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Numerical analysis of liquid ammonia spray and combustion

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This thesis is dedicated to
Zhao Yu Han,
for the delight, surprise and companionship you have provided me
throughout the 1575 days.

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Abstract

This thesis investigates liquid-ammonia injection and flashing-spray behaviour relevant to ammonia-fuelled gas turbines and related combustion systems, with an emphasis on how superheat, injector boundary conditions and modelling assumptions influence spray penetration, morphology and droplet-scale statistics. Chapter 1 reviews the constraints associated with ammonia combustion and motivates the need for spray models that account for latent-heat-driven cooling and near-nozzle phase-change effects. Chapter 3 examines ammonia–methane co-firing in a gas-turbine combustor. The model reproduces the principal recirculation topology but overpredicts liquid penetration, identifying limitations in the representation of superheated injection. Chapter 4 develops an Eulerian–Lagrangian workflow in ANSYS Fluent for ammonia sprays in a constant-volume chamber and compares predicted macroscopic penetration with available measurements across several superheat conditions. The results show that agreement depends strongly on the specification and calibration of the injection momentum, and that the Rosin–Rammler distribution parameters require further calibration against matched experimental data. Chapter 5 uses compressible volume-of-fluid simulations coupled with a homogeneous relaxation model in OpenFOAM to investigate cavitation and flash-boiling dynamics within the nozzle and near field. Under flare-flashing conditions, the simulations indicate that the in-nozzle flow can remain subsonic and metastable while intense phase change occurs mainly after discharge. A stationary two-phase shock structure forms in the near field and can limit centreline momentum, providing a mechanism for the characteristic near-field morphologies and their sensitivity to nozzle geometry. Overall, the results identify the limitations of conventional spray-modelling assumptions for superheated ammonia and provide guidance on injection specification, the post-processing of droplet statistics and the interpretation of compressible two-phase structures near the nozzle.

Nomenclature

Abbreviations

CFD	Computational Fluid Dynamics
CSR	Catalytic Steam Reforming
CVC	Constant Volume Chamber
DBI	Diffuse Back-Illumination
DO	Discrete Ordinates (radiation model)
DPM	Discrete Phase Model
EDC	Eddy Dissipation Concept
FBN	Flash-Boiling Number
GDI	Gasoline Direct Injection
GHG	Greenhouse Gas
HB	Haber–Bosch process
HRM	Homogeneous Relaxation Model
ICE	Internal Combustion Engine
IRZ	Inner Recirculation Zone
KH–RT	Kelvin–Helmholtz / Rayleigh–Taylor breakup model
LES	Large-Eddy Simulation
LPT	Lagrangian Particle Tracking
MILD	Moderate or Intense Low Oxygen Dilution (combustion)
OEW	Oblique Evaporation Wave
PDF	Probability Density Function
PIV	Particle Image Velocimetry
ASOI	After Start of Injection
ppmv	Parts per million by volume
PIMPLE	Merged PISO–SIMPLE algorithm (OpenFOAM)
RANS	Reynolds-Averaged Navier–Stokes
RK3	Third-order Runge–Kutta scheme
RQL	Rich–Quench–Lean (combustion)
RNG	Renormalisation Group
SSP	Strong Stability Preserving
SST	Shear Stress Transport
UDF	User-Defined Function
VOF	Volume of Fluid

Symbols (alphabetical)

