-2.1477E-032	-7.8959E-033	-2.1429E-031	-4.1283E-032
118	0.3188	3.8498E-007	-4.3412E-032	-1.4117E-032	-2.1565E-032	-7.3592E-033	-2.0303E-031	-3.7596E-032
119	0.3250	3.6023E-007	-4.2412E-032	-1.4307E-032	-2.1643E-032	-6.8586E-033	-1.9229E-031	-3.4570E-032
120	0.3313	3.3933E-007	-4.1669E-032	-1.4525E-032	-2.1726E-032	-6.3979E-033	-1.8220E-031	-3.2069E-032
121	0.3375	3.2155E-007	-4.1171E-032	-1.4766E-032	-2.1829E-032	-5.9785E-033	-1.7282E-031	-2.9990E-032
122	0.3438	3.0632E-007	-4.0897E-032	-1.5029E-032	-2.1959E-032	-5.6002E-033	-1.6420E-031	-2.8253E-032
123	0.3500	2.9324E-007	-4.0821E-032	-1.5304E-032	-2.2119E-032	-5.2617E-033	-1.5634E-031	-2.6799E-032
124	0.3625	2.7242E-007	-4.1102E-032	-1.5842E-032	-2.2490E-032	-4.6934E-033	-1.4282E-031	-2.4569E-032
125	0.3750	2.5636E-007	-4.1951E-032	-1.6391E-032	-2.2979E-032	-4.2459E-033	-1.3184E-031	-2.2974E-032
126	0.3875	2.4380E-007	-4.3260E-032	-1.6925E-032	-2.3563E-032	-3.8972E-033	-1.2306E-031	-2.1855E-032
127	0.4000	2.3383E-007	-4.4933E-032	-1.7428E-032	-2.4216E-032	-3.6272E-033	-1.1612E-031	-2.1097E-032
128	0.4125	2.2582E-007	-4.6877E-032	-1.7887E-032	-2.4910E-032	-3.4189E-033	-1.1069E-031	-2.0617E-032
129	0.4250	2.1932E-007	-4.9036E-032	-1.8300E-032	-2.5629E-032	-3.2600E-033	-1.0652E-031	-2.0357E-032
130	0.4375	2.1397E-007	-5.1334E-032	-1.8664E-032	-2.6347E-032	-3.1380E-033	-1.0333E-031	-2.0266E-032

131	0.4500	2.0954E-007	-5.3759E-032	-1.8990E-032	-2.7072E-032	-3.0482E-033	-1.0104E-031	-2.0322E-032
132	0.4625	2.0582E-007	-5.6231E-032	-1.9290E-032	-2.7804E-032	-2.9787E-033	-9.9338E-032	-2.0490E-032
133	0.4750	2.0267E-007	-5.8714E-032	-1.9539E-032	-2.8470E-032	-2.9326E-033	-9.8134E-032	-2.0755E-032
134	0.4812	2.0128E-007	-6.0014E-032	-1.9642E-032	-2.8745E-032	-2.9163E-033	-9.7833E-032	-2.0819E-032
135	0.4875	2.0005E-007	-6.1167E-032	-1.9733E-032	-2.8992E-032	-2.8966E-033	-9.7387E-032	-2.0936E-032
136	0.4906	1.9951E-007	-6.1423E-032	-1.9750E-032	-2.9007E-032	-2.8844E-033	-9.6960E-032	-2.0931E-032
137	0.4938	1.9906E-007	-6.1770E-032	-1.9770E-032	-2.9109E-032	-2.8803E-033	-9.6588E-032	-2.0947E-032
138	0.4969	1.9877E-007	-6.1543E-032	-1.9654E-032	-2.8993E-032	-2.8724E-033	-9.6315E-032	-2.0908E-032
139	0.5000	1.9877E-007	-6.1575E-032	-1.9653E-032	-2.8993E-032	-2.8724E-033	-9.6315E-032	-2.0908E-032

	X(cm)	MOLE FRACTIONS:						
		CO	CO2	HCO	CH2O	CH2OH	CH3O	CH3OH
1	0.0000	-5.3807E-066	-2.9841E-059	-7.7390E-067	-2.0510E-057	-3.3699E-068	-2.0136E-062	-2.9989E-059
2	0.0500	-2.4627E-064	-1.6846E-057	-4.1852E-065	-1.1175E-055	-1.8633E-066	-1.1134E-060	-1.6660E-057
3	0.0750	-4.8895E-063	1.9043E-054	-7.9521E-064	-2.0595E-054	-3.7003E-065	-3.4298E-059	-3.5648E-056
4	0.1000	-1.2138E-061	4.1736E-054	-2.0128E-062	-5.1873E-053	-9.3797E-064	-1.0906E-057	-9.9029E-055
5	0.1125	-1.2337E-060	-1.4316E-054	-2.0906E-061	-5.3796E-052	-9.7239E-063	-1.1924E-056	-1.1158E-053
6	0.1250	-1.5749E-059	8.2684E-054	-2.8293E-060	-7.2708E-051	-1.2946E-061	-1.5373E-055	-1.5945E-052
7	0.1313	-8.9191E-059	2.6469E-053	-1.6853E-059	-4.3278E-050	-7.6042E-061	-8.0540E-055	-9.8944E-052
8	0.1344	-2.9465E-058	-3.8426E-053	-5.8475E-059	-1.5009E-049	-2.6012E-060	-2.3856E-054	-3.5235E-051
9	0.1375	-1.1344E-057	-5.4352E-052	-2.3820E-058	-6.1100E-049	-1.0433E-059	-8.1124E-054	-1.4691E-050
10	0.1383	-1.7577E-057	-5.2992E-052	-3.7647E-058	-9.6538E-049	-1.6387E-059	-1.1772E-053	-2.3429E-050
11	0.1391	-2.8676E-057	-3.5423E-052	-6.3000E-058	-1.6150E-048	-2.7237E-059	-1.8014E-053	-3.9613E-050
12	0.1398	-4.8522E-057	-5.0655E-052	-1.0950E-057	-2.8060E-048	-4.7022E-059	-2.8739E-053	-6.9589E-050
13	0.1406	-8.4098E-057	-7.5620E-054	-1.9483E-057	-4.9903E-048	-8.3140E-059	-4.7353E-053	-1.2511E-049
14	0.1414	-1.4800E-056	-1.0486E-051	-3.5142E-057	-8.9963E-048	-1.4915E-058	-8.0069E-053	-2.2796E-049
15	0.1422	-2.6298E-056	-1.3859E-051	-6.3892E-057	-1.6344E-047	-2.6992E-058	-1.3846E-052	-4.1845E-049
16	0.1438	-7.6902E-056	-1.3435E-051	-1.9363E-056	-4.9435E-047	-8.1376E-058	-3.9834E-052	-1.2865E-048
17	0.1469	-4.2561E-055	-1.3364E-051	-1.1098E-055	-2.8126E-046	-4.6695E-057	-2.3012E-051	-7.4615E-048
18	0.1500	-2.0402E-054	-1.3599E-051	-5.1855E-055	-1.2863E-045	-2.2257E-056	-1.2554E-050	-3.4685E-047
19	0.1625	-1.4072E-052	-2.4703E-051	-2.1147E-053	-3.8837E-044	-1.1617E-054	-5.9659E-049	-1.0714E-045
20	0.1656	-1.2334E-050	-5.1774E-051	-1.2016E-052	-1.2629E-043	-7.6774E-054	-5.3487E-048	-3.5357E-045
21	0.1688	-9.1484E-049	-1.2207E-050	-3.2342E-051	-5.0565E-043	-7.1160E-053	-4.2194E-047	-1.4387E-044
22	0.1750	-2.0504E-046	-1.0960E-049	-2.0146E-048	-5.0641E-042	-3.4581E-051	-8.8937E-046	-1.4673E-043
23	0.1875	-1.7501E-043	-2.7485E-047	-6.6210E-045	-1.0546E-040	-8.7071E-049	-5.1854E-044	-3.0886E-042
24	0.1938	-6.7027E-041	-1.7407E-045	-1.1031E-041	-6.5769E-040	-3.3643E-047	-9.3667E-043	-1.8722E-041
25	0.2000	2.0427E-040	-1.2345E-043	1.1218E-040	-4.8928E-039	-1.3164E-045	-1.4731E-041	-1.3031E-040
26	0.2031	2.0322E-040	-1.9590E-042	-1.2187E-041	-1.7247E-038	-1.3637E-044	-8.0411E-041	-4.0847E-040
27	0.2047	5.3072E-040	-1.1186E-041	-1.2232E-040	-4.6200E-038	-5.7681E-044	-2.2491E-040	-8.1675E-040
28	0.2063	1.8799E-039	-7.4890E-041	5.0679E-040	-1.3066E-037	-2.3518E-043	-6.4851E-040	-1.7565E-039
29	0.2078	-3.3658E-038	-5.3561E-040	1.1398E-038	-3.6573E-037	-1.1190E-042	-1.8846E-039	-3.8336E-039
30	0.2086	-6.5389E-037	-1.6348E-039	-9.6044E-039	-6.9288E-037	-2.7793E-042	-3.2632E-039	-5.6952E-039
31	0.2094	-4.2516E-036	-5.4457E-039	-1.6697E-038	-1.2879E-036	-6.5636E-042	-5.7427E-039	-8.5325E-039
32	0.2102	-2.5818E-035	-1.9136E-038	-7.1880E-038	-2.1877E-036	-1.4040E-041	-1.0056E-038	-1.2634E-038
33	0.2109	-1.5324E-034	-7.0139E-038	-3.8436E-037	-3.6516E-036	-3.2760E-041	-1.6743E-038	-1.8335E-038
34	0.2113	-4.3823E-034	-1.4167E-037	-9.8348E-038	-5.0714E-036	-4.9712E-041	-2.1003E-038	-2.1683E-038
35	0.2117	-1.1638E-033	-2.9835E-037	-4.4437E-038	-6.8002E-036	-7.8822E-041	-2.5865E-038	-2.5568E-038
36	0.2121	-2.9929E-033	-6.4977E-037	-2.1221E-038	-8.3026E-036	-1.0687E-040	-2.9998E-038	-2.9841E-038
37	0.2125	-7.4917E-033	-1.4582E-036	-7.8797E-039	-9.3246E-036	-1.4963E-040	-3.3169E-038	-3.4631E-038
38	0.2129	-1.8256E-032	-3.3707E-036	-2.8106E-038	-1.0025E-035	-1.6270E-040	-3.6771E-038	-4.0249E-038
39	0.2133	-4.3063E-032	-8.0413E-036	-3.0953E-038	-1.0322E-035	-1.8720E-040	-3.8718E-038	-4.5979E-038
40	0.2137	-9.7776E-032	-1.9860E-035	-4.5894E-038	-1.0480E-035	-2.1595E-040	-3.8928E-038	-5.1731E-038
41	0.2141	-2.1284E-031	-5.0944E-035	-9.1892E-038	-1.0610E-035	-2.4964E-040	-3.7317E-038	-5.7467E-038
42	0.2145	-4.4255E-031	-7.6958E-035	-2.0175E-037	-1.0744E-035	-2.9506E-040	-3.3653E-038	-6.3226E-038
43	0.2148	-8.7618E-031	-2.1274E-034	-4.4840E-037	-1.2364E-035	-3.7277E-040	-3.4220E-038	-7.2359E-038
44	0.2156	-2.7671E-030	-5.5165E-034	-1.7298E-036	-1.6521E-035	-6.0896E-040	-2.9960E-038	-9.4460E-038
45	0.2164	-7.3437E-030	-1.4809E-033	-5.2750E-036	-2.4824E-035	-1.2119E-039	-3.5857E-038	-1.1484E-037
46	0.2172	-1.7177E-029	-3.6471E-033	-1.5106E-035	-3.8248E-035	-2.3667E-039	-3.4297E-038	-1.3827E-037
47	0.2180	-3.6986E-029	-7.7512E-033	-4.0223E-035	-6.2890E-035	-4.8862E-039	-3.0802E-038	-1.6768E-037
48	0.2188	-7.5690E-029	-1.6084E-032	-1.0145E-034	-1.0870E-034	-1.0547E-038	-3.0426E-038	-2.1055E-037
49	0.2195	-1.5007E-028	-3.5544E-032	-2.4635E-034	-1.9364E-034	-2.3332E-038	-3.7311E-038	-2.7939E-037
50	0.2203	-2.9128E-028	-7.5210E-032	-5.8103E-034	-3.5038E-034	-5.2090E-038	-5.6071E-038	-3.9456E-037
51	0.2211	-5.5633E-028	-1.6818E-031	-1.3373E-033	-6.3776E-034	-1.1615E-037	-9.3649E-038	-5.8883E-037
52	0.2219	-1.0481E-027	-3.9406E-031	-3.0185E-033	-1.1602E-033	-2.5764E-037	-1.6150E-037	-9.1435E-037
53	0.2234	-3.2529E-027	-2.4421E-030	-1.2831E-032	-3.4450E-033	-1.0831E-036	-4.4043E-037	-2.1994E-036
54	0.2250	-9.1665E-027	-1.6599E-029	-4.7285E-032	-9.1496E-033	-3.8813E-036	-1.0592E-036	-4.9262E-036
55	0.2258	-1.5656E-026	-4.4272E-029	-9.1036E-032	-1.4885E-032	-7.2175E-036	-1.6241E-036	-7.2860E-036
56	0.2266	-2.6853E-026	-1.1999E-028	-1.7397E-031	-2.4245E-032	-1.3256E-035	-2.4834E-036	-1.0782E-035
57	0.2270	-3.5399E-026	-1.9854E-028	-2.4119E-031	-3.0994E-032	-1.7916E-035	-3.0690E-036	-1.3112E-035
58	0.2273	-4.6819E-026	-3.3024E-028	-3.3465E-031	-3.9690E-032	-2.4179E-035	-3.7944E-036	-1.5963E-035
59	0.2277	-6.2008E-026	-5.5258E-028	-4.6364E-031	-5.0802E-032	-3.2505E-035	-4.6846E-036	-1.9422E-035

60	0.2279	-7.1449E-026	-7.1692E-028	-5.4591E-031	-5.7476E-032	-3.7644E-035	-5.2024E-036	-2.1416E-035
61	0.2281	-8.2393E-026	-9.3297E-028	-6.4295E-031	-6.5038E-032	-4.3572E-035	-5.7766E-036	-2.3615E-035
62	0.2283	-9.5059E-026	-1.2187E-027	-7.5717E-031	-7.3589E-032	-5.0390E-035	-6.4117E-036	-2.6034E-035
63	0.2285	-1.0970E-025	-1.5992E-027	-8.9137E-031	-8.3236E-032	-5.8210E-035	-7.1123E-036	-2.8690E-035
64	0.2287	-1.2660E-025	-2.1106E-027	-1.0487E-030	-9.4098E-032	-6.7153E-035	-7.8831E-036	-3.1599E-035
65	0.2289	-1.4608E-025	-2.8049E-027	-1.2330E-030	-1.0630E-031	-7.7353E-035	-8.7290E-036	-3.4777E-035
66	0.2291	-1.6850E-025	-3.7596E-027	-1.4482E-030	-1.1997E-031	-8.8953E-035	-9.6548E-036	-3.8242E-035
67	0.2293	-1.9426E-025	-5.0919E-027	-1.6992E-030	-1.3527E-031	-1.0211E-034	-1.0665E-035	-4.2010E-035
68	0.2295	-2.2383E-025	-6.9825E-027	-1.9914E-030	-1.5233E-031	-1.1698E-034	-1.1765E-035	-4.6098E-035
69	0.2297	-2.5770E-025	-9.7160E-027	-2.3308E-030	-1.7133E-031	-1.3376E-034	-1.2960E-035	-5.0521E-035
70	0.2299	-2.9644E-025	-1.3747E-026	-2.7242E-030	-1.9244E-031	-1.5262E-034	-1.4254E-035	-5.5295E-035
71	0.2301	-3.4067E-025	-1.9808E-026	-3.1794E-030	-2.1585E-031	-1.7377E-034	-1.5653E-035	-6.0436E-035
72	0.2303	-3.9110E-025	-2.9088E-026	-3.7049E-030	-2.4174E-031	-1.9742E-034	-1.7161E-035	-6.5958E-035
73	0.2305	-4.4849E-025	-4.3483E-026	-4.3105E-030	-2.7033E-031	-2.2380E-034	-1.8782E-035	-7.1874E-035
74	0.2307	-5.1371E-025	-6.5925E-026	-5.0070E-030	-3.0184E-031	-2.5313E-034	-2.0523E-035	-7.8199E-035
75	0.2309	-5.8771E-025	-1.0066E-025	-5.8067E-030	-3.3650E-031	-2.8569E-034	-2.2388E-035	-8.4942E-035
76	0.2311	-6.7158E-025	-1.5323E-025	-6.7234E-030	-3.7455E-031	-3.2171E-034	-2.4381E-035	-9.2116E-035
77	0.2313	-7.6651E-025	-2.2985E-025	-7.7724E-030	-4.1626E-031	-3.6150E-034	-2.6508E-035	-9.9729E-035
78	0.2314	-8.7385E-025	-3.3645E-025	-8.9714E-030	-4.6191E-031	-4.0532E-034	-2.8773E-035	-1.0779E-034
79	0.2316	-9.9513E-025	-4.7855E-025	-1.0340E-029	-5.1179E-031	-4.5350E-034	-3.1182E-035	-1.1630E-034
80	0.2318	-1.1320E-024	-6.6264E-025	-1.1901E-029	-5.6621E-031	-5.0635E-034	-3.3739E-035	-1.2528E-034
81	0.2320	-1.2865E-024	-8.9880E-025	-1.3679E-029	-6.2550E-031	-5.6420E-034	-3.6447E-035	-1.3471E-034
82	0.2324	-1.6543E-024	-1.5779E-024	-1.7975E-029	-7.5968E-031	-6.9595E-034	-4.2325E-035	-1.5497E-034
83	0.2328	-2.1146E-024	-2.6916E-024	-2.3448E-029	-9.1599E-031	-8.5040E-034	-4.8791E-035	-1.7692E-034
84	0.2336	-3.3780E-024	-7.3366E-024	-3.8853E-029	-1.3027E-030	-1.2350E-033	-6.3463E-035	-2.2570E-034
85	0.2344	-5.2571E-024	-1.8605E-023	-6.2412E-029	-1.8009E-030	-1.7303E-033	-8.0305E-035	-2.7966E-034
86	0.2352	-8.0339E-024	-4.4044E-023	-9.8041E-029	-2.4405E-030	-2.3608E-033	-9.9702E-035	-3.3849E-034
87	0.2359	-1.2110E-023	-9.7434E-023	-1.5136E-028	-3.2620E-030	-3.1585E-033	-1.2224E-034	-4.0241E-034
88	0.2367	-1.8052E-023	-2.0137E-022	-2.3030E-028	-4.3180E-030	-4.1642E-033	-1.4869E-034	-4.7202E-034
89	0.2375	-2.6642E-023	-3.8858E-022	-3.4586E-028	-5.6743E-030	-5.4269E-033	-1.7992E-034	-5.4815E-034
90	0.2383	-3.8933E-023	-6.9985E-022	-5.1285E-028	-7.4103E-030	-7.0035E-033	-2.1688E-034	-6.3161E-034
91	0.2391	-5.6305E-023	-1.1773E-021	-7.5052E-028	-9.6173E-030	-8.9551E-033	-2.6053E-034	-7.2298E-034
92	0.2398	-8.0490E-023	-1.8549E-021	-1.0829E-027	-1.2395E-029	-1.1343E-032	-3.1171E-034	-8.2251E-034
93	0.2406	-1.1359E-022	-2.7507E-021	-1.5387E-027	-1.5846E-029	-1.4224E-032	-3.7110E-034	-9.2999E-034
94	0.2414	-1.5804E-022	-3.8666E-021	-2.1507E-027	-2.0070E-029	-1.7644E-032	-4.3911E-034	-1.0448E-033
95	0.2422	-2.1660E-022	-5.1937E-021	-2.9550E-027	-2.5159E-029	-2.1635E-032	-5.1591E-034	-1.1660E-033
96	0.2430	-2.9228E-022	-6.7187E-021	-3.9895E-027	-3.1193E-029	-2.6212E-032	-6.0140E-034	-1.2924E-033
97	0.2437	-3.8832E-022	-8.4282E-021	-5.2930E-027	-3.8236E-029	-3.1377E-032	-6.9526E-034	-1.4228E-033
98	0.2445	-5.0811E-022	-1.0310E-020	-6.9044E-027	-4.6342E-029	-3.7116E-032	-7.9702E-034	-1.5559E-033
99	0.2453	-6.5517E-022	-1.2356E-020	-8.8610E-027	-5.5547E-029	-4.3404E-032	-9.0609E-034	-1.6905E-033
100	0.2461	-8.3312E-022	-1.4545E-020	-1.1199E-026	-6.5879E-029	-5.0206E-032	-1.0218E-033	-1.8258E-033
101	0.2469	-1.0457E-021	-1.6864E-020	-1.3951E-026	-7.7348E-029	-5.7478E-032	-1.1435E-033	-1.9605E-033
102	0.2484	-1.5864E-021	-2.1845E-020	-2.0779E-026	-1.0360E-028	-7.3180E-032	-1.4003E-033	-2.2243E-033
103	0.2500	-2.2806E-021	-2.7177E-020	-2.9221E-026	-1.3284E-028	-8.9256E-032	-1.6542E-033	-2.4602E-033
104	0.2516	-3.1399E-021	-3.2731E-020	-3.9252E-026	-1.6458E-028	-1.0524E-031	-1.8993E-033	-2.6657E-033
105	0.2531	-4.1718E-021	-3.8335E-020	-5.0791E-026	-1.9840E-028	-1.2082E-031	-2.1329E-033	-2.8445E-033
106	0.2562	-6.7682E-021	-4.9045E-020	-7.7912E-026	-2.7119E-028	-1.5023E-031	-2.5639E-033	-3.1421E-033
107	0.2594	-9.8924E-021	-5.8593E-020	-1.0757E-025	-3.4288E-028	-1.7367E-031	-2.8895E-033	-3.3298E-033
108	0.2625	-1.3431E-020	-6.6566E-020	-1.3806E-025	-4.1181E-028	-1.9159E-031	-3.1260E-033	-3.4427E-033
109	0.2656	-1.7257E-020	-7.2889E-020	-1.6800E-025	-4.7725E-028	-2.0490E-031	-3.2926E-033	-3.5103E-033
110	0.2688	-2.1246E-020	-7.7699E-020	-1.9634E-025	-5.3894E-028	-2.1450E-031	-3.4057E-033	-3.5514E-033
111	0.2750	-2.9350E-020	-8.3447E-020	-2.4629E-025	-6.5276E-028	-2.2632E-031	-3.5336E-033	-3.6060E-033
112	0.2812	-3.7141E-020	-8.6295E-020	-2.8500E-025	-7.5209E-028	-2.2995E-031	-3.5510E-033	-3.6198E-033
113	0.2875	-4.4351E-020	-8.7360E-020	-3.1299E-025	-8.3984E-028	-2.2858E-031	-3.5061E-033	-3.6158E-033
114	0.2938	-5.0851E-020	-8.7412E-020	-3.3159E-025	-9.1792E-028	-2.2411E-031	-3.4249E-033	-3.6035E-033
115	0.3000	-5.6604E-020	-8.6933E-020	-3.4239E-025	-9.8760E-028	-2.1768E-031	-3.3220E-033	-3.5859E-033
116	0.3063	-6.1628E-020	-8.6215E-020	-3.4695E-025	-1.0498E-027	-2.1003E-031	-3.2065E-033	-3.5641E-033
117	0.3125	-6.5971E-020	-8.5423E-020	-3.4669E-025	-1.1052E-027	-2.0166E-031	-3.0842E-033	-3.5383E-033
118	0.3188	-6.9695E-020	-8.4651E-020	-3.4282E-025	-1.1544E-027	-1.9293E-031	-2.9591E-033	-3.5088E-033
119	0.3250	-7.2868E-020	-8.3943E-020	-3.3633E-025	-1.1979E-027	-1.8410E-031	-2.8343E-033	-3.4758E-033
120	0.3313	-7.5556E-020	-8.3319E-020	-3.2804E-025	-1.2363E-027	-1.7536E-031	-2.7117E-033	-3.4399E-033
121	0.3375	-7.7821E-020	-8.2784E-020	-3.1858E-025	-1.2698E-027	-1.6685E-031	-2.5929E-033	-3.4013E-033
122	0.3438	-7.9717E-020	-8.2334E-020	-3.0845E-025	-1.2991E-027	-1.5867E-031	-2.4788E-033	-3.3607E-033
123	0.3500	-8.1289E-020	-8.1967E-020	-2.9801E-025	-1.3242E-027	-1.5089E-031	-2.3703E-033	-3.3184E-033
124	0.3625	-8.3523E-020	-8.1495E-020	-2.7718E-025	-1.3617E-027	-1.3664E-031	-2.1709E-033	-3.2285E-033
125	0.3750	-8.5039E-020	-8.1215E-020	-2.5747E-025	-1.3890E-027	-1.2410E-031	-1.9945E-033	-3.1389E-033
126	0.3875	-8.6021E-020	-8.1077E-020	-2.3937E-025	-1.4082E-027	-1.1315E-031	-1.8394E-033	-3.0512E-033
127	0.4000	-8.6607E-020	-8.1055E-020	-2.2301E-025	-1.4209E-027	-1.0363E-031	-1.7037E-033	-2.9670E-033
128	0.4125	-8.6898E-020	-8.1028E-020	-2.0840E-025	-1.4284E-027	-9.5381E-032	-1.5850E-033	-2.8870E-033
129	0.4250	-8.6949E-020	-8.1054E-020	-1.9527E-025	-1.4324E-027	-8.8164E-032	-1.4804E-033	-2.8116E-033
130	0.4375	-8.6863E-020	-8.0977E-020	-1.8366E-025	-1.4332E-027	-8.1924E-032	-1.3894E-033	-2.7412E-033

131	0.4500	-8.6595E-020	-8.0922E-020	-1.7339E-025	-1.4319E-027	-7.6512E-032	-1.3094E-033	-2.6771E-033
132	0.4625	-8.6208E-020	-8.0990E-020	-1.6417E-025	-1.4298E-027	-7.1741E-032	-1.2388E-033	-2.6167E-033
133	0.4750	-8.5544E-020	-7.9234E-020	-1.5583E-025	-1.4218E-027	-6.7589E-032	-1.1760E-033	-2.5600E-033
134	0.4812	-8.5122E-020	-7.7403E-020	-1.5163E-025	-1.4152E-027	-6.5646E-032	-1.1473E-033	-2.5254E-033
135	0.4875	-8.4354E-020	-7.2891E-020	-1.4825E-025	-1.4080E-027	-6.3954E-032	-1.1223E-033	-2.4981E-033
136	0.4906	-8.3966E-020	-7.1376E-020	-1.4661E-025	-1.3999E-027	-6.3218E-032	-1.1099E-033	-2.4821E-033
137	0.4938	-8.3452E-020	-6.9176E-020	-1.4525E-025	-1.3953E-027	-6.2741E-032	-1.1008E-033	-2.4707E-033
138	0.4969	-8.3240E-020	-6.7542E-020	-1.4442E-025	-1.3894E-027	-6.2319E-032	-1.0946E-033	-2.4501E-033
139	0.5000	-8.3240E-020	-6.7542E-020	-1.4442E-025	-1.3894E-027	-6.2319E-032	-1.0946E-033	-2.4501E-033

X(cm) MOLE FRACTIONS:

		C2H	C2H2	C2H3	C2H4	C2H5	C2H6	HCCO
1	0.0000	-4.0654E-105	-1.2062E-090	-1.2493E-100	-9.3251E-092	-2.4685E-099	-1.0831E-093	-3.2195E-099
2	0.0500	-2.1973E-103	-6.5796E-089	-6.8747E-099	-5.1684E-090	-1.4828E-097	-6.5544E-092	-1.1776E-097
3	0.0750	-4.7191E-102	-1.3951E-087	-1.5381E-097	-1.1128E-088	-4.0720E-096	-1.5364E-090	-2.9614E-096
4	0.1000	-1.2987E-100	-3.8318E-086	-4.2558E-096	-3.1051E-087	-1.9781E-094	-4.6778E-089	-9.4721E-095
5	0.1125	-1.4502E-099	-4.2751E-085	-4.7554E-095	-3.5152E-086	-6.0940E-093	-5.7425E-088	-1.2217E-093
6	0.1250	-2.0463E-098	-6.0270E-084	-6.7120E-094	-5.0323E-085	-2.1524E-091	-8.9499E-087	-1.9944E-092
7	0.1313	-1.2547E-097	-3.6938E-083	-4.1165E-093	-3.1256E-084	-3.2053E-090	-5.9870E-086	-1.4038E-091
8	0.1344	-4.4162E-097	-1.2999E-082	-1.4494E-092	-1.1127E-083	-1.9690E-089	-2.2739E-085	-5.6143E-091
9	0.1375	-1.8162E-096	-5.3445E-082	-5.9660E-092	-4.6343E-083	-1.2486E-088	-1.0180E-084	-2.6431E-090
10	0.1383	-2.8788E-096	-8.4709E-082	-9.4593E-092	-7.3865E-083	-2.3954E-088	-1.6752E-084	-4.5662E-090
11	0.1391	-4.8306E-096	-1.4213E-081	-1.5881E-091	-1.2479E-082	-4.8140E-088	-2.9435E-084	-8.2993E-090
12	0.1398	-8.4158E-096	-2.4760E-081	-2.7687E-091	-2.1902E-082	-9.8939E-088	-5.3912E-084	-1.5643E-089
13	0.1406	-1.5001E-095	-4.4132E-081	-4.9397E-091	-3.9338E-082	-2.0545E-087	-1.0115E-083	-3.0110E-089
14	0.1414	-2.7097E-095	-7.9712E-081	-8.9337E-091	-7.1602E-082	-4.2862E-087	-1.9232E-083	-5.8558E-089
15	0.1422	-4.9315E-095	-1.4506E-080	-1.6286E-090	-1.3130E-081	-8.9608E-087	-3.6827E-083	-1.1421E-088
16	0.1438	-1.4953E-094	-4.3981E-080	-4.9620E-090	-4.0301E-081	-3.3657E-086	-1.2110E-082	-3.8139E-088
17	0.1469	-8.5333E-094	-2.5090E-079	-2.8811E-089	-2.3327E-080	-2.5597E-085	-7.5988E-082	-2.4524E-087
18	0.1500	-3.9146E-093	-1.1504E-078	-1.3983E-088	-1.0826E-079	-1.6659E-084	-3.7747E-081	-1.2955E-086
19	0.1625	-1.1947E-091	-3.4852E-077	-7.5325E-087	-3.3371E-078	-8.3251E-083	-1.2798E-079	-5.4854E-085
20	0.1656	-3.9576E-091	-1.1377E-076	-5.1672E-086	-1.1008E-077	-5.9035E-082	-4.4777E-079	-3.3746E-084
21	0.1688	-1.6497E-090	-4.5684E-076	-5.0098E-085	-4.4773E-077	-3.8163E-081	-1.9571E-078	-3.5552E-083
22	0.1750	-2.1247E-089	-4.5876E-075	-2.4992E-083	-4.5684E-076	-6.2402E-080	-2.1819E-077	-1.7589E-081
23	0.1875	-2.7279E-087	-9.5801E-074	-5.9854E-081	-9.6900E-075	-2.5440E-078	-5.0482E-076	-3.5473E-079
24	0.1938	-1.9757E-085	-5.9933E-073	-2.3368E-079	-6.1397E-074	-3.8205E-077	-3.4408E-075	-1.7556E-077
25	0.2000	-1.9761E-083	-4.4731E-072	-9.0111E-078	-4.6466E-073	-5.2691E-076	-2.8210E-074	-7.9010E-076
26	0.2031	-3.2948E-082	-1.6133E-071	-8.7064E-077	-1.6942E-072	-2.8690E-075	-1.0957E-073	-1.0109E-074
27	0.2047	-1.6993E-081	-3.6590E-071	-3.3391E-076	-3.8762E-072	-8.0303E-075	-2.6337E-073	-5.1207E-074
28	0.2063	-9.6368E-081	-9.1259E-071	-1.3864E-075	-9.7657E-072	-2.3841E-074	-7.0199E-073	-2.6794E-073
29	0.2078	-5.5811E-080	-2.3732E-070	-5.9004E-075	-2.5665E-071	-7.1143E-074	-1.9501E-072	-1.4293E-072
30	0.2086	-1.4155E-079	-4.0187E-070	-1.2980E-074	-4.3744E-071	-1.2856E-073	-3.4336E-072	-3.8445E-072
31	0.2094	-3.7060E-079	-7.0381E-070	-2.9441E-074	-7.7160E-071	-2.3915E-073	-6.2747E-072	-1.0400E-071
32	0.2102	-9.5154E-079	-1.2577E-069	-6.7974E-074	-1.3897E-070	-4.4986E-073	-1.1695E-071	-2.8602E-071
33	0.2109	-2.4351E-078	-2.2735E-069	-1.5772E-073	-2.5378E-070	-8.4567E-073	-2.1994E-071	-7.9846E-071
34	0.2113	-5.5103E-078	-3.0988E-069	-2.4631E-073	-3.4809E-070	-1.1682E-072	-3.0543E-071	-1.4157E-070
35	0.2117	-1.5297E-077	-4.2677E-069	-3.8767E-073	-4.8018E-070	-1.6258E-072	-4.2902E-071	-2.5171E-070
36	0.2121	-3.9613E-077	-5.9222E-069	-6.1231E-073	-6.5977E-070	-2.2694E-072	-6.0693E-071	-4.4806E-070
37	0.2125	-1.9901E-076	-8.2612E-069	-9.6839E-073	-8.9426E-070	-3.1610E-072	-8.6292E-071	-8.0368E-070
38	0.2129	-1.0597E-076	-1.1569E-068	-1.5438E-072	-1.2005E-069	-4.4565E-072	-1.2320E-070	-1.4079E-069
39	0.2133	-7.8266E-077	-1.6249E-068	-2.4661E-072	-1.6275E-069	-6.2805E-072	-1.7647E-070	-2.4476E-069
40	0.2137	-1.0450E-076	-2.2870E-068	-3.9529E-072	-2.2319E-069	-8.8695E-072	-2.5356E-070	-4.3156E-069
41	0.2141	-1.6994E-076	-3.2232E-068	-6.3519E-072	-3.0906E-069	-1.2565E-071	-3.6533E-070	-7.7708E-069
42	0.2145	-2.8250E-076	-4.5467E-068	-1.0228E-071	-4.3115E-069	-1.7859E-071	-5.2745E-070	-1.4253E-068
43	0.2148	-4.4991E-076	-6.4169E-068	-1.6518E-071	-6.0827E-069	-2.5492E-071	-7.6291E-070	-2.6317E-068
44	0.2156	-4.5965E-076	-1.2469E-067	-4.1269E-071	-1.1861E-068	-5.0749E-071	-1.5508E-069	-7.2721E-068
45	0.2164	-3.4103E-075	-2.3499E-067	-9.8379E-071	-2.2546E-068	-9.7642E-071	-3.0400E-069	-1.3351E-067
46	0.2172	-8.9480E-075	-4.3564E-067	-2.2875E-070	-4.2223E-068	-1.8470E-070	-5.8365E-069	-1.2368E-067
47	0.2180	-2.2660E-074	-8.0000E-067	-5.2295E-070	-7.8440E-068	-3.4560E-070	-1.1056E-068	-1.0833E-067
48	0.2188	-5.6801E-074	-1.4602E-066	-1.1830E-069	-1.4506E-067	-6.4191E-070	-2.0727E-068	-1.1486E-067
49	0.2195	-1.4154E-073	-2.6534E-066	-2.6550E-069	-2.6754E-067	-1.1856E-069	-3.8503E-068	-1.6726E-067
50	0.2203	-3.5156E-073	-4.8043E-066	-5.9133E-069	-4.9250E-067	-2.1797E-069	-7.0867E-068	-3.2541E-067
51	0.2211	-8.7212E-073	-8.6697E-066	-1.3075E-068	-9.0535E-067	-3.9895E-069	-1.2917E-067	-7.6418E-067
52	0.2219	-2.1750E-072	-1.5594E-065	-2.8819E-068	-1.6622E-066	-7.2689E-069	-2.3296E-067	-2.0095E-066
53	0.2234	-1.2148E-071	-4.5653E-065	-1.2002E-067	-5.0510E-066	-2.1615E-068	-6.7468E-067	-1.1849E-065
54	0.2250	-6.2426E-071	-1.2263E-064	-4.4576E-067	-1.4189E-065	-5.8635E-068	-1.7081E-066	-7.2282E-065
55	0.2258	-1.4633E-070	-2.0608E-064	-8.9066E-067	-2.4629E-065	-9.9317E-068	-2.6943E-066	-2.0434E-064
56	0.2266	-3.4947E-070	-3.5266E-064	-1.8137E-066	-4.3611E-065	-1.7115E-067	-4.2778E-066	-5.6231E-064
57	0.2270	-5.4948E-070	-4.6725E-064	-2.6433E-066	-5.8880E-065	-2.2752E-067	-5.4132E-066	-9.6079E-064
58	0.2273	-8.7170E-070	-6.2409E-064	-3.8944E-066	-8.0166E-065	-3.0479E-067	-6.8801E-066	-1.6344E-063
59	0.2277	-1.3915E-069	-8.3834E-064	-5.7846E-066	-1.0976E-064	-4.1027E-067	-8.7658E-066	-2.7690E-063