α	Phase volume fraction (-)
α_L, α_G	Liquid and vapour volume fractions (-)
α_f	Heat transfer coefficient for flash evaporation (W/m ² K)
α_k	Inverse effective Prandtl number for k (-)
α_ε	Inverse effective Prandtl number for ε (-)
α_v	Vapour volume fraction in HRM (-)
β	RNG k - ε model constant (-)
χ	Instantaneous vapour mass fraction in HRM (-)
$\bar{\chi}$	Equilibrium vapour mass fraction in HRM (-)
$\dot{m}$	Total evaporation or mass flow rate (kg/s)
$\dot{m}_d$	Droplet evaporation rate (kg/s)
$\dot{m}_{\text{flash}}$	Flashing evaporation rate (kg/s)
$\dot{m}_h$	Heat-transfer-driven evaporation rate (kg/s)
$\dot{m}_L$	Liquid-phase volumetric mass source (kg/m ³ s)
$\dot{q}_p$	Heat transferred to a droplet (W)
Δp	Pressure difference (Pa)
ΔT	Temperature difference (K)
ε_p	Droplet emissivity (-)
η	RNG k - ε auxiliary variable (-)
η_0	RNG k - ε constant (-)
λ_g	Gas thermal conductivity (W/m K)
μ	Dynamic viscosity (Pa s)
μ_t	Turbulent (eddy) viscosity (Pa s)
ν_t	Turbulent kinematic viscosity (m ² /s)
Ω_{RT}	Rayleigh–Taylor instability growth rate (1/s)
ϕ	Global equivalence ratio (-)
π	Pi (-)
Pr	Prandtl number (-)
Pr _t	Turbulent Prandtl number (-)
ρ	Density (kg/m ³)
ρ_g	Gas density (kg/m ³)
ρ_l	Liquid density (kg/m ³)
ρ_p	Droplet density (kg/m ³)
ρ_v	Vapour density (kg/m ³)
σ	Stefan–Boltzmann constant (W/m ² K ⁴)
$\boldsymbol{\tau}$	Molecular stress tensor (Pa)
$\boldsymbol{\tau}_t$	Turbulent stress tensor (Pa)
τ_{RT}	Rayleigh–Taylor breakup time scale (s)
θ	HRM relaxation time scale (s)
θ_0	HRM empirical time constant (s)
θ_R	Radiation temperature (K)
φ	HRM pressure driving term (-)
A	Area (m ²)
A_{eff}	Effective injection area (m ²)

A_p	Droplet surface area (m ²)
a_p	Diagonal momentum-equation coefficient (kg/m ³ s)
B_M	Spalding mass transfer number (-)
B_T	Spalding heat transfer number (-)
C_a	Contraction coefficient (-)
C_d	Discharge coefficient (-)
C_D	Drag coefficient (-)
C_L	Levich constant (-)
C_μ	Turbulence-model constant (-)
C_{RT}	RT breakup radius constant (-)
C_τ	RT breakup time constant (-)
$C_{1\varepsilon}, C_{2\varepsilon}, C_{3\varepsilon}$	RNG k - ε constants (-)
$C_{\varepsilon 1}$	k - ε model constant (-)
c_p	Droplet specific heat capacity (J/kg K)
c_{pg}	Gas-mixture specific heat capacity (J/kg K)
c_{pv}	Vapour specific heat capacity (J/kg K)
D	Nozzle diameter / characteristic diameter (m)
$D_{i,m}$	Mass diffusivity in gas mixture (m ² /s)
D_e	Effective droplet diameter (m)
D_p	Droplet diameter (m)
d_d	Droplet diameter used in evaporation correlations (m)
d_{mean}	Rosin–Rammler characteristic diameter (m)
D_{eff}	Effective nozzle diameter (m)
$D^2\text{-law}$	Classical droplet evaporation scaling (-)
$Dv_{10}, Dv_{50}, Dv_{90}$	Volume-based percentile diameters (m)
E_{NH_3}	Energy fraction of ammonia in a blended fuel (-)
$F(d)$	Rosin–Rammler cumulative mass fraction (-)
F_{T_0}	Baseline heat-transfer correction factor (-)
F_T	Heat-transfer correction factor (-)
F_M	Mass-transfer correction factor (-)
FBN	Flash-boiling number (-)
F_D	Drag response coefficient (1/s)
F_x	Additional acceleration term (m/s ²)
g	Gravitational acceleration (m/s ²)
g_x	Gravitational acceleration component (m/s ²)
G	Incident radiation (W/m ²)
G_b	Buoyancy production term for turbulence (kg/m s ³)
G_k	Mean-strain production term for turbulence (kg/m s ³)
h	Convective heat transfer coefficient (W/m ² K)
h_{fg}	Latent heat of vaporisation (J/kg)
h_{SG}, h_{SL}	Saturated vapour/liquid enthalpy (J/kg)
h_g, h_s	Gas/surface enthalpy (J/kg)
$H(\mathbf{u})$	Off-diagonal momentum-equation contribution (kg/m ² s ²)
k	Thermal conductivity (W/m K)
k_{EFF}	Effective thermal conductivity (W/m K)
k_t	Turbulent thermal conductivity (W/m K)