60	0.2279	-1.7669E-069	-9.7473E-064	-7.0913E-066	-1.2886E-064	-4.7733E-067	-9.9058E-066	-3.6219E-063
61	0.2281	-2.2491E-069	-1.1357E-063	-8.7206E-066	-1.5161E-064	-5.5642E-067	-1.1206E-065	-4.7351E-063
62	0.2283	-2.8695E-069	-1.3256E-063	-1.0753E-065	-1.7866E-064	-6.4954E-067	-1.2687E-065	-6.1863E-063
63	0.2285	-3.6683E-069	-1.5494E-063	-1.3287E-065	-2.1082E-064	-7.5906E-067	-1.4370E-065	-8.0743E-063
64	0.2287	-4.6979E-069	-1.8130E-063	-1.6448E-065	-2.4901E-064	-8.8770E-067	-1.6282E-065	-1.0525E-062
65	0.2289	-6.0257E-069	-2.1235E-063	-2.0388E-065	-2.9432E-064	-1.0386E-066	-1.8449E-065	-1.3699E-062
66	0.2291	-7.7394E-069	-2.4888E-063	-2.5298E-065	-3.4802E-064	-1.2154E-066	-2.0901E-065	-1.7797E-062
67	0.2293	-9.9528E-069	-2.9184E-063	-3.1412E-065	-4.1162E-064	-1.4223E-066	-2.3672E-065	-2.3075E-062
68	0.2295	-1.2813E-068	-3.4233E-063	-3.9020E-065	-4.8686E-064	-1.6641E-066	-2.6796E-065	-2.9852E-062
69	0.2297	-1.6512E-068	-4.0164E-063	-4.8475E-065	-5.7578E-064	-1.9464E-066	-3.0313E-065	-3.8529E-062
70	0.2299	-2.1298E-068	-4.7128E-063	-6.0215E-065	-6.8079E-064	-2.2753E-066	-3.4266E-065	-4.9604E-062
71	0.2301	-2.7494E-068	-5.5298E-063	-7.4771E-065	-8.0464E-064	-2.6582E-066	-3.8699E-065	-6.3698E-062
72	0.2303	-3.5518E-068	-6.4879E-063	-9.2796E-065	-9.5057E-064	-3.1033E-066	-4.3662E-065	-8.1580E-062
73	0.2305	-4.5912E-068	-7.6107E-063	-1.1508E-064	-1.1223E-063	-3.6199E-066	-4.9209E-065	-1.0420E-061
74	0.2307	-5.9381E-068	-8.9258E-063	-1.4259E-064	-1.3243E-063	-4.2187E-066	-5.5396E-065	-1.3273E-061
75	0.2309	-7.6836E-068	-1.0465E-062	-1.7649E-064	-1.5614E-063	-4.9116E-066	-6.2284E-065	-1.6861E-061
76	0.2311	-9.9457E-068	-1.2266E-062	-2.1819E-064	-1.8395E-063	-5.7122E-066	-6.9937E-065	-2.1361E-061
77	0.2313	-1.2877E-067	-1.4372E-062	-2.6939E-064	-2.1653E-063	-6.6358E-066	-7.8425E-065	-2.6991E-061
78	0.2314	-1.6677E-067	-1.6832E-062	-3.3216E-064	-2.5464E-063	-7.6996E-066	-8.7820E-065	-3.4019E-061
79	0.2316	-2.1603E-067	-1.9704E-062	-4.0896E-064	-2.9917E-063	-8.9228E-066	-9.8199E-065	-4.2772E-061
80	0.2318	-2.7994E-067	-2.3057E-062	-5.0276E-064	-3.5114E-063	-1.0327E-065	-1.0964E-064	-5.3654E-061
81	0.2320	-3.6309E-067	-2.6966E-062	-6.1716E-064	-4.1169E-063	-1.1935E-065	-1.2223E-064	-6.7165E-061
82	0.2324	-6.0655E-067	-3.6723E-062	-9.2064E-064	-5.6246E-063	-1.5837E-065	-1.5111E-064	-1.0392E-060
83	0.2328	-1.0117E-066	-4.9702E-062	-1.3572E-063	-7.6175E-063	-2.0808E-065	-1.8520E-064	-1.5903E-060
84	0.2336	-2.6900E-066	-8.8385E-062	-2.7947E-063	-1.3480E-062	-3.4608E-065	-2.7080E-064	-3.5123E-060
85	0.2344	-6.9072E-066	-1.5251E-061	-5.4470E-063	-2.2886E-062	-5.5057E-065	-3.8107E-064	-7.3771E-060
86	0.2352	-1.7243E-065	-2.5857E-061	-1.0201E-062	-3.7711E-062	-8.4773E-065	-5.2048E-064	-1.4938E-059
87	0.2359	-4.2004E-065	-4.3377E-061	-1.8500E-062	-6.0658E-062	-1.2715E-064	-6.9455E-064	-2.9439E-059
88	0.2367	-1.0001E-064	-7.2316E-061	-3.2650E-062	-9.5553E-062	-1.8656E-064	-9.1002E-064	-5.6803E-059
89	0.2375	-2.3291E-064	-1.2013E-060	-5.6232E-062	-1.4771E-061	-2.6852E-064	-1.1749E-063	-1.0764E-058
90	0.2383	-5.3071E-064	-1.9918E-060	-9.4672E-062	-2.2434E-061	-3.7990E-064	-1.4980E-063	-2.0057E-058
91	0.2391	-1.1829E-063	-3.2975E-060	-1.5594E-061	-3.3503E-061	-5.2907E-064	-1.8890E-063	-3.6729E-058
92	0.2398	-2.5766E-063	-5.4482E-060	-2.5134E-061	-4.9218E-061	-7.2594E-064	-2.3569E-063	-6.6008E-058
93	0.2406	-5.4779E-063	-8.9706E-060	-3.9634E-061	-7.1137E-061	-9.8192E-064	-2.9102E-063	-1.1620E-057
94	0.2414	-1.1348E-062	-1.4689E-059	-6.1137E-061	-1.0116E-060	-1.3097E-063	-3.5554E-063	-1.9999E-057
95	0.2422	-2.2869E-062	-2.3861E-059	-9.2249E-061	-1.4154E-060	-1.7228E-063	-4.2972E-063	-3.3606E-057
96	0.2430	-4.4762E-062	-3.8358E-059	-1.3618E-060	-1.9486E-060	-2.2354E-063	-5.1375E-063	-5.5083E-057
97	0.2437	-8.5008E-062	-6.0887E-059	-1.9680E-060	-2.6403E-060	-2.8619E-063	-6.0756E-063	-8.8044E-057
98	0.2445	-1.5656E-061	-9.5266E-059	-2.7862E-060	-3.5224E-060	-3.6163E-063	-7.1085E-063	-1.3727E-056
99	0.2453	-2.7968E-061	-1.4676E-058	-3.8687E-060	-4.6292E-060	-4.5122E-063	-8.2309E-063	-2.0891E-056
100	0.2461	-4.8509E-061	-2.2252E-058	-5.2752E-060	-5.9969E-060	-5.5624E-063	-9.4346E-063	-3.1069E-056
101	0.2469	-8.1902E-061	-3.3213E-058	-7.0730E-060	-7.6624E-060	-6.7775E-063	-1.0708E-062	-4.5227E-056
102	0.2484	-2.1022E-060	-6.9149E-058	-1.2051E-059	-1.1989E-059	-9.7070E-063	-1.3406E-062	-8.9637E-056
103	0.2500	-4.7556E-060	-1.3134E-057	-1.8959E-059	-1.7539E-059	-1.3101E-062	-1.6025E-062	-1.6188E-055
104	0.2516	-9.7360E-060	-2.3216E-057	-2.8051E-059	-2.4324E-059	-1.6869E-062	-1.8416E-062	-2.7118E-055
105	0.2531	-1.8384E-059	-3.8692E-057	-3.9523E-059	-3.2318E-059	-2.0920E-062	-2.0512E-062	-4.2725E-055
106	0.2562	-5.3141E-059	-9.2031E-057	-6.9909E-059	-5.1695E-059	-2.9568E-062	-2.3761E-062	-9.1709E-055
107	0.2594	-1.2126E-058	-1.8069E-056	-1.0620E-058	-7.2387E-059	-3.7148E-062	-2.5160E-062	-1.6500E-054
108	0.2625	-2.3593E-058	-3.1174E-056	-1.4571E-058	-9.2630E-059	-4.3151E-062	-2.5107E-062	-2.6286E-054
109	0.2656	-4.0870E-058	-4.8921E-056	-1.8605E-058	-1.1129E-058	-4.7516E-062	-2.4146E-062	-3.8352E-054
110	0.2688	-6.4848E-058	-7.1434E-056	-2.2545E-058	-1.2778E-058	-5.0424E-062	-2.2709E-062	-5.2391E-054
111	0.2750	-1.3528E-057	-1.3075E-055	-2.9875E-058	-1.5440E-058	-5.3179E-062	-1.9535E-062	-8.5161E-054
112	0.2812	-2.3609E-057	-2.0593E-055	-3.5782E-058	-1.7167E-058	-5.2583E-062	-1.6299E-062	-1.2150E-053
113	0.2875	-3.6693E-057	-2.9454E-055	-4.0309E-058	-1.8165E-058	-5.0170E-062	-1.3428E-062	-1.5928E-053
114	0.2938	-5.2550E-057	-3.9383E-055	-4.3634E-058	-1.8653E-058	-4.6942E-062	-1.1030E-062	-1.9695E-053
115	0.3000	-7.0850E-057	-5.0134E-055	-4.5965E-058	-1.8799E-058	-4.3464E-062	-9.0756E-063	-2.3348E-053
116	0.3063	-9.1233E-057	-6.1500E-055	-4.7500E-058	-1.8724E-058	-4.0035E-062	-7.4980E-063	-2.6824E-053
117	0.3125	-1.1335E-056	-7.3328E-055	-4.8422E-058	-1.8516E-058	-3.6814E-062	-6.2291E-063	-3.0093E-053
118	0.3188	-1.3689E-056	-8.5504E-055	-4.8881E-058	-1.8235E-058	-3.3866E-062	-5.2093E-063	-3.3149E-053
119	0.3250	-1.6158E-056	-9.7959E-055	-4.9010E-058	-1.7923E-058	-3.1218E-062	-4.3891E-063	-3.5998E-053
120	0.3313	-1.8723E-056	-1.1066E-054	-4.8915E-058	-1.7609E-058	-2.8869E-062	-3.7284E-063	-3.8664E-053
121	0.3375	-2.1366E-056	-1.2359E-054	-4.8678E-058	-1.7314E-058	-2.6803E-062	-3.1950E-063	-4.1168E-053
122	0.3438	-2.4074E-056	-1.3674E-054	-4.8363E-058	-1.7048E-058	-2.4997E-062	-2.7634E-063	-4.3536E-053
123	0.3500	-2.6827E-056	-1.5008E-054	-4.8012E-058	-1.6818E-058	-2.3427E-062	-2.4135E-063	-4.5782E-053
124	0.3625	-3.2295E-056	-1.7666E-054	-4.7259E-058	-1.6457E-058	-2.0889E-062	-1.8995E-063	-4.9835E-053
125	0.3750	-3.7926E-056	-2.0439E-054	-4.6655E-058	-1.6256E-058	-1.8972E-062	-1.5481E-063	-5.3735E-053
126	0.3875	-4.3726E-056	-2.3347E-054	-4.6270E-058	-1.6208E-058	-1.7535E-062	-1.3047E-063	-5.7572E-053
127	0.4000	-4.9691E-056	-2.6402E-054	-4.6113E-058	-1.6298E-058	-1.6467E-062	-1.1336E-063	-6.1412E-053
128	0.4125	-5.5823E-056	-2.9619E-054	-4.6179E-058	-1.6506E-058	-1.5683E-062	-1.0117E-063	-6.5304E-053
129	0.4250	-6.2163E-056	-3.3003E-054	-4.6493E-058	-1.6839E-058	-1.5130E-062	-9.2539E-064	-6.9329E-053
130	0.4375	-6.8602E-056	-3.6534E-054	-4.6911E-058	-1.7253E-058	-1.4749E-062	-8.6405E-064	-7.3377E-053

131	0.4500	-7.5391E-056	-4.0315E-054	-4.7637E-058	-1.7791E-058	-1.4537E-062	-8.2100E-064	-7.7696E-053
132	0.4625	-8.2765E-056	-4.4472E-054	-4.8774E-058	-1.8510E-058	-1.4542E-062	-8.0106E-064	-8.2753E-053
133	0.4750	-9.1351E-056	-4.9315E-054	-5.0603E-058	-1.9462E-058	-1.4778E-062	-7.9854E-064	-8.8646E-053
134	0.4812	-9.6092E-056	-5.1891E-054	-5.1721E-058	-2.0076E-058	-1.5026E-062	-8.0262E-064	-9.1748E-053
135	0.4875	-1.0214E-055	-5.5307E-054	-5.3792E-058	-2.0933E-058	-1.5416E-062	-8.1322E-064	-9.7088E-053
136	0.4906	-1.0486E-055	-5.6707E-054	-5.4884E-058	-2.1372E-058	-1.5685E-062	-8.2573E-064	-9.9141E-053
137	0.4938	-1.0719E-055	-5.7931E-054	-5.5668E-058	-2.1751E-058	-1.5916E-062	-8.3602E-064	-1.0106E-052
138	0.4969	-1.0816E-055	-5.8549E-054	-5.6497E-058	-2.2042E-058	-1.6115E-062	-8.4441E-064	-1.0137E-052
139	0.5000	-1.0816E-055	-5.8549E-054	-5.6497E-058	-2.2042E-058	-1.6115E-062	-8.4441E-064	-1.0137E-052

	X(cm)	MOLE FRACTIONS:						
		CH2CO	HCCOH	N	NH	NH2	NH3	NNH
1	0.0000	-7.0201E-090	-4.8889E-098	2.0265E-034	5.4237E-028	7.2491E-030	1.1493E-029	1.7964E-019
2	0.0500	-4.4495E-088	-3.0987E-096	6.8152E-033	1.5460E-026	2.1055E-028	4.4833E-028	8.3879E-018
3	0.0750	-1.0909E-086	-7.5967E-095	1.5514E-032	1.9949E-026	3.0855E-028	7.8654E-028	8.8531E-018
4	0.1000	-3.4775E-085	-2.4217E-093	4.2223E-031	2.2493E-026	4.6410E-028	1.5862E-027	8.9173E-018
5	0.1125	-4.4562E-084	-3.1031E-092	1.1000E-029	2.8953E-026	1.4248E-027	4.3201E-027	8.9297E-018
6	0.1250	-7.2639E-083	-5.0582E-091	2.4860E-028	1.0687E-025	1.2128E-026	2.6145E-026	8.9387E-018
7	0.1313	-5.0549E-082	-3.5200E-090	2.2885E-027	5.0669E-025	5.8972E-026	9.2843E-026	8.9440E-018
8	0.1344	-1.9877E-081	-1.3841E-089	9.1770E-027	1.4555E-024	1.6029E-025	2.1830E-025	8.9486E-018
9	0.1375	-9.2487E-081	-6.4403E-089	3.7462E-026	4.4976E-024	4.6842E-025	5.9337E-025	8.9573E-018
10	0.1383	-1.5487E-080	-1.0785E-088	5.8234E-026	6.3011E-024	6.4301E-025	8.0424E-025	8.9612E-018
11	0.1391	-2.7807E-080	-1.9364E-088	9.2511E-026	9.0064E-024	9.0131E-025	1.1282E-024	8.9661E-018
12	0.1398	-5.2136E-080	-3.6305E-088	1.4889E-025	1.3056E-023	1.2828E-024	1.6276E-024	8.9723E-018
13	0.1406	-1.0018E-079	-6.9759E-088	2.4148E-025	1.9108E-023	1.8457E-024	2.3993E-024	8.9803E-018
14	0.1414	-1.9505E-079	-1.3582E-087	3.9335E-025	2.8148E-023	2.6757E-024	3.5944E-024	8.9905E-018
15	0.1422	-3.8239E-079	-2.6628E-087	6.4234E-025	4.1639E-023	3.8988E-024	5.4488E-024	9.0037E-018
16	0.1438	-1.3049E-078	-9.0867E-087	1.6176E-024	8.8532E-023	8.0808E-024	1.2241E-023	9.0419E-018
17	0.1469	-8.5452E-078	-5.9504E-086	7.5231E-024	3.2461E-022	2.8494E-023	4.8196E-023	9.1922E-018
18	0.1500	-4.4015E-077	-3.0650E-085	3.1497E-023	1.0708E-021	8.9586E-023	1.6096E-022	9.5776E-018
19	0.1625	-1.5688E-075	-1.0925E-083	8.6852E-022	2.0317E-020	1.5566E-021	3.0201E-021	1.7218E-017
20	0.1656	-5.6658E-075	-3.9453E-083	3.8834E-021	6.2055E-020	4.1704E-021	6.8042E-021	3.5271E-017
21	0.1688	-2.5736E-074	-1.7921E-082	1.6156E-020	1.9546E-019	1.2017E-020	1.8318E-020	8.0005E-017
22	0.1750	-3.0064E-073	-2.0935E-081	1.5460E-019	1.3385E-018	7.4386E-020	1.1251E-019	3.7949E-016
23	0.1875	-7.2815E-072	-5.0704E-080	3.6110E-018	2.0566E-017	9.8210E-019	1.3738E-018	4.8484E-015
24	0.1938	-5.1608E-071	-3.5935E-079	3.3238E-017	1.1937E-016	4.5834E-018	4.7182E-018	2.9749E-014
25	0.2000	-4.4185E-070	-3.0760E-078	2.8957E-016	7.1193E-016	2.2758E-017	1.8411E-017	1.5846E-013
26	0.2031	-1.7828E-069	-1.2398E-077	1.1505E-015	2.1194E-015	5.8571E-017	3.9322E-017	4.2644E-013
27	0.2047	-4.4263E-069	-3.0732E-077	2.5704E-015	3.9921E-015	1.0136E-016	6.1745E-017	7.1407E-013
28	0.2063	-1.2255E-068	-8.4907E-077	5.9223E-015	7.8075E-015	1.8285E-016	1.0309E-016	1.1887E-012
29	0.2078	-3.5490E-068	-2.4509E-076	1.3779E-014	1.5571E-014	3.3722E-016	1.7960E-016	1.9716E-012
30	0.2086	-6.4353E-068	-4.4289E-076	2.1629E-014	2.2479E-014	4.6570E-016	2.4224E-016	2.5524E-012
31	0.2094	-1.2173E-067	-8.3420E-076	3.4415E-014	3.2874E-014	6.5070E-016	3.3309E-016	3.3068E-012
32	0.2102	-2.3595E-067	-1.6084E-075	5.5169E-014	4.8527E-014	9.1667E-016	4.6527E-016	4.2864E-012
33	0.2109	-4.6375E-067	-3.1401E-075	8.8754E-014	7.2134E-014	1.2984E-015	6.5800E-016	5.5581E-012
34	0.2113	-6.6304E-067	-4.4683E-075	1.1328E-013	8.8468E-014	1.5513E-015	7.8769E-016	6.3356E-012
35	0.2117	-9.6159E-067	-6.4454E-075	1.4514E-013	1.0892E-013	1.8589E-015	9.4814E-016	7.2254E-012
36	0.2121	-1.4082E-066	-9.3883E-075	1.8649E-013	1.3454E-013	2.2326E-015	1.1469E-015	8.2438E-012
37	0.2125	-2.0756E-066	-1.3769E-074	2.4009E-013	1.6665E-013	2.6866E-015	1.3934E-015	9.4096E-012
38	0.2129	-3.0666E-066	-2.0288E-074	3.0949E-013	2.0689E-013	3.2378E-015	1.6993E-015	1.0745E-011
39	0.2133	-4.5490E-066	-2.9991E-074	3.9926E-013	2.5732E-013	3.9065E-015	2.0792E-015	1.2275E-011
40	0.2137	-6.7741E-066	-4.4432E-074	5.1527E-013	3.2053E-013	4.7173E-015	2.5514E-015	1.4029E-011
41	0.2141	-1.0123E-065	-6.5924E-074	6.6504E-013	3.9965E-013	5.6997E-015	3.1388E-015	1.6042E-011
42	0.2145	-1.5173E-065	-9.7913E-074	8.5819E-013	4.9856E-013	6.8892E-015	3.8696E-015	1.8353E-011
43	0.2148	-2.2811E-065	-1.4553E-073	1.1070E-012	6.2192E-013	8.3284E-015	4.7795E-015	2.1009E-011
44	0.2156	-4.9422E-065	-3.1047E-073	1.8187E-012	9.5867E-013	1.2109E-014	7.2683E-015	2.7537E-011
45	0.2164	-5.1221E-065	-6.3781E-073	2.9416E-012	1.4551E-012	1.7452E-014	1.0953E-014	3.6137E-011
46	0.2172	-5.1188E-065	-1.2882E-072	4.7073E-012	2.1765E-012	2.4991E-014	1.6400E-014	4.7503E-011
47	0.2180	-5.2386E-065	-2.5840E-072	7.4727E-012	3.2123E-012	3.5610E-014	2.4437E-014	6.2573E-011
48	0.2188	-5.8956E-065	-5.1744E-072	1.1786E-011	4.6877E-012	5.0557E-014	3.6268E-014	8.2606E-011
49	0.2195	-7.8189E-065	-1.0375E-071	1.8486E-011	6.7817E-012	7.1595E-014	5.3636E-014	1.0929E-010
50	0.2203	-1.2554E-064	-2.0875E-071	2.8851E-011	9.7541E-012	1.0122E-013	7.9042E-014	1.4490E-010
51	0.2211	-2.3529E-064	-4.2224E-071	4.4820E-011	1.3986E-011	1.4299E-013	1.1605E-013	1.9241E-010
52	0.2219	-4.8496E-064	-8.6027E-071	6.9308E-011	2.0044E-011	2.0194E-013	1.6967E-013	2.5578E-010
53	0.2234	-1.9296E-063	-3.1393E-070	1.5660E-010	4.0099E-011	3.9242E-013	3.4719E-013	4.4985E-010
54	0.2250	-7.6278E-063	-1.0918E-069	3.3285E-010	7.8133E-011	7.4144E-013	6.6534E-013	7.8054E-010
55	0.2258	-1.6855E-062	-2.2361E-069	4.8282E-010	1.0917E-010	1.0232E-012	9.1119E-013	1.0224E-009
56	0.2266	-3.7764E-062	-4.7629E-069	6.9815E-010	1.5253E-010	1.4159E-012	1.2459E-012	1.3336E-009
57	0.2270	-5.7920E-062	-7.2193E-069	8.3896E-010	1.8037E-010	1.6686E-012	1.4567E-012	1.5204E-009
58	0.2273	-8.9482E-062	-1.1136E-068	1.0077E-009	2.1331E-010	1.9684E-012	1.7038E-012	1.7314E-009
59	0.2277	-1.3856E-061	-1.7416E-068	1.2089E-009	2.5212E-010	2.3230E-012	1.9927E-012	1.9690E-009

60	0.2279	-1.7315E-061	-2.2003E-068	1.3235E-009	2.7406E-010	2.5241E-012	2.1549E-012	2.0987E-009
61	0.2281	-2.1677E-061	-2.7944E-068	1.4486E-009	2.9787E-010	2.7430E-012	2.3304E-012	2.2361E-009
62	0.2283	-2.7168E-061	-3.5648E-068	1.5849E-009	3.2367E-010	2.9810E-012	2.5202E-012	2.3816E-009
63	0.2285	-3.4062E-061	-4.5648E-068	1.7332E-009	3.5162E-010	3.2395E-012	2.7252E-012	2.5357E-009
64	0.2287	-4.2702E-061	-5.8646E-068	1.8943E-009	3.8184E-010	3.5201E-012	2.9463E-012	2.6986E-009
65	0.2289	-5.3506E-061	-7.5560E-068	2.0692E-009	4.1449E-010	3.8242E-012	3.1846E-012	2.8708E-009
66	0.2291	-6.6987E-061	-9.7593E-068	2.2586E-009	4.4970E-010	4.1534E-012	3.4411E-012	3.0527E-009
67	0.2293	-8.3776E-061	-1.2632E-067	2.4634E-009	4.8763E-010	4.5096E-012	3.7168E-012	3.2447E-009
68	0.2295	-1.0464E-060	-1.6382E-067	2.6846E-009	5.2844E-010	4.8944E-012	4.0129E-012	3.4472E-009
69	0.2297	-1.3051E-060	-2.1279E-067	2.9230E-009	5.7229E-010	5.3096E-012	4.3305E-012	3.6605E-009
70	0.2299	-1.6252E-060	-2.7679E-067	3.1798E-009	6.1934E-010	5.7573E-012	4.6706E-012	3.8852E-009
71	0.2301	-2.0205E-060	-3.6047E-067	3.4557E-009	6.6976E-010	6.2392E-012	5.0344E-012	4.1215E-009
72	0.2303	-2.5077E-060	-4.6990E-067	3.7517E-009	7.2371E-010	6.7575E-012	5.4231E-012	4.3700E-009
73	0.2305	-3.1066E-060	-6.1303E-067	4.0690E-009	7.8136E-010	7.3141E-012	5.8378E-012	4.6310E-009
74	0.2307	-3.8416E-060	-8.0026E-067	4.4084E-009	8.4289E-010	7.9112E-012	6.2797E-012	4.9049E-009
75	0.2309	-4.7417E-060	-1.0452E-066	4.7709E-009	9.0847E-010	8.5509E-012	6.7498E-012	5.1921E-009
76	0.2311	-5.8418E-060	-1.3655E-066	5.1576E-009	9.7827E-010	9.2353E-012	7.2493E-012	5.4929E-009
77	0.2313	-7.1838E-060	-1.7844E-066	5.5693E-009	1.0525E-009	9.9668E-012	7.7793E-012	5.8078E-009
78	0.2314	-8.8179E-060	-2.3320E-066	6.0072E-009	1.1313E-009	1.0747E-011	8.3408E-012	6.1370E-009
79	0.2316	-1.0804E-059	-3.0478E-066	6.4721E-009	1.2149E-009	1.1580E-011	8.9348E-012	6.4810E-009
80	0.2318	-1.3214E-059	-3.9832E-066	6.9651E-009	1.3034E-009	1.2465E-011	9.5623E-012	6.8400E-009
81	0.2320	-1.6134E-059	-5.2056E-066	7.4871E-009	1.3970E-009	1.3407E-011	1.0224E-011	7.2143E-009
82	0.2324	-2.3808E-059	-8.7727E-066	8.6207E-009	1.6003E-009	1.5465E-011	1.1653E-011	8.0103E-009
83	0.2328	-3.4698E-059	-1.4656E-065	9.8754E-009	1.8255E-009	1.7764E-011	1.3222E-011	8.8704E-009
84	0.2336	-6.9907E-059	-3.7846E-065	1.2763E-008	2.3454E-009	2.3127E-011	1.6782E-011	1.0790E-008
85	0.2344	-1.3379E-058	-9.3466E-065	1.6145E-008	2.9594E-009	2.9525E-011	2.0853E-011	1.2974E-008
86	0.2352	-2.4763E-058	-2.2311E-064	2.0021E-008	3.6701E-009	3.6984E-011	2.5383E-011	1.5419E-008
87	0.2359	-4.4709E-058	-5.1628E-064	2.4374E-008	4.4756E-009	4.5469E-011	3.0287E-011	1.8110E-008
88	0.2367	-7.9132E-058	-1.1594E-063	2.9162E-008	5.3694E-009	5.4877E-011	3.5450E-011	2.1022E-008
89	0.2375	-1.3766E-057	-2.5275E-063	3.4323E-008	6.3406E-009	6.5048E-011	4.0730E-011	2.4121E-008
90	0.2383	-2.3565E-057	-5.3480E-063	3.9779E-008	7.3748E-009	7.5773E-011	4.5975E-011	2.7364E-008
91	0.2391	-3.9686E-057	-1.0978E-062	4.5435E-008	8.4544E-009	8.6811E-011	5.1035E-011	3.0702E-008
92	0.2398	-6.5704E-057	-2.1844E-062	5.1190E-008	9.5602E-009	9.7921E-011	5.5774E-011	3.4084E-008
93	0.2406	-1.0680E-056	-4.2106E-062	5.6937E-008	1.0673E-008	1.0887E-010	6.0085E-011	3.7458E-008
94	0.2414	-1.7024E-056	-7.8580E-062	6.2570E-008	1.1773E-008	1.1948E-010	6.3895E-011	4.0775E-008
95	0.2422	-2.6586E-056	-1.4196E-061	6.7989E-008	1.2845E-008	1.2960E-010	6.7169E-011	4.3991E-008
96	0.2430	-4.0649E-056	-2.4833E-061	7.3103E-008	1.3872E-008	1.3914E-010	6.9905E-011	4.7068E-008
97	0.2437	-6.0850E-056	-4.2097E-061	7.7837E-008	1.4844E-008	1.4807E-010	7.2138E-011	4.9975E-008
98	0.2445	-8.9207E-056	-6.9238E-061	8.2128E-008	1.5751E-008	1.5640E-010	7.3923E-011	5.2687E-008
99	0.2453	-1.2817E-055	-1.1066E-060	8.5933E-008	1.6589E-008	1.6418E-010	7.5335E-011	5.5190E-008
100	0.2461	-1.8069E-055	-1.7221E-060	8.9223E-008	1.7354E-008	1.7149E-010	7.6457E-011	5.7475E-008
101	0.2469	-2.5028E-055	-2.6172E-060	9.1985E-008	1.8045E-008	1.7842E-010	7.7373E-011	5.9537E-008
102	0.2484	-4.5408E-055	-5.5894E-060	9.5917E-008	1.9204E-008	1.9144E-010	7.8846E-011	6.2994E-008
103	0.2500	-7.5771E-055	-1.0749E-059	9.8093E-008	2.0114E-008	2.0407E-010	8.0376E-011	6.5679E-008
104	0.2516	-1.1845E-054	-1.9060E-059	9.8788E-008	2.0806E-008	2.1678E-010	8.2313E-011	6.7692E-008
105	0.2531	-1.7567E-054	-3.1666E-059	9.8319E-008	2.1312E-008	2.2985E-010	8.4874E-011	6.9138E-008
106	0.2562	-3.4156E-054	-7.4740E-059	9.4801E-008	2.1864E-008	2.5755E-010	9.2265E-011	7.0640E-008
107	0.2594	-5.6537E-054	-1.4587E-058	8.9873E-008	2.2036E-008	2.8696E-010	1.0214E-010	7.1053E-008
108	0.2625	-8.3849E-054	-2.5014E-058	8.4542E-008	2.1958E-008	3.1728E-010	1.1400E-010	7.0808E-008
109	0.2656	-1.1486E-053	-3.9046E-058	7.9360E-008	2.1722E-008	3.4771E-010	1.2727E-010	7.0178E-008
110	0.2688	-1.4828E-053	-5.6778E-058	7.4590E-008	2.1391E-008	3.7756E-010	1.4145E-010	6.9330E-008
111	0.2750	-2.1877E-053	-1.0339E-057	6.6588E-008	2.0574E-008	4.3371E-010	1.7119E-010	6.7298E-008
112	0.2812	-2.8704E-053	-1.6348E-057	6.0366E-008	1.9687E-008	4.8589E-010	2.0176E-010	6.5127E-008
113	0.2875	-3.4968E-053	-2.3614E-057	5.5640E-008	1.8791E-008	5.3412E-010	2.3272E-010	6.2935E-008
114	0.2938	-4.0538E-053	-3.2054E-057	5.2131E-008	1.7916E-008	5.7871E-010	2.6390E-010	6.0770E-008
115	0.3000	-4.5405E-053	-4.1608E-057	4.9617E-008	1.7077E-008	6.2010E-010	2.9527E-010	5.8655E-008
116	0.3063	-4.9619E-053	-5.2238E-057	4.7925E-008	1.6285E-008	6.5874E-010	3.2688E-010	5.6603E-008
117	0.3125	-5.3272E-053	-6.3932E-057	4.6922E-008	1.5543E-008	6.9508E-010	3.5881E-010	5.4621E-008
118	0.3188	-5.6452E-053	-7.6687E-057	4.6500E-008	1.4856E-008	7.2957E-010	3.9119E-010	5.2713E-008
119	0.3250	-5.9247E-053	-9.0510E-057	4.6568E-008	1.4225E-008	7.6264E-010	4.2414E-010	5.0885E-008
120	0.3313	-6.1745E-053	-1.0543E-056	4.7047E-008	1.3652E-008	7.9474E-010	4.5781E-010	4.9138E-008
121	0.3375	-6.4019E-053	-1.2146E-056	4.7867E-008	1.3136E-008	8.2627E-010	4.9236E-010	4.7475E-008
122	0.3438	-6.6119E-053	-1.3863E-056	4.8966E-008	1.2677E-008	8.5761E-010	5.2795E-010	4.5897E-008
123	0.3500	-6.8079E-053	-1.5688E-056	5.0281E-008	1.2274E-008	8.8904E-010	5.6465E-010	4.4405E-008
124	0.3625	-7.1538E-053	-1.9577E-056	5.3314E-008	1.1627E-008	9.5256E-010	6.4141E-010	4.1690E-008
125	0.3750	-7.4826E-053	-2.3935E-056	5.6705E-008	1.1153E-008	1.0200E-009	7.2487E-010	3.9256E-008
126	0.3875	-7.8017E-053	-2.8784E-056	6.0257E-008	1.0829E-008	1.0932E-009	8.1668E-010	3.7079E-008
127	0.4000	-8.1141E-053	-3.4135E-056	6.3820E-008	1.0631E-008	1.1731E-009	9.1798E-010	3.5132E-008
128	0.4125	-8.4232E-053	-3.9997E-056	6.7293E-008	1.0537E-008	1.2601E-009	1.0296E-009	3.3392E-008
129	0.4250	-8.7346E-053	-4.6409E-056	7.0612E-008	1.0528E-008	1.3542E-009	1.1519E-009	3.1835E-008
130	0.4375	-9.0384E-053	-5.3303E-056	7.3742E-008	1.0586E-008	1.4553E-009	1.2852E-009	3.0441E-008

131	0.4500	-9.3692E-053	-6.0872E-056	7.6673E-008	1.0699E-008	1.5629E-009	1.4293E-009	2.9196E-008
132	0.4625	-9.7398E-053	-6.9210E-056	7.9417E-008	1.0856E-008	1.6764E-009	1.5837E-009	2.8090E-008
133	0.4750	-1.0215E-052	-7.8835E-056	8.2019E-008	1.1054E-008	1.7955E-009	1.7474E-009	2.7128E-008
134	0.4812	-1.0474E-052	-8.4018E-056	8.3305E-008	1.1171E-008	1.8565E-009	1.8313E-009	2.6715E-008
135	0.4875	-1.0893E-052	-9.0128E-056	8.4573E-008	1.1297E-008	1.9168E-009	1.9134E-009	2.6372E-008
136	0.4906	-1.1031E-052	-9.2633E-056	8.5174E-008	1.1361E-008	1.9445E-009	1.9509E-009	2.6238E-008
137	0.4938	-1.1171E-052	-9.4826E-056	8.5700E-008	1.1419E-008	1.9681E-009	1.9826E-009	2.6140E-008
138	0.4969	-1.1255E-052	-9.5674E-056	8.6056E-008	1.1458E-008	1.9835E-009	2.0033E-009	2.6086E-008
139	0.5000	-1.1255E-052	-9.5674E-056	8.6056E-008	1.1458E-008	1.9835E-009	2.0033E-009	2.6086E-008

	X(cm)	MOLE FRACTIONS:						
		NO	NO2	N2O	HNO	CN	HCN	H2CN
1	0.0000	2.3286E-027	1.6519E-032	2.8929E-022	5.2721E-029	-4.7549E-078	-4.0476E-064	-6.7064E-066
2	0.0500	1.0729E-025	8.5605E-031	1.6529E-020	2.3996E-027	-2.2093E-076	-2.2176E-062	-3.7049E-064
3	0.0750	1.6964E-025	1.9143E-030	2.5171E-020	3.7682E-027	-4.7459E-075	-4.7021E-061	-9.9551E-063
4	0.1000	2.3818E-025	5.3273E-030	3.3939E-020	5.2177E-027	-1.3079E-073	-1.2932E-059	-3.1537E-061
5	0.1125	2.9235E-025	2.2212E-029	3.8345E-020	6.9022E-027	-1.4623E-072	-1.4442E-058	-4.0006E-060
6	0.1250	5.3243E-025	2.3762E-028	4.2771E-020	1.7994E-026	-2.0678E-071	-2.0405E-057	-6.1266E-059
7	0.1313	1.2766E-024	1.3595E-027	4.4989E-020	5.3604E-026	-1.2708E-070	-1.2529E-056	-4.0182E-058
8	0.1344	2.8264E-024	4.5854E-027	4.6100E-020	1.2300E-025	-4.4855E-070	-4.4185E-056	-1.4720E-057
9	0.1375	8.0065E-024	1.8046E-026	4.7213E-020	3.3968E-025	-1.8501E-069	-1.8218E-055	-6.2531E-057
10	0.1383	1.1229E-023	2.8087E-026	4.7492E-020	4.6548E-025	-2.9406E-069	-2.8911E-055	-1.0036E-056
11	0.1391	1.6524E-023	4.6098E-026	4.7771E-020	6.6608E-025	-4.9442E-069	-4.8587E-055	-1.7061E-056
12	0.1398	2.5265E-023	7.8406E-026	4.8050E-020	9.8807E-025	-8.6308E-069	-8.4793E-055	-3.0100E-056
13	0.1406	3.9752E-023	1.3636E-025	4.8331E-020	1.5078E-024	-1.5415E-068	-1.5142E-054	-5.4296E-056
14	0.1414	6.3839E-023	2.4033E-025	4.8612E-020	2.3511E-024	-2.7900E-068	-2.7402E-054	-9.9192E-056
15	0.1422	1.0400E-022	4.2685E-025	4.8894E-020	3.7253E-024	-5.0873E-068	-4.9962E-054	-1.8249E-055
16	0.1438	2.6523E-022	1.2441E-024	4.9466E-020	9.0988E-024	-1.5458E-067	-1.5195E-053	-5.6282E-055
17	0.1469	1.2351E-021	6.7717E-024	5.0660E-020	4.0272E-023	-8.8435E-067	-8.6994E-053	-3.2814E-054
18	0.1500	4.7698E-021	2.9851E-023	5.2033E-020	1.4891E-022	-4.0687E-066	-3.9998E-052	-1.5401E-053
19	0.1625	1.1289E-019	8.5504E-022	6.3900E-020	3.3119E-021	-1.2479E-064	-1.2165E-050	-4.8346E-052
20	0.1656	3.0294E-019	2.6978E-021	7.4234E-020	8.2978E-021	-4.1672E-064	-3.9759E-050	-1.6603E-051
21	0.1688	9.9370E-019	1.0392E-020	1.0585E-019	2.5428E-020	-1.7698E-063	-1.6002E-049	-6.9206E-051
22	0.1750	7.8720E-018	9.9064E-020	4.0046E-019	1.8618E-019	-2.4960E-062	-1.6123E-048	-7.2113E-050
23	0.1875	1.2797E-016	1.9624E-018	5.2550E-018	2.7505E-018	-3.4910E-060	-3.3762E-047	-1.5773E-048
24	0.1938	6.1130E-016	1.1394E-017	2.0693E-017	1.1309E-017	-2.4308E-058	-2.1142E-046	-1.0517E-047
25	0.2000	3.4395E-015	7.6666E-017	9.2515E-017	5.2986E-017	-2.2152E-056	-1.5811E-045	-8.2425E-047
26	0.2031	9.8421E-015	2.3449E-016	2.0522E-016	1.2779E-016	-3.6275E-055	-5.7115E-045	-3.0794E-046
27	0.2047	1.8954E-014	4.6372E-016	3.2768E-016	2.1876E-016	-1.8836E-054	-1.2974E-044	-7.1323E-046
28	0.2063	3.9709E-014	9.9394E-016	5.6632E-016	4.0582E-016	-1.0643E-053	-3.2423E-044	-1.8137E-045
29	0.2078	8.7111E-014	2.1937E-015	1.0407E-015	7.9455E-016	-6.0750E-053	-8.4492E-044	-4.7969E-045
30	0.2086	1.3368E-013	3.3262E-015	1.4587E-015	1.1483E-015	-1.5514E-052	-1.4331E-043	-8.1976E-045
31	0.2094	2.1080E-013	5.1499E-015	2.1190E-015	1.7060E-015	-4.0750E-052	-2.5144E-043	-1.4489E-044
32	0.2102	3.3865E-013	8.0584E-015	3.1786E-015	2.5883E-015	-1.0820E-051	-4.5006E-043	-2.6114E-044
33	0.2109	5.5079E-013	1.2638E-014	4.9007E-015	3.9869E-015	-2.8812E-051	-8.1479E-043	-4.7574E-044
34	0.2113	7.0936E-013	1.5873E-014	6.1756E-015	4.9928E-015	-4.7792E-051	-1.1103E-042	-6.5092E-044
35	0.2117	9.2066E-013	2.0020E-014	7.8805E-015	6.2983E-015	-8.0544E-051	-1.5287E-042	-8.9984E-044
36	0.2121	1.2023E-012	2.5317E-014	1.0168E-014	7.9926E-015	-1.3529E-050	-2.1181E-042	-1.2533E-043
37	0.2125	1.5776E-012	3.2052E-014	1.3242E-014	1.0190E-014	-2.2129E-050	-2.9494E-042	-1.7550E-043
38	0.2129	2.0779E-012	4.0574E-014	1.7378E-014	1.3038E-014	-3.7844E-050	-4.1210E-042	-2.4666E-043
39	0.2133	2.7446E-012	5.1298E-014	2.2939E-014	1.6724E-014	-6.3520E-050	-5.7769E-042	-3.4753E-043
40	0.2137	3.6325E-012	6.4709E-014	3.0404E-014	2.1488E-014	-1.0668E-049	-8.1187E-042	-4.9040E-043
41	0.2141	4.8145E-012	8.1370E-014	4.0401E-014	2.7629E-014	-1.7953E-049	-1.1431E-041	-6.9258E-043
42	0.2145	6.3870E-012	1.0192E-013	5.3742E-014	3.5530E-014	-3.0301E-049	-1.6112E-041	-9.7843E-043
43	0.2148	8.4770E-012	1.2706E-013	7.1481E-014	4.5666E-014	-5.1529E-049	-2.2735E-041	-1.3822E-042
44	0.2156	1.4710E-011	1.9341E-013	1.2423E-013	7.4413E-014	-1.4392E-048	-4.4151E-041	-2.6865E-042
45	0.2164	2.4943E-011	2.8317E-013	2.0846E-013	1.1816E-013	-3.6043E-048	-8.2913E-041	-5.0486E-042
46	0.2172	4.1641E-011	4.0070E-013	3.4115E-013	1.8357E-013	-8.9947E-048	-1.5321E-040	-9.2981E-042
47	0.2180	6.8708E-011	5.5040E-013	5.4894E-013	2.7968E-013	-2.2265E-047	-2.8044E-040	-1.6889E-041
48	0.2188	1.1230E-010	7.3677E-013	8.7417E-013	4.1870E-013	-5.4556E-047	-5.1000E-040	-3.0338E-041
49	0.2195	1.8200E-010	9.6474E-013	1.3847E-012	6.1709E-013	-1.3256E-046	-9.2258E-040	-5.3931E-041
50	0.2203	2.9267E-010	1.2401E-012	2.1891E-012	8.9725E-013	-3.2019E-046	-1.6609E-039	-9.4867E-041
51	0.2211	4.6703E-010	1.5691E-012	3.4616E-012	1.2895E-012	-7.7155E-046	-2.9754E-039	-1.6500E-040
52	0.2219	7.3944E-010	1.9567E-012	5.4791E-012	1.8338E-012	-1.8767E-045	-5.3033E-039	-2.8346E-040
53	0.2234	1.7296E-009	2.8754E-012	1.3040E-011	3.5201E-012	-9.7038E-045	-1.5231E-038	-7.5425E-040
54	0.2250	3.6855E-009	3.9204E-012	2.8375E-011	6.2675E-012	-4.6369E-044	-3.9733E-038	-1.7621E-039
55	0.2258	5.3081E-009	4.5483E-012	4.1305E-011	8.2635E-012	-1.0657E-043	-6.5114E-038	-2.6486E-039
56	0.2266	7.6420E-009	5.3087E-012	6.0325E-011	1.0887E-011	-2.4997E-043	-1.0822E-037	-3.9852E-039
57	0.2270	9.1752E-009	5.7576E-012	7.3035E-011	1.2499E-011	-3.9290E-043	-1.4089E-037	-4.8961E-039
58	0.2273	1.1032E-008	6.2675E-012	8.8675E-011	1.4364E-011	-6.2369E-043	-1.8464E-037	-6.0304E-039
59	0.2277	1.3271E-008	6.8467E-012	1.0785E-010	1.6516E-011	-9.9798E-043	-2.4310E-037	-7.4365E-039