K	Kinetic energy per unit mass (m^2/s^2)
K_{RT}	RT wavenumber ($1/\text{m}$)
L	KH–RT breakup length scale (m)
L/D	Nozzle length-to-diameter ratio (-)
L_v	Latent heat of vaporisation (J/kg)
Le	Lewis number (-)
m_p	Droplet mass (kg)
Nu	Nusselt number (-)
Nu^*	Modified Nusselt number (-)
n	Rosin–Rammler spread parameter (-)
P_{amb}	Ambient pressure (Pa)
P_{inj}	Injection pressure (Pa)
P_{sat}	Saturation pressure (Pa)
p	Pressure (Pa)
p_c	Critical pressure (Pa)
p_s	Saturation pressure (Pa)
P_r	Reduced pressure, $P_{\text{amb}}/P_{\text{sat}}$ (-)
$PNIP$	Particle Number in Parcel (-)
R	Gas constant (J/kg K)
R_{gas}	Gas constant used in L–K model (J/kg K)
R_p	Superheat parameter / pressure ratio, $P_{\text{sat}}(T_{\text{inj}})/P_{\text{amb}}$ (-)
Re	Reynolds number (-)
Re_d	Droplet Reynolds number (-)
S	Swirl number (-)
S_{mm}	Penetration distance (mm)
Sc_t	Turbulent Schmidt number (-)
Sh	Sherwood number (-)
Sh^*	Modified Sherwood number (-)
SI	Superheat index (-)
SMD	Sauter Mean Diameter (m)
T	Temperature (K)
T_b	Boiling temperature (K)
T_{bp}	Boiling point temperature (K)
T_d	Droplet temperature (K)
T_{inj}	Injection temperature (K)
T_p	Droplet temperature (K)
T_{∞}	Far-field gas temperature (K)
T_s	Surface temperature (K)
u	Continuous-phase velocity (m/s)
u_p	Droplet velocity (m/s)
U_0	Injection exit velocity (m/s)
v_0	Injection velocity (m/s)
We_g	Gas Weber number (-)
$Y_{Fs}, Y_{F\infty}$	Fuel mass fraction at droplet surface / far field (-)
Y_M	contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate (kg/m^3)
Y_{is}	Surface mass fraction of evaporating species (-)
ψ	Mixture compressibility, $\partial\rho/\partial p$ (s^2/m^2)

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Chapter 1

Introduction and literature review

1.1 Thesis scope and research narrative

This thesis investigates liquid-ammonia spray and combustion across three connected physical scales. The first scale is combustor-scale mixture formation and reaction, where spray evaporation interacts with swirl, recirculation and ammonia–methane chemistry. The second is the dispersed-spray scale, where individual superheated droplets undergo evaporation, cooling and momentum exchange after injection. The third is the near-nozzle scale, where cavitation, metastability, rapid phase change and two-phase compressibility determine the conditions delivered to the external spray. Treating these scales in sequence provides a coherent route from the practical combustion problem to the detailed mechanisms that govern flashing atomisation.

The literature review is organised according to this progression. It first establishes the motivation for ammonia as an energy carrier and reviews the combustion strategies, chemistry, turbulence and spray processes relevant to gas-turbine applications. It then focuses on experimental observations and Lagrangian modelling of flash-boiling ammonia sprays. Finally, it examines internal-nozzle cavitation, compressible two-phase flow and homogeneous-relaxation modelling, which are required to interpret the near-nozzle behaviour that cannot be resolved by a point-particle description.

1.2 Definition and scope of flashing and flash boiling

In this thesis, *flashing* denotes pressure-driven vapour generation when a liquid is rapidly exposed to a pressure below the saturation pressure corresponding to its temperature, such that $P < P_{\text{sat}}(T)$, or equivalently $T > T_{\text{sat}}(P)$. The liquid then enters

a superheated, metastable state and relaxes towards equilibrium through nucleation, bubble growth and evaporation. *Flash boiling* refers to the rapid boiling process that follows this depressurisation. Because nucleation and bubble growth require a finite time, satisfying the thermodynamic criterion does not imply instantaneous or complete vaporisation [22, 59].