60	0.2279	1.4560E-008	7.1663E-012	1.1904E-010	1.7714E-011	-1.2717E-042	-2.7963E-037	-8.2631E-039
61	0.2281	1.5981E-008	7.5088E-012	1.3149E-010	1.9004E-011	-1.6253E-042	-3.2220E-037	-9.1873E-039
62	0.2283	1.7544E-008	7.8759E-012	1.4533E-010	2.0392E-011	-2.0828E-042	-3.7179E-037	-1.0220E-038
63	0.2285	1.9263E-008	8.2690E-012	1.6071E-010	2.1885E-011	-2.6754E-042	-4.2949E-037	-1.1371E-038
64	0.2287	2.1152E-008	8.6896E-012	1.7778E-010	2.3488E-011	-3.4437E-042	-4.9659E-037	-1.2654E-038
65	0.2289	2.3225E-008	9.1393E-012	1.9672E-010	2.5210E-011	-4.4402E-042	-5.7456E-037	-1.4081E-038
66	0.2291	2.5497E-008	9.6197E-012	2.1770E-010	2.7057E-011	-5.7332E-042	-6.6509E-037	-1.5667E-038
67	0.2293	2.7987E-008	1.0133E-011	2.4092E-010	2.9036E-011	-7.4112E-042	-7.7012E-037	-1.7426E-038
68	0.2295	3.0711E-008	1.0680E-011	2.6661E-010	3.1157E-011	-9.5886E-042	-8.9188E-037	-1.9376E-038
69	0.2297	3.3688E-008	1.1263E-011	2.9499E-010	3.3427E-011	-1.2413E-041	-1.0329E-036	-2.1532E-038
70	0.2299	3.6940E-008	1.1884E-011	3.2631E-010	3.5855E-011	-1.6075E-041	-1.1962E-036	-2.3915E-038
71	0.2301	4.0487E-008	1.2546E-011	3.6085E-010	3.8450E-011	-2.0821E-041	-1.3851E-036	-2.6543E-038
72	0.2303	4.4352E-008	1.3250E-011	3.9888E-010	4.1222E-011	-2.6966E-041	-1.6034E-036	-2.9438E-038
73	0.2305	4.8560E-008	1.3998E-011	4.4073E-010	4.4182E-011	-3.4915E-041	-1.8555E-036	-3.2623E-038
74	0.2307	5.3137E-008	1.4795E-011	4.8672E-010	4.7339E-011	-4.5188E-041	-2.1464E-036	-3.6121E-038
75	0.2309	5.8108E-008	1.5641E-011	5.3721E-010	5.0705E-011	-5.8454E-041	-2.4820E-036	-3.9959E-038
76	0.2311	6.3504E-008	1.6539E-011	5.9259E-010	5.4290E-011	-7.5567E-041	-2.8687E-036	-4.4162E-038
77	0.2313	6.9354E-008	1.7494E-011	6.5326E-010	5.8106E-011	-9.7625E-041	-3.3141E-036	-4.8759E-038
78	0.2314	7.5689E-008	1.8507E-011	7.1966E-010	6.2164E-011	-1.2604E-040	-3.8265E-036	-5.3779E-038
79	0.2316	8.2544E-008	1.9582E-011	7.9226E-010	6.6477E-011	-1.6264E-040	-4.4158E-036	-5.9254E-038
80	0.2318	8.9952E-008	2.0722E-011	8.7155E-010	7.1057E-011	-2.0979E-040	-5.0930E-036	-6.5217E-038
81	0.2320	9.7952E-008	2.1931E-011	9.5807E-010	7.5915E-011	-2.7060E-040	-5.8705E-036	-7.1699E-038
82	0.2324	1.1584E-007	2.4561E-011	1.1544E-009	8.6502E-011	-4.4547E-040	-7.7690E-036	-8.6324E-038
83	0.2328	1.3639E-007	2.7476E-011	1.3841E-009	9.8268E-011	-7.3016E-040	-1.0221E-035	-1.0327E-037
84	0.2336	1.8636E-007	3.4211E-011	1.9561E-009	1.2553E-010	-1.8460E-039	-1.7236E-035	-1.4485E-037
85	0.2344	2.4902E-007	4.2124E-011	2.6898E-009	1.5776E-010	-4.4739E-039	-2.8197E-035	-1.9745E-037
86	0.2352	3.2618E-007	5.1331E-011	3.6092E-009	1.9531E-010	-1.0444E-038	-4.5189E-035	-2.6346E-037
87	0.2359	4.1946E-007	6.1927E-011	4.7343E-009	2.3845E-010	-2.3571E-038	-7.1319E-035	-3.4620E-037
88	0.2367	5.3031E-007	7.3975E-011	6.0786E-009	2.8728E-010	-5.1522E-038	-1.1118E-034	-4.5012E-037
89	0.2375	6.5980E-007	8.7494E-011	7.6469E-009	3.4173E-010	-1.0918E-037	-1.7147E-034	-5.8108E-037
90	0.2383	8.0866E-007	1.0246E-010	9.4338E-009	4.0155E-010	-2.2437E-037	-2.6184E-034	-7.4653E-037
91	0.2391	9.7716E-007	1.1883E-010	1.1423E-008	4.6629E-010	-4.4705E-037	-3.9603E-034	-9.5586E-037
92	0.2398	1.1652E-006	1.3648E-010	1.3587E-008	5.3541E-010	-8.6324E-037	-5.9322E-034	-1.2206E-036
93	0.2406	1.3721E-006	1.5531E-010	1.5890E-008	6.0821E-010	-1.6148E-036	-8.7974E-034	-1.5547E-036
94	0.2414	1.5972E-006	1.7517E-010	1.8291E-008	6.8396E-010	-2.9252E-036	-1.2911E-033	-1.9747E-036
95	0.2422	1.8391E-006	1.9591E-010	2.0744E-008	7.6190E-010	-5.1324E-036	-1.8742E-033	-2.5002E-036
96	0.2430	2.0964E-006	2.1738E-010	2.3204E-008	8.4127E-010	-8.7252E-036	-2.6898E-033	-3.1535E-036
97	0.2437	2.3675E-006	2.3942E-010	2.5627E-008	9.2137E-010	-1.4384E-035	-3.8154E-033	-3.9601E-036
98	0.2445	2.6508E-006	2.6191E-010	2.7975E-008	1.0015E-009	-2.3021E-035	-5.3479E-033	-4.9487E-036
99	0.2453	2.9446E-006	2.8473E-010	3.0217E-008	1.0812E-009	-3.5824E-035	-7.4073E-033	-6.1513E-036
100	0.2461	3.2472E-006	3.0778E-010	3.2326E-008	1.1599E-009	-5.4297E-035	-1.0140E-032	-7.6032E-036
101	0.2469	3.5569E-006	3.3098E-010	3.4283E-008	1.2372E-009	-8.0362E-035	-1.3725E-032	-9.3406E-036
102	0.2484	4.1936E-006	3.7769E-010	3.7699E-008	1.3866E-009	-1.6319E-034	-2.4096E-032	-1.3745E-035
103	0.2500	4.8406E-006	4.2404E-010	4.0532E-008	1.5272E-009	-3.0153E-034	-3.9655E-032	-1.9306E-035
104	0.2516	5.4894E-006	4.6967E-010	4.2832E-008	1.6581E-009	-5.1721E-034	-6.2112E-032	-2.6166E-035
105	0.2531	6.1331E-006	5.1430E-010	4.4672E-008	1.7788E-009	-8.3548E-034	-9.3530E-032	-3.4486E-035
106	0.2562	7.3873E-006	6.0015E-010	4.7198E-008	1.9903E-009	-1.8790E-033	-1.9104E-031	-5.5615E-035
107	0.2594	8.5867E-006	6.8021E-010	4.8876E-008	2.1673E-009	-3.5788E-033	-3.3847E-031	-8.0087E-035
108	0.2625	9.7238E-006	7.5413E-010	5.0012E-008	2.3150E-009	-6.0869E-033	-5.4524E-031	-1.0717E-034
109	0.2656	1.0797E-005	8.2208E-010	5.0805E-008	2.4383E-009	-9.5277E-033	-8.1872E-031	-1.3612E-034
110	0.2688	1.1807E-005	8.8451E-010	5.1379E-008	2.5415E-009	-1.3998E-032	-1.1648E-030	-1.6637E-034
111	0.2750	1.3633E-005	9.9426E-010	5.2121E-008	2.6992E-009	-2.6297E-032	-2.0975E-030	-2.3005E-034
112	0.2812	1.5283E-005	1.0910E-009	5.2645E-008	2.8144E-009	-4.2838E-032	-3.2893E-030	-2.8693E-034
113	0.2875	1.6791E-005	1.1786E-009	5.3064E-008	2.8992E-009	-6.3481E-032	-4.7216E-030	-3.3621E-034
114	0.2938	1.8181E-005	1.2601E-009	5.3439E-008	2.9619E-009	-8.7870E-032	-6.3665E-030	-3.7764E-034
115	0.3000	1.9477E-005	1.3379E-009	5.3807E-008	3.0086E-009	-1.1555E-031	-8.1934E-030	-4.1147E-034
116	0.3063	2.0697E-005	1.4136E-009	5.4190E-008	3.0437E-009	-1.4601E-031	-1.0173E-029	-4.3837E-034
117	0.3125	2.1856E-005	1.4887E-009	5.4605E-008	3.0707E-009	-1.7881E-031	-1.2281E-029	-4.5920E-034
118	0.3188	2.2967E-005	1.5645E-009	5.5065E-008	3.0924E-009	-2.1351E-031	-1.4496E-029	-4.7497E-034
119	0.3250	2.4041E-005	1.6418E-009	5.5578E-008	3.1109E-009	-2.4976E-031	-1.6804E-029	-4.8666E-034
120	0.3313	2.5087E-005	1.7213E-009	5.6152E-008	3.1283E-009	-2.8731E-031	-1.9194E-029	-4.9518E-034
121	0.3375	2.6112E-005	1.8035E-009	5.6790E-008	3.1459E-009	-3.2595E-031	-2.1662E-029	-5.0135E-034
122	0.3438	2.7123E-005	1.8888E-009	5.7495E-008	3.1649E-009	-3.6552E-031	-2.4203E-029	-5.0588E-034
123	0.3500	2.8123E-005	1.9773E-009	5.8265E-008	3.1865E-009	-4.0586E-031	-2.6813E-029	-5.0936E-034
124	0.3625	3.0103E-005	2.1637E-009	5.9989E-008	3.2406E-009	-4.8788E-031	-3.2228E-029	-5.1552E-034
125	0.3750	3.2081E-005	2.3638E-009	6.1935E-008	3.3086E-009	-5.7289E-031	-3.7949E-029	-5.2051E-034
126	0.3875	3.4066E-005	2.5768E-009	6.4079E-008	3.3917E-009	-6.6161E-031	-4.4060E-029	-5.2637E-034
127	0.4000	3.6063E-005	2.8016E-009	6.6386E-008	3.4900E-009	-7.5458E-031	-5.0622E-029	-5.3399E-034
128	0.4125	3.8072E-005	3.0369E-009	6.8816E-008	3.6023E-009	-8.5195E-031	-5.7679E-029	-5.4365E-034
129	0.4250	4.0094E-005	3.2810E-009	7.1329E-008	3.7274E-009	-9.5384E-031	-6.5243E-029	-5.5536E-034
130	0.4375	4.2126E-005	3.5324E-009	7.3889E-008	3.8637E-009	-1.0601E-030	-7.3319E-029	-5.6883E-034

131	0.4500	4.4166E-005	3.7895E-009	7.6460E-008	4.0098E-009	-1.1707E-030	-8.1903E-029	-5.8400E-034
132	0.4625	4.6211E-005	4.0501E-009	7.9005E-008	4.1642E-009	-1.2839E-030	-9.0932E-029	-6.0068E-034
133	0.4750	4.8257E-005	4.3115E-009	8.1480E-008	4.3258E-009	-1.3976E-030	-1.0026E-028	-6.1847E-034
134	0.4812	4.9272E-005	4.4402E-009	8.2674E-008	4.4086E-009	-1.4550E-030	-1.0480E-028	-6.2772E-034
135	0.4875	5.0263E-005	4.5637E-009	8.3792E-008	4.4910E-009	-1.5083E-030	-1.0914E-028	-6.3735E-034
136	0.4906	5.0726E-005	4.6202E-009	8.4298E-008	4.5298E-009	-1.5304E-030	-1.1107E-028	-6.4314E-034
137	0.4938	5.1131E-005	4.6687E-009	8.4728E-008	4.5637E-009	-1.5514E-030	-1.1276E-028	-6.4783E-034
138	0.4969	5.1409E-005	4.7012E-009	8.5018E-008	4.5868E-009	-1.5639E-030	-1.1380E-028	-6.5354E-034
139	0.5000	5.1409E-005	4.7012E-009	8.5018E-008	4.5868E-009	-1.5639E-030	-1.1380E-028	-6.5354E-034

	X(cm)	MOLE FRACTIONS:						
		HCNN	HCNO	HOCN	HNCO	NCO	N2	AR
1	0.0000	-1.1949E-076	-4.1002E-068	-1.9405E-069	-4.8197E-063	-2.4520E-069	5.4022E-001	0.0000E+000
2	0.0500	-4.3708E-075	-2.3335E-066	-1.1043E-067	-2.7430E-061	-1.3897E-067	5.4022E-001	0.0000E+000
3	0.0750	-9.6367E-074	-5.1545E-065	-2.4394E-066	-6.0590E-060	-8.8919E-066	5.4022E-001	0.0000E+000
4	0.1000	-2.3556E-072	-1.4765E-063	-6.9876E-065	-1.7356E-058	-5.1037E-064	5.4022E-001	0.0000E+000
5	0.1125	-2.3347E-071	-1.7127E-062	-8.1055E-064	-2.0132E-057	-1.1358E-062	5.4022E-001	0.0000E+000
6	0.1250	-2.7619E-070	-2.5154E-061	-1.1904E-062	-2.9567E-056	-2.5274E-061	5.4022E-001	0.0000E+000
7	0.1313	-1.4486E-069	-1.5974E-060	-7.5599E-062	-1.8777E-055	-2.2972E-060	5.4022E-001	0.0000E+000
8	0.1344	-4.3890E-069	-5.7977E-060	-2.7438E-061	-6.8150E-055	-1.0164E-059	5.4022E-001	0.0000E+000
9	0.1375	-1.5074E-068	-2.4676E-059	-1.1678E-060	-2.9005E-054	-4.9852E-059	5.4022E-001	0.0000E+000
10	0.1383	-2.2167E-068	-3.9703E-059	-1.8789E-060	-4.6669E-054	-8.4763E-059	5.4022E-001	0.0000E+000
11	0.1391	-3.3856E-068	-6.7857E-059	-3.2114E-060	-7.9763E-054	-1.5236E-058	5.4022E-001	0.0000E+000
12	0.1398	-5.3148E-068	-1.2061E-058	-5.7078E-060	-1.4177E-053	-2.8294E-058	5.4022E-001	0.0000E+000
13	0.1406	-8.4995E-068	-2.1944E-058	-1.0385E-059	-2.5794E-053	-5.3484E-058	5.4022E-001	0.0000E+000
14	0.1414	-1.3758E-067	-4.0462E-058	-1.9149E-059	-4.7561E-053	-1.0205E-057	5.4022E-001	0.0000E+000
15	0.1422	-2.2444E-067	-7.5156E-058	-3.5568E-059	-8.8342E-053	-1.9566E-057	5.4022E-001	0.0000E+000
16	0.1438	-5.6835E-067	-2.3547E-057	-1.1144E-058	-2.7679E-052	-6.4322E-057	5.4022E-001	0.0000E+000
17	0.1469	-2.6354E-066	-1.3964E-056	-6.6087E-058	-1.6414E-051	-4.0856E-056	5.4022E-001	0.0000E+000
18	0.1500	-1.0646E-065	-6.6143E-056	-3.1303E-057	-7.7747E-051	-2.1295E-055	5.4022E-001	0.0000E+000
19	0.1625	-5.3715E-064	-2.0982E-054	-9.9298E-056	-2.4663E-049	-7.8218E-054	5.4022E-001	0.0000E+000
20	0.1656	-5.2957E-062	-7.0443E-054	-3.3337E-055	-8.2800E-049	-3.4833E-053	5.4022E-001	0.0000E+000
21	0.1688	-1.1273E-059	-2.9274E-053	-1.3854E-054	-3.4409E-048	-1.7108E-052	5.4022E-001	0.0000E+000
22	0.1750	-7.4895E-057	-3.0677E-052	-1.4518E-053	-3.6058E-047	-2.0906E-051	5.4022E-001	0.0000E+000
23	0.1875	-1.9088E-053	-6.6800E-051	-3.1614E-052	-7.8516E-046	-5.6991E-050	5.4024E-001	0.0000E+000
24	0.1938	-2.0435E-050	-4.3274E-050	-2.0480E-051	-5.0860E-045	-5.2097E-049	5.4026E-001	0.0000E+000
25	0.2000	-8.0085E-048	-3.3565E-049	-1.5884E-050	-3.9442E-044	-5.1358E-048	5.4032E-001	0.0000E+000
26	0.2031	3.0125E-045	-1.2486E-048	-5.9081E-050	-1.4663E-043	-2.3038E-047	5.4039E-001	0.0000E+000
27	0.2047	7.2019E-045	-2.9022E-048	-1.3732E-049	-3.4060E-043	-5.9642E-047	5.4044E-001	0.0000E+000
28	0.2063	5.8816E-044	-7.4458E-048	-3.5230E-049	-8.7316E-043	-1.6786E-046	5.4052E-001	0.0000E+000
29	0.2078	5.3988E-043	-1.9950E-047	-9.4308E-049	-2.3348E-042	-4.8897E-046	5.4063E-001	0.0000E+000
30	0.2086	2.8352E-043	-3.4492E-047	-1.6259E-048	-4.0214E-042	-8.8972E-046	5.4070E-001	0.0000E+000
31	0.2094	-1.3971E-042	-6.1902E-047	-2.9055E-048	-7.1774E-042	-1.6793E-045	5.4079E-001	0.0000E+000
32	0.2102	-4.7163E-042	-1.1211E-046	-5.3029E-048	-1.3081E-041	-3.2387E-045	5.4089E-001	0.0000E+000
33	0.2109	-5.4851E-041	-2.0639E-046	-9.7950E-048	-2.4120E-041	-6.3322E-045	5.4101E-001	0.0000E+000
34	0.2113	-7.7179E-041	-2.7990E-046	-1.3513E-047	-3.3237E-041	-9.0341E-045	5.4107E-001	0.0000E+000
35	0.2117	-1.3028E-040	-3.7826E-046	-1.8854E-047	-4.6313E-041	-1.3058E-044	5.4115E-001	0.0000E+000
36	0.2121	-1.7844E-040	-5.0735E-046	-2.6525E-047	-6.5061E-041	-1.9058E-044	5.4122E-001	0.0000E+000
37	0.2125	-1.0578E-040	-5.9792E-046	-3.7542E-047	-9.1937E-041	-2.8021E-044	5.4131E-001	0.0000E+000
38	0.2129	-1.5106E-040	-6.8529E-046	-5.3364E-047	-1.3045E-040	-4.1439E-044	5.4140E-001	0.0000E+000
39	0.2133	-9.6890E-041	-7.8042E-046	-7.6084E-047	-1.8563E-040	-6.1583E-044	5.4150E-001	0.0000E+000
40	0.2137	-5.4538E-041	-9.0200E-046	-1.0871E-046	-2.6464E-040	-9.1914E-044	5.4161E-001	0.0000E+000
41	0.2141	-4.1726E-041	-1.0689E-045	-1.5554E-046	-3.7775E-040	-1.3773E-043	5.4173E-001	0.0000E+000
42	0.2145	-6.1982E-041	-1.3027E-045	-2.2279E-046	-5.3958E-040	-2.0719E-043	5.4185E-001	0.0000E+000
43	0.2148	-1.1009E-040	-1.7305E-045	-3.1931E-046	-7.7102E-040	-3.1280E-043	5.4198E-001	0.0000E+000
44	0.2156	6.7650E-040	-2.9430E-045	-6.3830E-046	-1.5317E-039	-6.9033E-043	5.4228E-001	0.0000E+000
45	0.2164	-3.0149E-040	-3.5887E-045	-1.2358E-045	-2.9421E-039	-1.4899E-042	5.4262E-001	0.0000E+000
46	0.2172	-1.1799E-040	-3.7749E-045	-2.3557E-045	-5.5509E-039	-3.1997E-042	5.4300E-001	0.0000E+000
47	0.2180	-3.1655E-041	-3.8629E-045	-4.4568E-045	-1.0362E-038	-6.8790E-042	5.4343E-001	0.0000E+000
48	0.2188	-7.6606E-042	-4.0315E-045	-8.4047E-045	-1.9204E-038	-1.4836E-041	5.4391E-001	0.0000E+000
49	0.2195	-1.9585E-042	-4.4483E-045	-1.5838E-044	-3.5390E-038	-3.2123E-041	5.4445E-001	0.0000E+000
50	0.2203	-9.6086E-043	-5.3878E-045	-2.9876E-044	-6.4883E-038	-6.9849E-041	5.4505E-001	0.0000E+000
51	0.2211	-1.5154E-042	-7.3655E-045	-5.6498E-044	-1.1835E-037	-1.5251E-040	5.4571E-001	0.0000E+000
52	0.2219	-3.6138E-042	-1.1383E-044	-1.0726E-043	-2.1472E-037	-3.3430E-040	5.4644E-001	0.0000E+000
53	0.2234	-1.8125E-041	-3.1341E-044	-3.4810E-043	-6.3467E-037	-1.3540E-039	5.4809E-001	0.0000E+000
54	0.2250	-7.5935E-041	-9.3054E-044	-1.0801E-042	-1.6930E-036	-5.0001E-039	5.5001E-001	0.0000E+000
55	0.2258	-1.5268E-040	-1.7250E-043	-2.0512E-042	-2.8051E-036	-1.0000E-038	5.5107E-001	0.0000E+000
56	0.2266	-2.9766E-040	-3.2779E-043	-4.0197E-042	-4.7163E-036	-2.0119E-038	5.5220E-001	0.0000E+000
57	0.2270	-4.1415E-040	-4.5992E-043	-5.7760E-042	-6.1760E-036	-2.8876E-038	5.5280E-001	0.0000E+000
58	0.2273	-5.7299E-040	-6.5070E-043	-8.4029E-042	-8.1436E-036	-4.1644E-038	5.5340E-001	0.0000E+000
59	0.2277	-7.8714E-040	-9.2482E-043	-1.2334E-041	-1.0787E-035	-6.0146E-038	5.5402E-001	0.0000E+000

60	0.2279	-9.2113E-040	-1.1061E-042	-1.5034E-041	-1.2445E-035	-7.2442E-038	5.5434E-001	0.0000E+000
61	0.2281	-1.0765E-039	-1.3255E-042	-1.8387E-041	-1.4383E-035	-8.7360E-038	5.5466E-001	0.0000E+000
62	0.2283	-1.2560E-039	-1.5905E-042	-2.2549E-041	-1.6647E-035	-1.0543E-037	5.5498E-001	0.0000E+000
63	0.2285	-1.4628E-039	-1.9102E-042	-2.7714E-041	-1.9287E-035	-1.2728E-037	5.5530E-001	0.0000E+000
64	0.2287	-1.7003E-039	-2.2952E-042	-3.4125E-041	-2.2364E-035	-1.5366E-037	5.5563E-001	0.0000E+000
65	0.2289	-1.9721E-039	-2.7582E-042	-4.2083E-041	-2.5947E-035	-1.8546E-037	5.5596E-001	0.0000E+000
66	0.2291	-2.2824E-039	-3.3143E-042	-5.1960E-041	-3.0113E-035	-2.2374E-037	5.5629E-001	0.0000E+000
67	0.2293	-2.6353E-039	-3.9811E-042	-6.4219E-041	-3.4954E-035	-2.6973E-037	5.5662E-001	0.0000E+000
68	0.2295	-3.0354E-039	-4.7795E-042	-7.9435E-041	-4.0572E-035	-3.2489E-037	5.5696E-001	0.0000E+000
69	0.2297	-3.4878E-039	-5.7341E-042	-9.8320E-041	-4.7086E-035	-3.9093E-037	5.5729E-001	0.0000E+000
70	0.2299	-3.9976E-039	-6.8737E-042	-1.2176E-040	-5.4630E-035	-4.6986E-037	5.5763E-001	0.0000E+000
71	0.2301	-4.5704E-039	-8.2322E-042	-1.5084E-040	-6.3358E-035	-5.6401E-037	5.5797E-001	0.0000E+000
72	0.2303	-5.2122E-039	-9.8491E-042	-1.8691E-040	-7.3445E-035	-6.7611E-037	5.5830E-001	0.0000E+000
73	0.2305	-5.9291E-039	-1.1771E-041	-2.3166E-040	-8.5090E-035	-8.0934E-037	5.5864E-001	0.0000E+000
74	0.2307	-6.7279E-039	-1.4051E-041	-2.8716E-040	-9.8520E-035	-9.6740E-037	5.5898E-001	0.0000E+000
75	0.2309	-7.6154E-039	-1.6754E-041	-3.5596E-040	-1.1399E-034	-1.1546E-036	5.5932E-001	0.0000E+000
76	0.2311	-8.5991E-039	-1.9951E-041	-4.4122E-040	-1.3180E-034	-1.3760E-036	5.5965E-001	0.0000E+000
77	0.2313	-9.6867E-039	-2.3729E-041	-5.4687E-040	-1.5227E-034	-1.6374E-036	5.5999E-001	0.0000E+000
78	0.2314	-1.0886E-038	-2.8186E-041	-6.7773E-040	-1.7578E-034	-1.9456E-036	5.6032E-001	0.0000E+000
79	0.2316	-1.2207E-038	-3.3437E-041	-8.3977E-040	-2.0276E-034	-2.3088E-036	5.6066E-001	0.0000E+000
80	0.2318	-1.3657E-038	-3.9615E-041	-1.0404E-039	-2.3369E-034	-2.7362E-036	5.6099E-001	0.0000E+000
81	0.2320	-1.5247E-038	-4.6875E-041	-1.2887E-039	-2.6910E-034	-3.2391E-036	5.6132E-001	0.0000E+000
82	0.2324	-1.8867E-038	-6.5168E-041	-1.9620E-039	-3.5520E-034	-4.5111E-036	5.6197E-001	0.0000E+000
83	0.2328	-2.3127E-038	-8.9742E-041	-2.9668E-039	-4.6554E-034	-6.2350E-036	5.6261E-001	0.0000E+000
84	0.2336	-3.3741E-038	-1.6367E-040	-6.4544E-039	-7.7757E-034	-1.1526E-035	5.6387E-001	0.0000E+000
85	0.2344	-4.7508E-038	-2.8560E-040	-1.3516E-038	-1.2537E-033	-2.0548E-035	5.6509E-001	0.0000E+000
86	0.2352	-6.5152E-038	-4.8253E-040	-2.7495E-038	-1.9706E-033	-3.5694E-035	5.6625E-001	0.0000E+000
87	0.2359	-8.7614E-038	-7.9402E-040	-5.4449E-038	-3.0361E-033	-6.0753E-035	5.6736E-001	0.0000E+000
88	0.2367	-1.1606E-037	-1.2768E-039	-1.0502E-037	-4.5992E-033	-1.0165E-034	5.6842E-001	0.0000E+000
89	0.2375	-1.5186E-037	-2.0101E-039	-1.9724E-037	-6.8618E-033	-1.6748E-034	5.6943E-001	0.0000E+000
90	0.2383	-1.9654E-037	-3.1013E-039	-3.6065E-037	-1.0092E-032	-2.7187E-034	5.7038E-001	0.0000E+000
91	0.2391	-2.5167E-037	-4.6914E-039	-6.4186E-037	-1.4638E-032	-4.3467E-034	5.7129E-001	0.0000E+000
92	0.2398	-3.1875E-037	-6.9586E-039	-1.1117E-036	-2.0937E-032	-6.8388E-034	5.7216E-001	0.0000E+000
93	0.2406	-3.9905E-037	-1.0120E-038	-1.8736E-036	-2.9523E-032	-1.0575E-033	5.7299E-001	0.0000E+000
94	0.2414	-4.9350E-037	-1.4429E-038	-3.0731E-036	-4.1032E-032	-1.6054E-033	5.7378E-001	0.0000E+000
95	0.2422	-6.0261E-037	-2.0173E-038	-4.9077E-036	-5.6196E-032	-2.3908E-033	5.7454E-001	0.0000E+000
96	0.2430	-7.2638E-037	-2.7664E-038	-7.6353E-036	-7.5834E-032	-3.4908E-033	5.7526E-001	0.0000E+000
97	0.2437	-8.6439E-037	-3.7231E-038	-1.1583E-035	-1.0085E-031	-4.9973E-033	5.7596E-001	0.0000E+000
98	0.2445	-1.0158E-036	-4.9211E-038	-1.7152E-035	-1.3220E-031	-7.0169E-033	5.7663E-001	0.0000E+000
99	0.2453	-1.1793E-036	-6.3938E-038	-2.4827E-035	-1.7093E-031	-9.6699E-033	5.7728E-001	0.0000E+000
100	0.2461	-1.3534E-036	-8.1741E-038	-3.5179E-035	-2.1813E-031	-1.3090E-032	5.7789E-001	0.0000E+000
101	0.2469	-1.5362E-036	-1.0294E-037	-4.8895E-035	-2.7496E-031	-1.7429E-032	5.7849E-001	0.0000E+000
102	0.2484	-1.9198E-036	-1.5657E-037	-8.9156E-035	-4.2140E-031	-2.9429E-032	5.7961E-001	0.0000E+000
103	0.2500	-2.2989E-036	-2.2422E-037	-1.5044E-034	-6.1146E-031	-4.6511E-032	5.8064E-001	0.0000E+000
104	0.2516	-2.6591E-036	-3.0595E-037	-2.3889E-034	-8.4960E-031	-6.9718E-032	5.8159E-001	0.0000E+000
105	0.2531	-2.9925E-036	-4.0132E-037	-3.6118E-034	-1.1398E-030	-1.0005E-031	5.8248E-001	0.0000E+000
106	0.2562	-3.5655E-036	-6.3095E-037	-7.3456E-034	-1.8902E-030	-1.8560E-031	5.8408E-001	0.0000E+000
107	0.2594	-3.9615E-036	-8.9265E-037	-1.3024E-033	-2.8228E-030	-3.0492E-031	5.8550E-001	0.0000E+000
108	0.2625	-4.2088E-036	-1.1753E-036	-2.1004E-033	-3.9208E-030	-4.5977E-031	5.8680E-001	0.0000E+000
109	0.2656	-4.3466E-036	-1.4711E-036	-3.1579E-033	-5.1631E-030	-6.4991E-031	5.8800E-001	0.0000E+000
110	0.2688	-4.4091E-036	-1.7756E-036	-4.4983E-033	-6.5277E-030	-8.7341E-031	5.8911E-001	0.0000E+000
111	0.2750	-4.4138E-036	-2.4062E-036	-8.1067E-033	-9.5660E-030	-1.4082E-030	5.9113E-001	0.0000E+000
112	0.2812	-4.3140E-036	-3.0676E-036	-1.3004E-032	-1.2883E-029	-2.0402E-030	5.9294E-001	0.0000E+000
113	0.2875	-4.1754E-036	-3.7812E-036	-1.9306E-032	-1.6435E-029	-2.7485E-030	5.9460E-001	0.0000E+000
114	0.2938	-4.0310E-036	-4.5774E-036	-2.7106E-032	-2.0197E-029	-3.5130E-030	5.9612E-001	0.0000E+000
115	0.3000	-3.8956E-036	-5.4914E-036	-3.6483E-032	-2.4153E-029	-4.3169E-030	5.9753E-001	0.0000E+000
116	0.3063	-3.7752E-036	-6.5617E-036	-4.7506E-032	-2.8299E-029	-5.1472E-030	5.9884E-001	0.0000E+000
117	0.3125	-3.6717E-036	-7.8295E-036	-6.0237E-032	-3.2636E-029	-5.9939E-030	6.0007E-001	0.0000E+000
118	0.3188	-3.5846E-036	-9.3372E-036	-7.4731E-032	-3.7169E-029	-6.8505E-030	6.0121E-001	0.0000E+000
119	0.3250	-3.5128E-036	-1.1128E-035	-9.1040E-032	-4.1907E-029	-7.7130E-030	6.0229E-001	0.0000E+000
120	0.3313	-3.4544E-036	-1.3246E-035	-1.0921E-031	-4.6862E-029	-8.5794E-030	6.0329E-001	0.0000E+000
121	0.3375	-3.4073E-036	-1.5733E-035	-1.2930E-031	-5.2046E-029	-9.4493E-030	6.0424E-001	0.0000E+000
122	0.3438	-3.3697E-036	-1.8629E-035	-1.5132E-031	-5.7470E-029	-1.0323E-029	6.0512E-001	0.0000E+000
123	0.3500	-3.3396E-036	-2.1966E-035	-1.7529E-031	-6.3136E-029	-1.1200E-029	6.0595E-001	0.0000E+000
124	0.3625	-3.2917E-036	-3.0080E-035	-2.2862E-031	-7.5123E-029	-1.2942E-029	6.0744E-001	0.0000E+000
125	0.3750	-3.2582E-036	-4.0289E-035	-2.9030E-031	-8.8288E-029	-1.4741E-029	6.0876E-001	0.0000E+000
126	0.3875	-3.2331E-036	-5.2945E-035	-3.6124E-031	-1.0285E-028	-1.6624E-029	6.0994E-001	0.0000E+000
127	0.4000	-3.2124E-036	-6.8345E-035	-4.4214E-031	-1.1897E-028	-1.8605E-029	6.1098E-001	0.0000E+000
128	0.4125	-3.1934E-036	-8.6760E-035	-5.3369E-031	-1.3671E-028	-2.0694E-029	6.1192E-001	0.0000E+000
129	0.4250	-3.1743E-036	-1.0839E-034	-6.3613E-031	-1.5615E-028	-2.2887E-029	6.1276E-001	0.0000E+000
130	0.4375	-3.1572E-036	-1.3342E-034	-7.4972E-031	-1.7726E-028	-2.5192E-029	6.1351E-001	0.0000E+000

131	0.4500	-3.1410E-036	-1.6200E-034	-8.7429E-031	-2.0001E-028	-2.7559E-029	6.1417E-001	0.0000E+000
132	0.4625	-3.1234E-036	-1.9395E-034	-1.0092E-030	-2.2427E-028	-3.0028E-029	6.1476E-001	0.0000E+000
133	0.4750	-3.1048E-036	-2.2885E-034	-1.1497E-030	-2.4857E-028	-3.2449E-029	6.1525E-001	0.0000E+000
134	0.4812	-3.0960E-036	-2.4652E-034	-1.2207E-030	-2.6021E-028	-3.3550E-029	6.1544E-001	0.0000E+000
135	0.4875	-3.0829E-036	-2.6359E-034	-1.2819E-030	-2.7075E-028	-3.4523E-029	6.1559E-001	0.0000E+000
136	0.4906	-3.0739E-036	-2.7095E-034	-1.3078E-030	-2.7494E-028	-3.4804E-029	6.1564E-001	0.0000E+000
137	0.4938	-3.0646E-036	-2.7763E-034	-1.3315E-030	-2.7821E-028	-3.5150E-029	6.1568E-001	0.0000E+000
138	0.4969	-3.0516E-036	-2.8162E-034	-1.3406E-030	-2.7976E-028	-3.5144E-029	6.1569E-001	0.0000E+000
139	0.5000	-3.0516E-036	-2.8162E-034	-1.3406E-030	-2.7976E-028	-3.5144E-029	6.1569E-001	0.0000E+000

	X(cm)	MOLE FRACTIONS:						
		C3H7	C3H8	CH2CHO	CH3CHO	K	KO	HKO
1	0.0000	-1.4080E-130	-1.8366E-128	-3.9581E-096	-3.8067E-092	9.2238E-019	1.3688E-019	3.1601E-011
2	0.0500	-1.0823E-128	-1.4173E-126	-2.5193E-094	-2.4328E-090	6.8165E-017	8.5579E-018	2.8176E-009
3	0.0750	-3.5275E-127	-4.2064E-125	-2.2976E-092	-6.0123E-089	7.2138E-017	9.0336E-018	4.2077E-009
4	0.1000	-1.4375E-125	-1.6305E-123	-2.5158E-090	-1.9324E-087	7.2855E-017	9.0996E-018	5.5943E-009
5	0.1125	-2.3171E-124	-2.5106E-122	-1.1373E-088	-2.4950E-086	7.3054E-017	9.1125E-018	6.2865E-009
6	0.1250	-4.6879E-123	-4.9558E-121	-4.4745E-087	-4.0992E-085	7.3225E-017	9.1218E-018	6.9778E-009
7	0.1313	-3.9496E-122	-4.0901E-120	-6.9524E-086	-2.8720E-084	7.3317E-017	9.1273E-018	7.3232E-009
8	0.1344	-1.8255E-121	-1.8721E-119	-4.3819E-085	-1.1360E-083	7.3379E-017	9.1321E-018	7.4959E-009
9	0.1375	-1.0097E-120	-1.0300E-118	-2.8607E-084	-5.3207E-083	7.3475E-017	9.1410E-018	7.6684E-009
10	0.1383	-1.8342E-120	-1.8677E-118	-5.5712E-084	-8.9364E-083	7.3513E-017	9.1450E-018	7.7116E-009
11	0.1391	-3.6397E-120	-3.7022E-118	-1.1420E-083	-1.6105E-082	7.3559E-017	9.1500E-018	7.7547E-009
12	0.1398	-7.5926E-120	-7.7201E-118	-2.3989E-083	-3.0318E-082	7.3616E-017	9.1563E-018	7.7978E-009
13	0.1406	-1.6246E-119	-1.6520E-117	-5.0953E-083	-5.8496E-082	7.3688E-017	9.1645E-018	7.8409E-009
14	0.1414	-3.5190E-119	-3.5793E-117	-1.0875E-082	-1.1436E-081	7.3778E-017	9.1749E-018	7.8841E-009
15	0.1422	-7.6658E-119	-7.8005E-117	-2.3259E-082	-2.2512E-081	7.3892E-017	9.1884E-018	7.9272E-009
16	0.1438	-3.0752E-118	-3.1314E-116	-9.0478E-082	-7.7311E-081	7.4218E-017	9.2273E-018	8.0134E-009
17	0.1469	-2.4184E-117	-2.4625E-115	-7.1431E-081	-5.0989E-080	7.5476E-017	9.3807E-018	8.1858E-009
18	0.1500	-1.4615E-116	-1.4844E-114	-4.7766E-080	-2.6410E-079	7.8667E-017	9.7737E-018	8.3583E-009
19	0.1625	-6.4629E-115	-6.5381E-113	-2.4669E-078	-9.4811E-078	1.4160E-016	1.7568E-017	9.0519E-009
20	0.1656	-2.7271E-114	-2.7145E-112	-1.7589E-077	-3.4244E-077	2.9018E-016	3.5970E-017	9.2295E-009
21	0.1688	-1.4760E-113	-1.4585E-111	-1.1645E-076	-1.5583E-076	6.5837E-016	8.1583E-017	9.4197E-009
22	0.1750	-2.1139E-112	-2.0786E-110	-1.9623E-075	-1.8223E-075	3.1222E-015	3.8704E-016	9.9543E-009
23	0.1875	-6.2798E-111	-6.1150E-109	-8.1796E-074	-4.3742E-074	3.9534E-014	4.9433E-015	1.4213E-008
24	0.1938	-5.3880E-110	-5.1246E-108	-1.2653E-072	-2.9678E-073	2.3661E-013	3.0273E-014	2.5519E-008
25	0.2000	-5.6419E-109	-5.2599E-107	-1.8501E-071	-2.3832E-072	1.1694E-012	1.5975E-013	7.4426E-008
26	0.2031	-2.7276E-108	-2.4568E-106	-1.1196E-070	-8.7216E-072	2.9304E-012	4.2342E-013	1.3665E-007
27	0.2047	-7.8389E-108	-6.8625E-106	-3.4301E-070	-1.9937E-071	4.6730E-012	6.9859E-013	1.8925E-007
28	0.2063	-2.5509E-107	-2.1727E-105	-1.1156E-069	-5.0540E-071	7.3487E-012	1.1338E-012	2.7025E-007
29	0.2078	-8.6954E-107	-7.1800E-105	-3.6563E-069	-1.3263E-070	1.1452E-011	1.8006E-012	3.8850E-007
30	0.2086	-1.7517E-106	-1.4112E-104	-7.0429E-069	-2.2351E-070	1.4320E-011	2.2592E-012	4.6221E-007
31	0.2094	-3.7181E-106	-2.9201E-104	-1.4012E-068	-3.8993E-070	1.7864E-011	2.8066E-012	5.4908E-007
32	0.2102	-8.0874E-106	-6.1963E-104	-2.8203E-068	-6.9238E-070	2.2193E-011	3.4384E-012	6.4849E-007
33	0.2109	-1.7737E-105	-1.3271E-103	-5.6747E-068	-1.2365E-069	2.7383E-011	4.1337E-012	7.5779E-007
34	0.2113	-2.6910E-105	-1.9856E-103	-8.1511E-068	-1.6670E-069	3.0318E-011	4.4986E-012	8.1414E-007
35	0.2117	-4.1504E-105	-3.0204E-103	-1.1819E-067	-2.2685E-069	3.3442E-011	4.8582E-012	8.7070E-007
36	0.2121	-6.4654E-105	-4.6427E-103	-1.7215E-067	-3.1064E-069	3.6711E-011	5.1976E-012	9.2598E-007
37	0.2125	-1.0150E-104	-7.1805E-103	-2.5092E-067	-4.2697E-069	4.0062E-011	5.4979E-012	9.7821E-007
38	0.2129	-1.5965E-104	-1.1137E-102	-3.6490E-067	-5.8781E-069	4.3412E-011	5.7363E-012	1.0254E-006
39	0.2133	-2.5204E-104	-1.7337E-102	-5.2783E-067	-8.0921E-069	4.6663E-011	5.8872E-012	1.0654E-006
40	0.2137	-3.9962E-104	-2.7072E-102	-7.5718E-067	-1.1125E-068	4.9718E-011	5.9253E-012	1.0963E-006
41	0.2141	-6.3640E-104	-4.2383E-102	-1.0733E-066	-1.5261E-068	5.2498E-011	5.8325E-012	1.1168E-006
42	0.2145	-1.0176E-103	-6.6497E-102	-1.4961E-066	-2.0877E-068	5.4962E-011	5.6071E-012	1.1263E-006
43	0.2148	-1.6347E-103	-1.0482E-101	-2.0358E-066	-2.8481E-068	5.7122E-011	5.2762E-012	1.1250E-006
44	0.2156	-4.0017E-103	-2.4747E-101	-3.4016E-066	-5.1702E-068	6.0576E-011	4.5189E-012	1.0942E-006
45	0.2164	-9.3584E-103	-5.5498E-101	-5.4959E-066	-9.0216E-068	6.3860E-011	3.9715E-012	1.0483E-006
46	0.2172	-2.1350E-102	-1.2114E-100	-7.5208E-066	-1.5500E-067	6.7661E-011	3.8922E-012	1.0044E-006
47	0.2180	-4.8358E-102	-2.6151E-100	-9.7444E-066	-2.6750E-067	7.2561E-011	4.2299E-012	9.7330E-007
48	0.2188	-1.0940E-101	-5.6166E-100	-1.2955E-065	-4.7002E-067	7.9143E-011	4.8469E-012	9.6046E-007
49	0.2195	-2.4764E-101	-1.2021E-099	-1.8857E-065	-8.4500E-067	8.8066E-011	5.6697E-012	9.6759E-007
50	0.2203	-5.6152E-101	-2.5635E-099	-3.1026E-065	-1.5514E-066	1.0009E-010	6.7015E-012	9.9471E-007
51	0.2211	-1.2770E-100	-5.4435E-099	-5.6864E-065	-2.8931E-066	1.1616E-010	7.9989E-012	1.0412E-006
52	0.2219	-2.9183E-100	-1.1500E-098	-1.1163E-064	-5.4479E-066	1.3747E-010	9.6727E-012	1.1068E-006
53	0.2234	-1.2646E-099	-4.3283E-098	-3.9960E-064	-1.7423E-065	2.0249E-010	1.5050E-011	1.3015E-006
54	0.2250	-4.9540E-099	-1.4215E-097	-1.3737E-063	-5.0942E-065	3.1755E-010	2.8150E-011	1.6115E-006
55	0.2258	-1.0503E-098	-2.6765E-097	-2.7594E-063	-9.0181E-065	4.1792E-010	4.5302E-011	1.8821E-006
56	0.2266	-2.2930E-098	-5.1863E-097	-5.6159E-063	-1.6297E-064	5.8579E-010	8.5974E-011	2.3441E-006
57	0.2270	-3.4769E-098	-7.3620E-097	-8.1542E-063	-2.2204E-064	7.1652E-010	1.2574E-010	2.7053E-006
58	0.2273	-5.3435E-098	-1.0588E-096	-1.1917E-062	-3.0506E-064	8.9935E-010	1.8963E-010	3.2066E-006
59	0.2277	-8.2722E-098	-1.5347E-096	-1.7444E-062	-4.2101E-064	1.1543E-009	2.9100E-010	3.8911E-006