Flash boiling is distinguished here from conventional evaporation, heat-driven boiling and cavitation. Surface evaporation can occur below the boiling point and is governed mainly by interfacial heat and mass transfer, while conventional boiling follows sustained heating to the saturation temperature at the prevailing pressure. Cavitation results from a local pressure reduction within the liquid, commonly inside a nozzle, and its vapour structures may collapse if the pressure recovers. During flashing injection, however, vapour structures can continue to grow after discharge because the surrounding pressure remains below the liquid saturation pressure. Cavitation and flash boiling may therefore coexist and interact in ammonia injectors, but they describe different dominant mechanisms [97, 21].

The scope of this thesis covers pressure-driven phase change at three connected scales: its effect on evaporation, mixture preparation and combustion in a swirl combustor; the finite-rate evaporation and cooling of superheated Lagrangian droplets; and the resolved interaction of in-nozzle cavitation, metastability, relaxation-controlled phase change and compressible near-nozzle flow. The superheat pressure ratio used throughout the thesis is

$$R_p = \frac{P_{\text{sat}}(T_{\text{inj}})}{P_{\text{amb}}}, \quad (1.1)$$

where $P_{\text{sat}}(T_{\text{inj}})$ is the saturation pressure at the injection temperature and P_{amb} is the ambient pressure. A value $R_p > 1$ indicates that flashing is thermodynamically possible following exposure to the ambient pressure, whereas geometry, residence time and the relaxation time scale determine where and how rapidly it develops. The term *flare flashing* is reserved for the strongly flashing regime associated with intense near-nozzle vapour generation and radial spray expansion [114, 50, 70].

1.3 Homogeneous relaxation model and relaxation time scale

The homogeneous relaxation model (HRM) represents finite-rate phase change by allowing the local vapour mass fraction to relax towards its thermodynamic-equilibrium value rather than imposing instantaneous equilibrium. If χ is the instantaneous

vapour mass fraction and $\bar{\chi}$ is the equilibrium vapour mass fraction, the relaxation relation is written as

$$\frac{D\chi}{Dt} = \frac{\bar{\chi} - \chi}{\theta}, \quad (1.2)$$

where θ is the relaxation time scale. A small value of θ produces rapid approach to equilibrium, whereas a large value preserves a metastable liquid state over a longer residence time. HRM is therefore suitable for flows in which the hydrodynamic and phase-change time scales are comparable, including flashing through short nozzles and rapid near-nozzle expansion [22, 29].

The empirical Downar–Zapolski correlation expresses the relaxation time as $\theta = \theta_0 \alpha_v^{-0.54} \varphi^{-1.76}$, where α_v is the vapour volume fraction, φ is a dimensionless pressure-driving term and θ_0 is an empirical time constant [22]. The constant θ_0 controls the overall phase-change rate and was originally calibrated using flashing-water data. Its direct application to ammonia is therefore uncertain because nucleation behaviour and thermophysical properties differ between fluids. In this thesis, θ_0 is treated as a calibration and sensitivity parameter and is assessed against measured ammonia spray angles.

The HRM assumes that the phases share a common pressure and velocity field at the resolved scale. It does not resolve individual bubbles or nucleation sites; their combined effect is represented through the relaxation law. The model is coupled here with a compressible volume-of-fluid formulation so that delayed vaporisation, changes in mixture sound speed and near-nozzle shock structures can be represented within one Eulerian framework. The detailed implementation and ammonia-specific sensitivity analysis are presented in Sections 2.4 and Chapter 5.

1.4 Ammonia as an energy carrier and combustion fuel

1.4.1 Energy context and motivation

Reducing greenhouse-gas emissions requires low-carbon energy carriers that can connect variable renewable generation with transport, industry and dispatchable power production. Solar, wind and tidal resources are intrinsically intermittent and geographically constrained, so their energy must often be stored in electrical, thermal, mechanical or chemical form. Chemical fuels remain attractive where high energy

density, long-duration storage and transportability are required. Hydrogen and ammonia are therefore widely considered as potential renewable-energy vectors, provided that their production is decarbonised [45, 93].