60	0.2279	-1.0353E-097	-1.8565E-096	-2.1160E-062	-4.9590E-064	1.3164E-009	3.6113E-010	4.3171E-006
61	0.2281	-1.3003E-097	-2.2533E-096	-2.5706E-062	-5.8518E-064	1.5072E-009	4.4746E-010	4.8103E-006
62	0.2283	-1.6373E-097	-2.7418E-096	-3.1248E-062	-6.9143E-064	1.7298E-009	5.5221E-010	5.3748E-006
63	0.2285	-2.0653E-097	-3.3424E-096	-3.7988E-062	-8.1763E-064	1.9864E-009	6.7704E-010	6.0122E-006
64	0.2287	-2.6081E-097	-4.0797E-096	-4.6162E-062	-9.6723E-064	2.2783E-009	8.2246E-010	6.7207E-006
65	0.2289	-3.2953E-097	-4.9834E-096	-5.6049E-062	-1.1442E-063	2.6052E-009	9.8719E-010	7.4940E-006
66	0.2291	-4.1639E-097	-6.0889E-096	-6.7977E-062	-1.3532E-063	2.9642E-009	1.1673E-009	8.3206E-006
67	0.2293	-5.2598E-097	-7.4394E-096	-8.2332E-062	-1.5995E-063	3.3502E-009	1.3557E-009	9.1832E-006
68	0.2295	-6.6403E-097	-9.0860E-096	-9.9566E-062	-1.8892E-063	3.7549E-009	1.5416E-009	1.0059E-005
69	0.2297	-8.3758E-097	-1.1090E-095	-1.2020E-061	-2.2291E-063	4.1678E-009	1.7114E-009	1.0922E-005
70	0.2299	-1.0553E-096	-1.3525E-095	-1.4486E-061	-2.6274E-063	4.5764E-009	1.8497E-009	1.1741E-005
71	0.2301	-1.3280E-096	-1.6477E-095	-1.7425E-061	-3.0929E-063	4.9675E-009	1.9422E-009	1.2491E-005
72	0.2303	-1.6687E-096	-2.0050E-095	-2.0919E-061	-3.6359E-063	5.3290E-009	1.9794E-009	1.3147E-005
73	0.2305	-2.0935E-096	-2.4365E-095	-2.5064E-061	-4.2680E-063	5.6517E-009	1.9595E-009	1.3695E-005
74	0.2307	-2.6220E-096	-2.9567E-095	-2.9971E-061	-5.0024E-063	5.9303E-009	1.8906E-009	1.4130E-005
75	0.2309	-3.2780E-096	-3.5823E-095	-3.5767E-061	-5.8538E-063	6.1644E-009	1.7898E-009	1.4459E-005
76	0.2311	-4.0906E-096	-4.3334E-095	-4.2598E-061	-6.8389E-063	6.3573E-009	1.6788E-009	1.4695E-005
77	0.2313	-5.0947E-096	-5.2329E-095	-5.0630E-061	-7.9761E-063	6.5155E-009	1.5779E-009	1.4859E-005
78	0.2314	-6.3328E-096	-6.3080E-095	-6.0055E-061	-9.2861E-063	6.6461E-009	1.5010E-009	1.4970E-005
79	0.2316	-7.8562E-096	-7.5902E-095	-7.1091E-061	-1.0792E-062	6.7561E-009	1.4529E-009	1.5046E-005
80	0.2318	-9.7269E-096	-9.1158E-095	-8.3981E-061	-1.2520E-062	6.8505E-009	1.4304E-009	1.5099E-005
81	0.2320	-1.2020E-095	-1.0927E-094	-9.8997E-061	-1.4497E-062	6.9330E-009	1.4256E-009	1.5138E-005
82	0.2324	-1.8146E-095	-1.5551E-094	-1.3628E-060	-1.9293E-062	7.0703E-009	1.4543E-009	1.5194E-005
83	0.2328	-2.6969E-095	-2.1805E-094	-1.8505E-060	-2.5380E-062	7.1786E-009	1.4914E-009	1.5234E-005
84	0.2336	-5.6038E-095	-4.0666E-094	-3.2515E-060	-4.2269E-062	7.3251E-009	1.5771E-009	1.5291E-005
85	0.2344	-1.0839E-094	-7.0869E-094	-5.4255E-060	-6.7053E-062	7.3998E-009	1.6597E-009	1.5335E-005
86	0.2352	-1.9893E-094	-1.1754E-093	-8.7583E-060	-1.0281E-061	7.4193E-009	1.7390E-009	1.5373E-005
87	0.2359	-3.4976E-094	-1.8730E-093	-1.3808E-059	-1.5369E-061	7.3987E-009	1.8145E-009	1.5407E-005
88	0.2367	-5.9263E-094	-2.8850E-093	-2.1380E-059	-2.2526E-061	7.3509E-009	1.8870E-009	1.5439E-005
89	0.2375	-9.7196E-094	-4.3141E-093	-3.2617E-059	-3.2486E-061	7.2863E-009	1.9573E-009	1.5469E-005
90	0.2383	-1.5483E-093	-6.2840E-093	-4.9109E-059	-4.6192E-061	7.2126E-009	2.0262E-009	1.5498E-005
91	0.2391	-2.4022E-093	-8.9401E-093	-7.3008E-059	-6.4827E-061	7.1353E-009	2.0940E-009	1.5524E-005
92	0.2398	-3.6377E-093	-1.2448E-092	-1.0713E-058	-8.9829E-061	7.0581E-009	2.1613E-009	1.5550E-005
93	0.2406	-5.3850E-093	-1.6990E-092	-1.5504E-058	-1.2289E-060	6.9836E-009	2.2282E-009	1.5574E-005
94	0.2414	-7.8026E-093	-2.2758E-092	-2.2107E-058	-1.6592E-060	6.9137E-009	2.2951E-009	1.5597E-005
95	0.2422	-1.1077E-092	-2.9946E-092	-3.1033E-058	-2.2109E-060	6.8501E-009	2.3622E-009	1.5619E-005
96	0.2430	-1.5420E-092	-3.8744E-092	-4.2863E-058	-2.9071E-060	6.7948E-009	2.4299E-009	1.5640E-005
97	0.2437	-2.1069E-092	-4.9327E-092	-5.8244E-058	-3.7734E-060	6.7497E-009	2.4986E-009	1.5660E-005
98	0.2445	-2.8279E-092	-6.1854E-092	-7.7875E-058	-4.8374E-060	6.7172E-009	2.5691E-009	1.5680E-005
99	0.2453	-3.7321E-092	-7.6458E-092	-1.0251E-057	-6.1294E-060	6.6999E-009	2.6420E-009	1.5698E-005
100	0.2461	-4.8471E-092	-9.3242E-092	-1.3296E-057	-7.6833E-060	6.7006E-009	2.7183E-009	1.5716E-005
101	0.2469	-6.1997E-092	-1.1224E-091	-1.7011E-057	-9.5363E-060	6.7222E-009	2.7987E-009	1.5733E-005
102	0.2484	-9.6934E-092	-1.5657E-091	-2.6638E-057	-1.4246E-059	6.8372E-009	2.9754E-009	1.5765E-005
103	0.2500	-1.4034E-091	-2.0399E-091	-3.8836E-057	-2.0180E-059	7.0717E-009	3.1831E-009	1.5795E-005
104	0.2516	-1.9100E-091	-2.5155E-091	-5.3592E-057	-2.7451E-059	7.4485E-009	3.4302E-009	1.5821E-005
105	0.2531	-2.4754E-091	-2.9716E-091	-7.0795E-057	-3.6196E-059	7.9878E-009	3.7250E-009	1.5846E-005
106	0.2562	-3.7368E-091	-3.7846E-091	-1.1183E-056	-5.8681E-059	9.6023E-009	4.4796E-009	1.5889E-005
107	0.2594	-4.8496E-091	-4.2053E-091	-1.5378E-056	-8.4909E-059	1.2100E-008	5.5182E-009	1.5925E-005
108	0.2625	-5.6952E-091	-4.2722E-091	-1.9288E-056	-1.1330E-058	1.5637E-008	6.8935E-009	1.5956E-005
109	0.2656	-6.2627E-091	-4.0988E-091	-2.2681E-056	-1.4225E-058	2.0362E-008	8.6504E-009	1.5982E-005
110	0.2688	-6.5926E-091	-3.7935E-091	-2.5458E-056	-1.7039E-058	2.6403E-008	1.0822E-008	1.6004E-005
111	0.2750	-6.8041E-091	-3.0976E-091	-2.9377E-056	-2.2170E-058	4.2653E-008	1.6408E-008	1.6037E-005
112	0.2812	-6.5367E-091	-2.4021E-091	-3.1040E-056	-2.6115E-058	6.5761E-008	2.3906E-008	1.6056E-005
113	0.2875	-6.0498E-091	-1.8257E-091	-3.1136E-056	-2.8874E-058	9.6834E-008	3.3328E-008	1.6060E-005
114	0.2938	-5.4971E-091	-1.3835E-091	-3.0246E-056	-3.0622E-058	1.3694E-007	4.4522E-008	1.6050E-005
115	0.3000	-4.9521E-091	-1.0543E-091	-2.8787E-056	-3.1574E-058	1.8708E-007	5.7182E-008	1.6026E-005
116	0.3063	-4.4470E-091	-8.1130E-092	-2.7042E-056	-3.1926E-058	2.4815E-007	7.0870E-008	1.5986E-005
117	0.3125	-3.9938E-091	-6.3202E-092	-2.5200E-056	-3.1850E-058	3.2090E-007	8.5070E-008	1.5932E-005
118	0.3188	-3.5947E-091	-4.9911E-092	-2.3374E-056	-3.1479E-058	4.0584E-007	9.9247E-008	1.5864E-005
119	0.3250	-3.2470E-091	-3.9988E-092	-2.1632E-056	-3.0915E-058	5.0323E-007	1.1290E-007	1.5783E-005
120	0.3313	-2.9466E-091	-3.2523E-092	-2.0013E-056	-3.0237E-058	6.1306E-007	1.2563E-007	1.5687E-005
121	0.3375	-2.6884E-091	-2.6859E-092	-1.8535E-056	-2.9504E-058	7.3499E-007	1.3712E-007	1.5579E-005
122	0.3438	-2.4673E-091	-2.2525E-092	-1.7200E-056	-2.8755E-058	8.6831E-007	1.4718E-007	1.5460E-005
123	0.3500	-2.2783E-091	-1.9181E-092	-1.6004E-056	-2.8015E-058	1.0118E-006	1.5574E-007	1.5330E-005
124	0.3625	-1.9791E-091	-1.4564E-092	-1.3987E-056	-2.6599E-058	1.3194E-006	1.6829E-007	1.5051E-005
125	0.3750	-1.7595E-091	-1.1625E-092	-1.2378E-056	-2.5350E-058	1.6558E-006	1.7591E-007	1.4743E-005
126	0.3875	-1.6002E-091	-9.7113E-093	-1.1090E-056	-2.4278E-058	2.0124E-006	1.7957E-007	1.4415E-005
127	0.4000	-1.4860E-091	-8.4414E-093	-1.0050E-056	-2.3367E-058	2.3806E-006	1.8027E-007	1.4075E-005
128	0.4125	-1.4060E-091	-7.5933E-093	-9.2031E-057	-2.2603E-058	2.7531E-006	1.7885E-007	1.3729E-005
129	0.4250	-1.3557E-091	-7.0360E-093	-8.5247E-057	-2.1994E-058	3.1236E-006	1.7598E-007	1.3385E-005
130	0.4375	-1.3298E-091	-6.7027E-093	-7.9506E-057	-2.1468E-058	3.4872E-006	1.7217E-007	1.3045E-005

131	0.4500	-1.3246E-091	-6.5289E-093	-7.5034E-057	-2.1105E-058	3.8403E-006	1.6782E-007	1.2715E-005
132	0.4625	-1.3466E-091	-6.5300E-093	-7.1621E-057	-2.0914E-058	4.1799E-006	1.6320E-007	1.2396E-005
133	0.4750	-1.3942E-091	-6.6815E-093	-6.9759E-057	-2.1042E-058	4.5036E-006	1.5854E-007	1.2090E-005
134	0.4812	-1.4264E-091	-6.7943E-093	-6.9342E-057	-2.1241E-058	4.6584E-006	1.5629E-007	1.1943E-005
135	0.4875	-1.4614E-091	-6.9235E-093	-7.0144E-057	-2.1701E-058	4.8015E-006	1.5423E-007	1.1805E-005
136	0.4906	-1.4973E-091	-7.0903E-093	-7.0953E-057	-2.1931E-058	4.8647E-006	1.5333E-007	1.1743E-005
137	0.4938	-1.5265E-091	-7.2419E-093	-7.1272E-057	-2.2164E-058	4.9168E-006	1.5261E-007	1.1691E-005
138	0.4969	-1.5473E-091	-7.3293E-093	-7.2227E-057	-2.2379E-058	4.9498E-006	1.5216E-007	1.1657E-005
139	0.5000	-1.5473E-091	-7.3293E-093	-7.2227E-057	-2.2379E-058	4.9498E-006	1.5216E-007	1.1657E-005

	X(cm)	MOLE FRACTIONS:						
		KO2	HK	K2O	K2O2	K2CO3	K2H2O2	KHCO3
1	0.0000	1.4700E-005	4.8032E-023	3.4437E-023	5.3579E-021	1.8267E-056	5.9716E-015	2.3774E-039
2	0.0500	1.4697E-005	2.2853E-021	3.4180E-021	5.4010E-019	1.8771E-054	6.0296E-013	2.3745E-037
3	0.0750	1.4696E-005	3.3126E-021	6.0822E-021	9.3930E-019	-2.3645E-052	1.2680E-012	3.2193E-036
4	0.1000	1.4694E-005	4.1409E-021	9.6380E-021	1.4683E-018	1.3060E-052	2.4334E-012	-6.4752E-035
5	0.1125	1.4694E-005	4.5065E-021	1.1641E-020	1.7658E-018	-8.1064E-052	3.1706E-012	-7.4380E-035
6	0.1250	1.4693E-005	4.8327E-021	1.3862E-020	2.0954E-018	1.0035E-051	4.0751E-012	1.1995E-035
7	0.1313	1.4693E-005	4.9970E-021	1.5029E-020	2.2684E-018	-2.1903E-052	4.5731E-012	5.3358E-035
8	0.1344	1.4692E-005	5.1056E-021	1.5626E-020	2.3570E-018	-9.3510E-052	4.8344E-012	-2.7100E-034
9	0.1375	1.4692E-005	5.3189E-021	1.6238E-020	2.4475E-018	-3.0997E-049	5.1070E-012	-1.9920E-033
10	0.1383	1.4692E-005	5.4395E-021	1.6392E-020	2.4703E-018	7.8956E-051	5.1761E-012	-2.5824E-033
11	0.1391	1.4692E-005	5.6367E-021	1.6547E-020	2.4932E-018	-1.8488E-051	5.2461E-012	-3.2053E-033
12	0.1398	1.4692E-005	5.9674E-021	1.6703E-020	2.5163E-018	-5.4353E-049	5.3168E-012	-3.6125E-033
13	0.1406	1.4692E-005	6.5308E-021	1.6860E-020	2.5394E-018	8.1951E-049	5.3883E-012	-3.9193E-033
14	0.1414	1.4692E-005	7.5001E-021	1.7018E-020	2.5627E-018	-1.6296E-048	5.4606E-012	-4.7500E-033
15	0.1422	1.4692E-005	9.1766E-021	1.7178E-020	2.5862E-018	-9.0125E-050	5.5338E-012	-5.5526E-033
16	0.1438	1.4692E-005	1.6228E-020	1.7503E-020	2.6336E-018	3.4784E-049	5.6834E-012	-7.2910E-033
17	0.1469	1.4692E-005	6.1817E-020	1.8185E-020	2.7304E-018	-1.2263E-050	5.9950E-012	-1.0759E-032
18	0.1500	1.4692E-005	2.4575E-019	1.8950E-020	2.8293E-018	-1.0267E-051	6.3209E-012	-1.4988E-032
19	0.1625	1.4691E-005	6.5828E-018	2.5344E-020	3.2564E-018	-7.4180E-052	7.8374E-012	-8.0593E-032
20	0.1656	1.4691E-005	2.1397E-017	3.0239E-020	3.3655E-018	-1.5392E-051	8.2337E-012	-2.5447E-031
21	0.1688	1.4690E-005	8.1549E-017	4.7458E-020	3.4774E-018	2.3780E-050	8.6511E-012	-1.4228E-030
22	0.1750	1.4690E-005	7.5240E-016	2.7590E-019	3.7183E-018	-8.3257E-051	9.6362E-012	-2.4882E-029
23	0.1875	1.4679E-005	1.4733E-014	6.6769E-018	4.4334E-018	-1.2660E-051	1.4265E-011	-9.3161E-028
24	0.1938	1.4646E-005	9.0758E-014	4.6098E-017	5.1595E-018	5.0410E-051	2.4933E-011	-9.7428E-027
25	0.2000	1.4490E-005	6.1807E-013	3.9916E-016	7.2170E-018	-1.5254E-051	9.3403E-011	-1.2735E-025
26	0.2031	1.4277E-005	1.8541E-012	1.1969E-015	9.2298E-018	5.0746E-050	2.0718E-010	-7.3106E-025
27	0.2047	1.4082E-005	3.4444E-012	2.1889E-015	1.0837E-017	2.2972E-052	3.2729E-010	-2.4310E-024
28	0.2063	1.3754E-005	6.6648E-012	4.3167E-015	1.3501E-017	-7.2843E-051	5.6251E-010	-9.3783E-024
29	0.2078	1.3214E-005	1.2832E-011	8.5523E-015	1.8314E-017	-1.5438E-049	1.0025E-009	-3.7758E-023
30	0.2086	1.2840E-005	1.7694E-011	1.1796E-014	2.2317E-017	-3.0714E-049	1.3277E-009	-8.4756E-023
31	0.2094	1.2348E-005	2.4450E-011	1.6317E-014	2.8779E-017	-1.3442E-048	1.7740E-009	-2.0415E-022
32	0.2102	1.1704E-005	3.3599E-011	2.2392E-014	3.9628E-017	-3.8403E-048	2.3717E-009	-5.0730E-022
33	0.2109	1.0873E-005	4.5609E-011	3.0155E-014	5.8208E-017	-1.1720E-047	3.1434E-009	-1.2766E-021
34	0.2113	1.0377E-005	5.2788E-011	3.4596E-014	7.2424E-017	-2.2679E-047	3.5931E-009	-2.1044E-021
35	0.2117	9.8068E-006	6.0886E-011	3.9449E-014	9.2374E-017	-4.1009E-047	4.0954E-009	-3.5675E-021
36	0.2121	9.1553E-006	6.9903E-011	4.4641E-014	1.2053E-016	-7.9992E-047	4.6492E-009	-6.1524E-021
37	0.2125	8.4180E-006	7.9800E-011	5.0056E-014	1.6035E-016	-1.5594E-046	5.2505E-009	-1.0717E-020
38	0.2129	7.5959E-006	9.0492E-011	5.5544E-014	2.1661E-016	-3.0506E-046	5.8927E-009	-1.8776E-020
39	0.2133	6.6994E-006	1.0184E-010	6.0926E-014	2.9570E-016	-5.8496E-046	6.5662E-009	-3.2994E-020
40	0.2137	5.7514E-006	1.1368E-010	6.6011E-014	4.0590E-016	-8.5099E-046	7.2596E-009	-5.8065E-020
41	0.2141	4.7889E-006	1.2577E-010	7.0624E-014	5.5762E-016	2.5912E-044	7.9599E-009	-1.0226E-019
42	0.2145	3.8608E-006	1.3791E-010	7.4625E-014	7.6346E-016	1.8494E-044	8.6542E-009	-1.8053E-019
43	0.2148	3.0205E-006	1.4985E-010	7.7930E-014	1.0383E-015	4.3566E-044	9.3304E-009	-1.7893E-019
44	0.2156	1.7542E-006	1.7262E-010	8.2347E-014	1.8481E-015	-5.2855E-040	1.0596E-008	-1.7403E-019
45	0.2164	1.0338E-006	1.9376E-010	8.4787E-014	3.0143E-015	2.5114E-045	1.1751E-008	-1.6925E-019
46	0.2172	6.9947E-007	2.1404E-010	8.5770E-014	4.5658E-015	-6.1782E-041	1.2814E-008	-1.6859E-019
47	0.2180	5.5916E-007	2.3515E-010	8.5535E-014	6.4898E-015	1.5170E-038	1.3819E-008	-1.6433E-019
48	0.2188	4.9696E-007	2.5940E-010	8.4116E-014	8.7290E-015	8.8932E-045	1.4800E-008	-1.6623E-019
49	0.2195	4.6352E-007	2.8959E-010	8.1485E-014	1.1179E-014	-6.7139E-038	1.5794E-008	-1.7216E-019
50	0.2203	4.4104E-007	3.2878E-010	7.7631E-014	1.3691E-014	-9.5704E-044	1.6829E-008	-1.7238E-019
51	0.2211	4.2291E-007	3.8040E-010	7.2600E-014	1.6080E-014	-1.9764E-043	1.7931E-008	-1.7258E-019
52	0.2219	4.0616E-007	4.4872E-010	6.6537E-014	1.8132E-014	-4.5881E-043	1.9116E-008	-1.7279E-019
53	0.2234	3.7476E-007	6.5431E-010	5.2189E-014	2.0497E-014	-3.1433E-042	2.1752E-008	-1.7328E-019
54	0.2250	3.4580E-007	1.0097E-009	3.8990E-014	2.1009E-014	-2.7761E-041	2.4447E-008	-1.7385E-019
55	0.2258	3.3066E-007	1.3189E-009	3.5254E-014	2.1801E-014	-9.3095E-041	2.5782E-008	-1.7417E-019
56	0.2266	3.1424E-007	1.8266E-009	3.6868E-014	2.4725E-014	-3.5545E-040	2.7222E-008	-1.7451E-019
57	0.2270	3.0523E-007	2.2189E-009	4.1894E-014	2.8228E-014	-7.3870E-040	2.8118E-008	-1.7468E-019
58	0.2273	2.9516E-007	2.7559E-009	5.2090E-014	3.4305E-014	-1.6124E-039	2.9254E-008	-1.7487E-019
59	0.2277	2.8369E-007	3.4870E-009	7.0068E-014	4.4254E-014	-3.6850E-039	3.0750E-008	-1.7505E-019

60	0.2279	2.7719E-007	3.9448E-009	8.3242E-014	5.1291E-014	-5.6561E-039	3.1670E-008	-1.7515E-019
61	0.2281	2.6996E-007	4.4753E-009	1.0014E-013	6.0162E-014	-8.7769E-039	3.2729E-008	-1.7524E-019
62	0.2283	2.6182E-007	5.0845E-009	1.2141E-013	7.1178E-014	-1.3723E-038	3.3928E-008	-1.7534E-019
63	0.2285	2.5263E-007	5.7759E-009	1.4763E-013	8.4642E-014	-2.1604E-038	3.5254E-008	-1.7544E-019
64	0.2287	2.4222E-007	6.5503E-009	1.7925E-013	1.0082E-013	-3.4146E-038	3.6674E-008	-1.7554E-019
65	0.2289	2.3045E-007	7.4038E-009	2.1644E-013	1.1991E-013	-5.4098E-038	3.8131E-008	-1.7563E-019
66	0.2291	2.1717E-007	8.3275E-009	2.5895E-013	1.4197E-013	-8.5656E-038	3.9541E-008	-1.7573E-019
67	0.2293	2.0231E-007	9.3067E-009	3.0594E-013	1.6692E-013	-1.3519E-037	4.0796E-008	-1.7583E-019
68	0.2295	1.8589E-007	1.0321E-008	3.5589E-013	1.9446E-013	-2.1225E-037	4.1766E-008	-1.7593E-019
69	0.2297	1.6806E-007	1.1345E-008	4.0659E-013	2.2405E-013	-3.3071E-037	4.2313E-008	-1.7603E-019
70	0.2299	1.4916E-007	1.2349E-008	4.5529E-013	2.5497E-013	-5.1040E-037	4.2309E-008	-1.7612E-019
71	0.2301	1.2971E-007	1.3305E-008	4.9903E-013	2.8631E-013	-7.7891E-037	4.1656E-008	-1.7622E-019
72	0.2303	1.1039E-007	1.4185E-008	5.3512E-013	3.1706E-013	-1.1735E-036	4.0303E-008	-1.7631E-019
73	0.2305	9.2021E-008	1.4968E-008	5.6161E-013	3.4625E-013	-1.7439E-036	3.8265E-008	-1.7641E-019
74	0.2307	7.5376E-008	1.5641E-008	5.7769E-013	3.7302E-013	-2.5550E-036	3.5627E-008	-1.7650E-019
75	0.2309	6.1086E-008	1.6200E-008	5.8381E-013	3.9675E-013	-3.6894E-036	3.2529E-008	-1.7658E-019
76	0.2311	4.9489E-008	1.6649E-008	5.8143E-013	4.1705E-013	-5.2501E-036	2.9152E-008	-1.7667E-019
77	0.2313	4.0582E-008	1.6998E-008	5.7266E-013	4.3382E-013	-7.3626E-036	2.5683E-008	-1.7675E-019
78	0.2314	3.4049E-008	1.7263E-008	5.5967E-013	4.4715E-013	-1.0172E-035	2.2297E-008	-1.7683E-019
79	0.2316	2.9392E-008	1.7459E-008	5.4432E-013	4.5728E-013	-1.3837E-035	1.9127E-008	-1.7690E-019
80	0.2318	2.6066E-008	1.7600E-008	5.2798E-013	4.6453E-013	-1.8518E-035	1.6264E-008	-1.7696E-019
81	0.2320	2.3594E-008	1.7696E-008	5.1151E-013	4.6927E-013	-2.4361E-035	1.3749E-008	-1.7702E-019
82	0.2324	2.0225E-008	1.7782E-008	4.7972E-013	4.7219E-013	-3.9912E-035	9.7841E-009	-1.7710E-019
83	0.2328	1.7711E-008	1.7772E-008	4.5002E-013	4.6932E-013	-6.0686E-035	6.9544E-009	-1.7713E-019
84	0.2336	1.4131E-008	1.7534E-008	3.9742E-013	4.5149E-013	-1.1492E-034	3.6507E-009	-1.7699E-019
85	0.2344	1.1629E-008	1.7108E-008	3.5178E-013	4.2653E-013	-1.8004E-034	1.9820E-009	-1.7639E-019
86	0.2352	9.8033E-009	1.6552E-008	3.1241E-013	3.9876E-013	-2.5323E-034	1.1174E-009	-1.7506E-019
87	0.2359	8.4335E-009	1.5916E-008	2.7874E-013	3.7081E-013	-3.3455E-034	6.5236E-010	-1.7258E-019
88	0.2367	7.3871E-009	1.5236E-008	2.5022E-013	3.4425E-013	-4.2308E-034	3.9376E-010	-1.6843E-019
89	0.2375	6.5775E-009	1.4539E-008	2.2626E-013	3.1991E-013	-5.1520E-034	2.4554E-010	-1.6204E-019
90	0.2383	5.9450E-009	1.3844E-008	2.0622E-013	2.9808E-013	-6.0427E-034	1.5808E-010	-1.5294E-019
91	0.2391	5.4465E-009	1.3160E-008	1.8934E-013	2.7861E-013	-6.8154E-034	1.0500E-010	-1.4102E-019
92	0.2398	5.0502E-009	1.2494E-008	1.7476E-013	2.6098E-013	-7.3843E-034	7.1872E-011	-1.2668E-019
93	0.2406	4.7325E-009	1.1848E-008	1.6150E-013	2.4430E-013	-7.6931E-034	5.0638E-011	-1.1083E-019
94	0.2414	4.4749E-009	1.1226E-008	1.4846E-013	2.2741E-013	-7.7335E-034	3.6669E-011	-9.4657E-020
95	0.2422	4.2630E-009	1.0629E-008	1.3456E-013	2.0906E-013	-7.5429E-034	2.7246E-011	-7.9270E-020
96	0.2430	4.0856E-009	1.0060E-008	1.1899E-013	1.8827E-013	-7.1857E-034	2.0737E-011	-6.5452E-020
97	0.2437	3.9335E-009	9.5208E-009	1.0168E-013	1.6484E-013	-6.7304E-034	1.6138E-011	-5.3578E-020
98	0.2445	3.7993E-009	9.0150E-009	8.3514E-014	1.3965E-013	-6.2351E-034	1.2819E-011	-4.3690E-020
99	0.2453	3.6772E-009	8.5451E-009	6.6048E-014	1.1446E-013	-5.7354E-034	1.0374E-011	-3.5760E-020
100	0.2461	3.5627E-009	8.1132E-009	5.0769E-014	9.1211E-014	-5.2699E-034	8.5411E-012	-2.9263E-020
101	0.2469	3.4526E-009	7.7212E-009	3.8458E-014	7.1314E-014	-4.8457E-034	7.1421E-012	-2.4057E-020
102	0.2484	3.2380E-009	7.0578E-009	2.2340E-014	4.3413E-014	-4.1380E-034	5.2059E-012	-1.6557E-020
103	0.2500	3.0228E-009	6.5488E-009	1.3708E-014	2.6989E-014	-3.6044E-034	3.9620E-012	-1.1655E-020
104	0.2516	2.8092E-009	6.1847E-009	9.1128E-015	1.7810E-014	-3.2165E-034	3.1232E-012	-8.3880E-021
105	0.2531	2.6044E-009	5.9498E-009	6.5700E-015	1.2660E-014	-2.9415E-034	2.5337E-012	-6.1629E-021
106	0.2562	2.2488E-009	5.7887E-009	4.2297E-015	8.1610E-015	-2.6320E-034	1.7875E-012	-3.5242E-021
107	0.2594	1.9666E-009	5.9361E-009	3.3460E-015	6.3277E-015	-2.5253E-034	1.3383E-012	-2.1287E-021
108	0.2625	1.7535E-009	6.2931E-009	3.0450E-015	5.5010E-015	-2.5385E-034	1.0460E-012	-1.3475E-021
109	0.2656	1.5943E-009	6.7860E-009	3.0295E-015	5.0761E-015	-2.6237E-034	8.4445E-013	-8.8875E-022
110	0.2688	1.4738E-009	7.3618E-009	3.1808E-015	4.8504E-015	-2.7524E-034	6.9936E-013	-6.0811E-022
111	0.2750	1.3056E-009	8.6105E-009	3.7837E-015	4.7402E-015	-3.0830E-034	5.1020E-013	-3.1556E-022
112	0.2812	1.1859E-009	9.9158E-009	4.6661E-015	4.8694E-015	-3.4595E-034	3.9145E-013	-1.7872E-022
113	0.2875	1.0898E-009	1.1205E-008	5.7511E-015	5.0953E-015	-3.8576E-034	3.1149E-013	-1.0847E-022
114	0.2938	1.0056E-009	1.2443E-008	6.9818E-015	5.3226E-015	-4.2675E-034	2.5473E-013	-6.9571E-023
115	0.3000	9.2802E-010	1.3613E-008	8.3032E-015	5.4898E-015	-4.6855E-034	2.1277E-013	-4.6688E-023
116	0.3063	8.5496E-010	1.4705E-008	9.6591E-015	5.5605E-015	-5.1111E-034	1.8073E-013	-3.2541E-023
117	0.3125	7.8584E-010	1.5715E-008	1.0995E-014	5.5199E-015	-5.5447E-034	1.5563E-013	-2.3430E-023
118	0.3188	7.2083E-010	1.6640E-008	1.2260E-014	5.3708E-015	-5.9876E-034	1.3555E-013	-1.7358E-023
119	0.3250	6.6035E-010	1.7480E-008	1.3416E-014	5.1291E-015	-6.4411E-034	1.1921E-013	-1.3191E-023
120	0.3313	6.0477E-010	1.8235E-008	1.4434E-014	4.8179E-015	-6.9065E-034	1.0571E-013	-1.0258E-023
121	0.3375	5.5430E-010	1.8906E-008	1.5296E-014	4.4624E-015	-7.3846E-034	9.4435E-014	-8.1466E-024
122	0.3438	5.0899E-010	1.9495E-008	1.5998E-014	4.0865E-015	-7.8756E-034	8.4912E-014	-6.5966E-024
123	0.3500	4.6872E-010	2.0004E-008	1.6541E-014	3.7102E-015	-8.3783E-034	7.6816E-014	-5.4397E-024
124	0.3625	4.0272E-010	2.0780E-008	1.7201E-014	3.0184E-015	-9.4219E-034	6.4064E-014	-3.9082E-024
125	0.3750	3.5099E-010	2.1309E-008	1.7413E-014	2.4243E-015	-1.0504E-033	5.4283E-014	-2.9496E-024
126	0.3875	3.1039E-010	2.1627E-008	1.7294E-014	1.9406E-015	-1.1610E-033	4.6609E-014	-2.3186E-024
127	0.4000	2.7826E-010	2.1774E-008	1.6946E-014	1.5575E-015	-1.2735E-033	4.0476E-014	-1.8870E-024
128	0.4125	2.5247E-010	2.1785E-008	1.6450E-014	1.2580E-015	-1.3781E-033	3.5498E-014	-1.5767E-024
129	0.4250	2.3145E-010	2.1690E-008	1.5868E-014	1.0248E-015	-1.4802E-033	3.1406E-014	-1.3322E-024
130	0.4375	2.1405E-010	2.1518E-008	1.5241E-014	8.4284E-016	-1.5936E-033	2.8005E-014	-1.1554E-024

131	0.4500	1.9942E-010	2.1293E-008	1.4602E-014	7.0026E-016	-1.6772E-033	2.5151E-014	-1.0307E-024
132	0.4625	1.8694E-010	2.1036E-008	1.3970E-014	5.8782E-016	-1.7581E-033	2.2737E-014	-9.0130E-025
133	0.4750	1.7615E-010	2.0775E-008	1.3357E-014	4.9870E-016	-1.6561E-033	2.0678E-014	-7.7540E-025
134	0.4812	1.7126E-010	2.0655E-008	1.3061E-014	4.6129E-016	-1.5214E-033	1.9760E-014	-7.2928E-025
135	0.4875	1.6682E-010	2.0554E-008	1.2784E-014	4.2935E-016	-9.2110E-034	1.8939E-014	-4.9492E-025
136	0.4906	1.6484E-010	2.0517E-008	1.2660E-014	4.1596E-016	-9.9021E-034	1.8582E-014	-4.3962E-025
137	0.4938	1.6318E-010	2.0490E-008	1.2556E-014	4.0523E-016	-1.3415E-033	1.8288E-014	-4.2588E-025
138	0.4969	1.6208E-010	2.0476E-008	1.2487E-014	3.9850E-016	-1.0666E-033	1.8099E-014	-1.4915E-025
139	0.5000	1.6208E-010	2.0476E-008	1.2487E-014	3.9850E-016	-1.0666E-033	1.8099E-014	-1.4915E-025

	X(cm)	MOLE FRACTIONS: KCO3	KO3
1	0.0000	-3.7594E-036	3.4333E-013
2	0.0500	-3.7509E-034	3.3790E-011
3	0.0750	-4.2659E-032	5.1479E-011
4	0.1000	5.0956E-033	6.9300E-011
5	0.1125	-2.7597E-032	7.8223E-011
6	0.1250	1.3987E-031	8.7155E-011
7	0.1313	4.3633E-031	9.1623E-011
8	0.1344	-6.2668E-031	9.3859E-011
9	0.1375	-1.0108E-029	9.6097E-011
10	0.1383	-8.7965E-030	9.6657E-011
11	0.1391	-5.8599E-030	9.7217E-011
12	0.1398	-9.2617E-030	9.7777E-011
13	0.1406	-4.8525E-030	9.8339E-011
14	0.1414	-1.5038E-029	9.8901E-011
15	0.1422	-2.0566E-029	9.9465E-011
16	0.1438	-2.1675E-029	1.0060E-010
17	0.1469	-2.1029E-029	1.0293E-010
18	0.1500	-2.0660E-029	1.0547E-010
19	0.1625	-2.0736E-029	1.2480E-010
20	0.1656	-2.1121E-029	1.3739E-010
21	0.1688	-2.0864E-029	1.7320E-010
22	0.1750	-2.0806E-029	5.3529E-010
23	0.1875	-1.5333E-029	7.5271E-009
24	0.1938	-7.9547E-030	2.9856E-008
25	0.2000	-3.2586E-030	1.3778E-007
26	0.2031	-8.0036E-030	2.9005E-007
27	0.2047	-2.2687E-029	4.3278E-007
28	0.2063	-8.0445E-029	6.8128E-007
29	0.2078	-3.0911E-028	1.1022E-006
30	0.2086	-6.8443E-028	1.4022E-006
31	0.2094	-1.6366E-027	1.8066E-006
32	0.2102	-4.0595E-027	2.3489E-006
33	0.2109	-1.0244E-026	3.0674E-006
34	0.2113	-1.6939E-026	3.5055E-006
35	0.2117	-2.8837E-026	4.0170E-006
36	0.2121	-4.9990E-026	4.6109E-006
37	0.2125	-8.7542E-026	5.2941E-006
38	0.2129	-1.5280E-025	6.0676E-006
39	0.2133	-2.3748E-025	6.9239E-006
40	0.2137	3.0021E-025	7.8420E-006
41	0.2141	1.7969E-023	8.7866E-006
42	0.2145	5.0089E-022	9.7095E-006
43	0.2148	2.0983E-023	1.0556E-005
44	0.2156	3.0093E-023	1.1865E-005
45	0.2164	2.6200E-023	1.2643E-005
46	0.2172	1.6308E-023	1.3032E-005
47	0.2180	5.9208E-023	1.3214E-005
48	0.2188	2.4922E-023	1.3301E-005
49	0.2195	-5.0953E-023	1.3341E-005
50	0.2203	-2.2776E-024	1.3351E-005
51	0.2211	-2.2228E-024	1.3339E-005
52	0.2219	-2.4291E-024	1.3309E-005
53	0.2234	-3.0471E-024	1.3194E-005
54	0.2250	-4.2244E-024	1.2986E-005
55	0.2258	-5.3003E-024	1.2785E-005
56	0.2266	-7.0930E-024	1.2413E-005
57	0.2270	-8.4416E-024	1.2106E-005
58	0.2273	-1.0259E-023	1.1663E-005
59	0.2277	-1.2734E-023	1.1040E-005

60	0.2279	-1.4297E-023	1.0645E-005
61	0.2281	-1.6135E-023	1.0181E-005
62	0.2283	-1.8298E-023	9.6431E-006
63	0.2285	-2.0848E-023	9.0291E-006
64	0.2287	-2.3858E-023	8.3399E-006
65	0.2289	-2.7414E-023	7.5812E-006
66	0.2291	-3.1619E-023	6.7642E-006
67	0.2293	-3.6594E-023	5.9066E-006
68	0.2295	-4.2482E-023	5.0316E-006
69	0.2297	-4.9451E-023	4.1676E-006
70	0.2299	-5.7700E-023	3.3451E-006
71	0.2301	-6.7463E-023	2.5938E-006
72	0.2303	-7.9012E-023	1.9382E-006
73	0.2305	-9.2668E-023	1.3944E-006
74	0.2307	-1.0881E-022	9.6708E-007
75	0.2309	-1.2787E-022	6.5000E-007
76	0.2311	-1.5036E-022	4.2772E-007
77	0.2313	-1.7688E-022	2.7980E-007
78	0.2314	-2.0812E-022	1.8521E-007
79	0.2316	-2.4487E-022	1.2584E-007
80	0.2318	-2.8808E-022	8.8255E-008
81	0.2320	-3.3881E-022	6.3536E-008
82	0.2324	-4.6796E-022	3.5266E-008
83	0.2328	-6.4441E-022	2.0052E-008
84	0.2336	-1.2073E-021	6.8424E-009
85	0.2344	-2.2115E-021	2.4437E-009
86	0.2352	-3.9403E-021	9.1658E-010
87	0.2359	-6.7949E-021	3.6159E-010
88	0.2367	-1.1282E-020	1.5033E-010
89	0.2375	-1.7941E-020	6.5958E-011
90	0.2383	-2.7185E-020	3.0551E-011
91	0.2391	-3.9083E-020	1.4930E-011
92	0.2398	-5.3193E-020	7.6864E-012
93	0.2406	-6.8576E-020	4.1595E-012
94	0.2414	-8.4038E-020	2.3595E-012
95	0.2422	-9.8471E-020	1.3984E-012
96	0.2430	-1.1111E-019	8.6309E-013
97	0.2437	-1.2158E-019	5.5273E-013
98	0.2445	-1.2985E-019	3.6602E-013
99	0.2453	-1.3596E-019	2.4979E-013
100	0.2461	-1.4045E-019	1.7513E-013
101	0.2469	-1.4346E-019	1.2581E-013
102	0.2484	-1.4605E-019	6.9179E-014
103	0.2500	-1.4545E-019	4.0576E-014
104	0.2516	-1.4273E-019	2.5099E-014
105	0.2531	-1.3865E-019	1.6258E-014
106	0.2562	-1.2843E-019	7.7370E-015
107	0.2594	-1.1743E-019	4.1698E-015
108	0.2625	-1.0688E-019	2.5019E-015
109	0.2656	-9.7313E-020	1.6455E-015
110	0.2688	-8.8906E-020	1.1694E-015
111	0.2750	-7.5640E-020	7.1012E-016
112	0.2812	-6.5433E-020	5.0409E-016
113	0.2875	-5.7527E-020	3.9476E-016
114	0.2938	-5.1314E-020	3.2784E-016
115	0.3000	-4.6359E-020	2.8153E-016
116	0.3063	-4.2358E-020	2.4615E-016
117	0.3125	-3.9097E-020	2.1713E-016
118	0.3188	-3.6425E-020	1.9223E-016
119	0.3250	-3.4227E-020	1.7036E-016
120	0.3313	-3.2420E-020	1.5094E-016
121	0.3375	-3.0935E-020	1.3368E-016
122	0.3438	-2.9720E-020	1.1838E-016
123	0.3500	-2.8734E-020	1.0490E-016
124	0.3625	-2.7387E-020	8.3047E-017
125	0.3750	-2.6526E-020	6.6167E-017
126	0.3875	-2.5998E-020	5.3199E-017
127	0.4000	-2.5748E-020	4.3227E-017
128	0.4125	-2.5596E-020	3.5522E-017
129	0.4250	-2.5579E-020	2.9525E-017
130	0.4375	-2.5431E-020	2.4814E-017

131	0.4500	-2.5507E-020	2.1079E-017
132	0.4625	-2.5554E-020	1.8088E-017
133	0.4750	-2.5315E-020	1.5675E-017
134	0.4812	-2.2030E-020	1.4644E-017
135	0.4875	-2.0278E-020	1.3751E-017
136	0.4906	-1.4906E-020	1.3370E-017
137	0.4938	-1.8785E-020	1.3061E-017
138	0.4969	-1.5498E-020	1.2863E-017
139	0.5000	-1.5498E-020	1.2863E-017

Appendix:I

Table 2: Flame Speed Variation with Equivalence Ratio of CH_4/KCO_3 mixture

Equivalence Ratio	S_L of pure CH_4 (cm/s)	S_L of CH_4/ $0.001\%KCO_3$ mixture	S_L of CH_4/ $0.071\%KCO_3$ mixture
0.6	89	88	88
0.7	117	117	116
0.8	141	140	138
0.9	157	156	154
1	165	164	162
1.1	164	163	161
1.2	153	152	149
1.3	130	129	127
1.4	100	99	98
1.5	73	72	72
1.6	57	56	56
1.7	47	46	46
1.8	39	39	39