Hydrogen can be produced by several routes, including reforming of hydrocarbons or biomass-derived feedstocks and water electrolysis [49]. Its oxidation produces water without direct carbon dioxide emissions, and its gravimetric energy density is high. However, its low volumetric energy density under moderate storage conditions, broad flammability range and high burning velocity complicate storage, transport and leakage management [90]. Ammonia provides an alternative means of storing hydrogen in a carbon-free molecule. It is synthesised from nitrogen and hydrogen through the Haber–Bosch process and may be used directly as a fuel or cracked to produce a hydrogen-rich stream at the point of use [40]. Figure 1.1 summarises this renewable hydrogen–ammonia pathway.

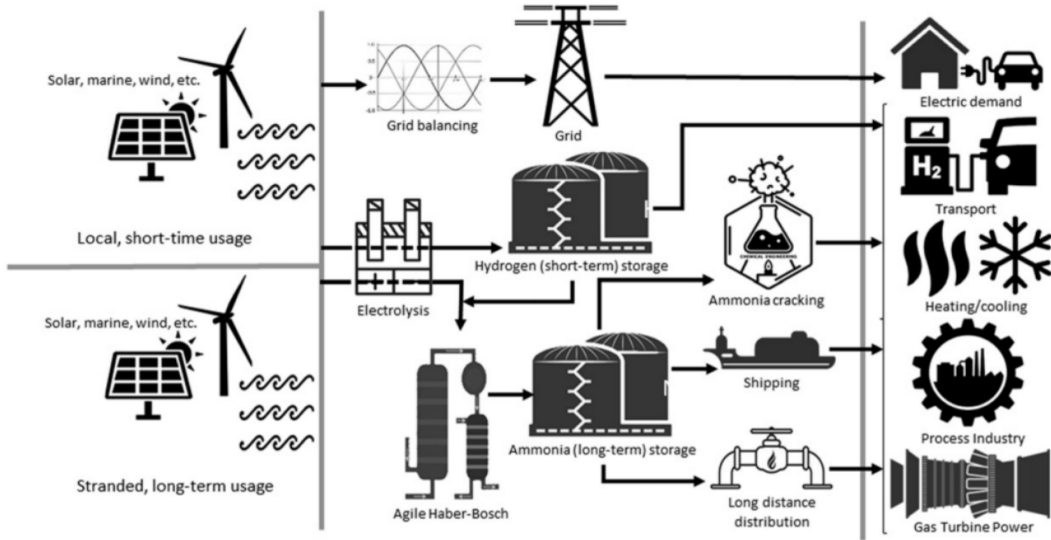


Figure 1.1: Carbon-free hydrogen/ammonia production approach [91].

Ammonia combustion has been investigated since the twentieth century, and early studies already identified its low flame-propagation rate and strong dependence of nitrogen-oxide emissions on mixture strength [78, 98]. Renewed interest in carbon-free fuels has highlighted the same practical challenges: low burning velocity, long ignition delay, restricted flame stability and the trade-off between NO_x formation and unburned ammonia [45, 23]. Fuel blending and staged combustion can mitigate these limitations. Ammonia–methane mixtures improve reactivity, while rich–quench–lean combustion, very-lean operation, MILD combustion and humidification offer alternative routes for controlling stability and emissions [65, 64, 92, 77, 81].

Supplying gaseous ammonia requires energy for vaporisation and preheating. Direct liquid injection can simplify fuel delivery and exploit injection hardware derived from conventional liquid-fuel systems [54]. Its success nevertheless depends on producing a sufficiently dispersed spray, because ammonia’s high latent heat and propensity to flash during depressurisation strongly affect evaporation, mixing and flame stabilisation [64].

1.5 Ammonia spray combustion in gas turbines

Ammonia benefits from an established production, storage and distribution infrastructure developed for the fertiliser industry and can be synthesised using renewable hydrogen [79, 16]. Its use has consequently been investigated in internal-combustion engines and gas turbines [74, 50, 70, 3, 66, 64, 35, 13, 84]. For gas-turbine applications, the central challenge is to combine rapid liquid-fuel preparation with stable heat release and acceptable emissions despite ammonia’s low reactivity, strong evaporative cooling and fuel-bound nitrogen.

1.5.1 Ammonia as fuel

Ammonia is carbon-free and has long been used as a chemical and fertiliser, but it has only recently been reconsidered as a potential energy vector and fuel [45, 93, 16]. Compared with hydrogen, ammonia has a higher volumetric energy density under moderate storage conditions (Figure 1.2) and can be liquefied at around 10 bar at ambient temperature, which simplifies storage and transport [91, 40]. Ammonia can also be cracked to produce hydrogen-rich mixtures, enabling flexible use in various applications [40, 49].

However, the combustion characteristics of ammonia are unfavourable. Its laminar burning velocity is significantly lower than that of typical hydrocarbons or hydrogen, the flammability range is narrow, and the ignition temperature is high [45, 23]. In addition, due to the fuel-bound nitrogen, ammonia flames tend to produce large amounts of NO_x through both fuel-N and thermal-N pathways [30, 46]. These drawbacks make it difficult to achieve stable and clean combustion when ammonia is used as the sole fuel.

To balance the feature in the low gravimetric energy density of liquid ammonia, research has therefore focused on fuel-blending strategies. Hydrogen is the first fuel that can be considered to mix with ammonia, as it has the most mass-energy density, fast-burning velocity, and high-burning temperature. Additionally, ammonia can be

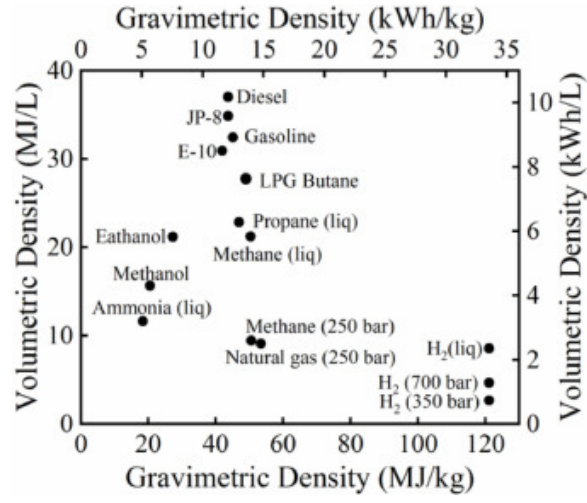


Figure 1.2: The gravimetric and volumetric densities of hydrogen, ammonia, and other fuels [90].

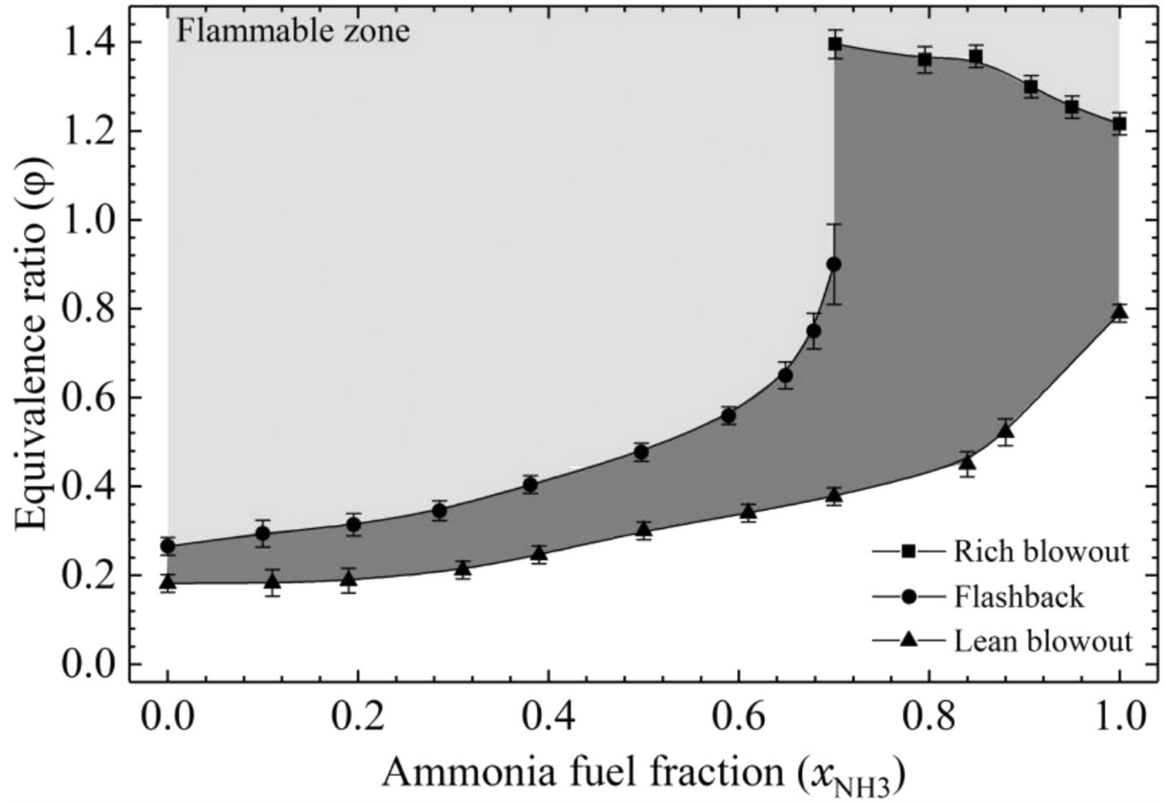


Figure 1.3: Flammable zone and stability zone of ammonia-hydrogen air combustion [42].

converted to hydrogen as a carrier which approaches even better[61]. According to [42, 41, 26], adding 10% to 30% of hydrogen to ammonia promotes the reactivity and flame speed, and Fig.1.3, modifies the lean blowout limit. However, Goldman et al.[31] reported that hydrogen has the potential to cause flashbacks if the proportion of ammonia is not enough. Mixing diesel with ammonia can be another approach, considering the high energy density. [74, 51] tried different ratios of diesel fuel energy with ammonia. They found that the fuel energy ratio of diesel between 40% to 60% was acceptable. Otherwise, the ammonia in the mixture was either incomplete combustion or too lean condition [74]. Mixing methane with ammonia is also an appropriate method to increase flame speed and flame temperature. In the following discussion, the equivalence ratio ϕ denotes the actual fuel-to-oxidiser ratio normalised by the stoichiometric fuel-to-oxidiser ratio, and the swirl number S denotes the non-dimensional measure of angular momentum relative to axial momentum in the inlet flow. It is also found that methane can promote the blow-off equivalence-ratio limit, as shown in Fig. 1.4, while requiring a larger mixing ratio than hydrogen [108].

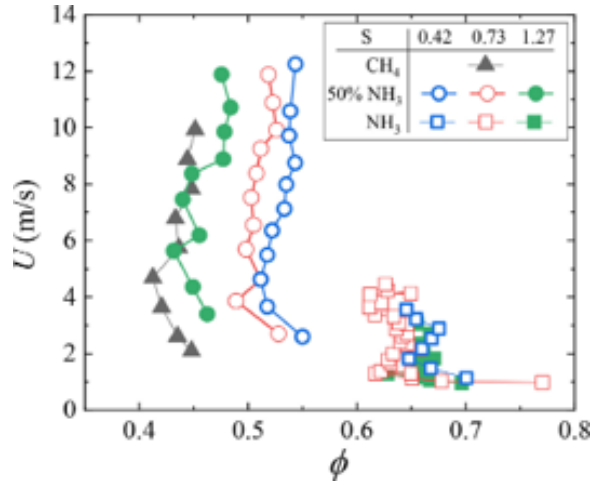


Figure 1.4: Blow-off equivalence ratio limits of swirled $\text{NH}_3\text{-CH}_4$ flame for different inlet air velocity and swirl number S [108].

Supplying gaseous ammonia requires additional energy and can delay ignition [69]. By contrast, direct liquid-ammonia injection can increase the rate of energy delivery to the combustor. Okafor et al. [69] studied liquid-ammonia spray combustion with swirled air preheated to 500 K. They used the recirculation of heat and radicals in a strongly swirling flow ($S > 0.6$) to enhance flame stability. Images of pure liquid-ammonia spray flames and ammonia-methane co-fired flames were compared (Fig. 1.5). Methane addition shortened the ammonia flame. However, the large

latent heat of ammonia strongly affected spray-combustion emissions, and combustion efficiency decreased as ϕ increased [69, 107]. The associated reduction in O, H and OH radical production increased unburned NH_3 and N_2 emissions and shifted the optimum equivalence ratio towards leaner conditions [69, 107].

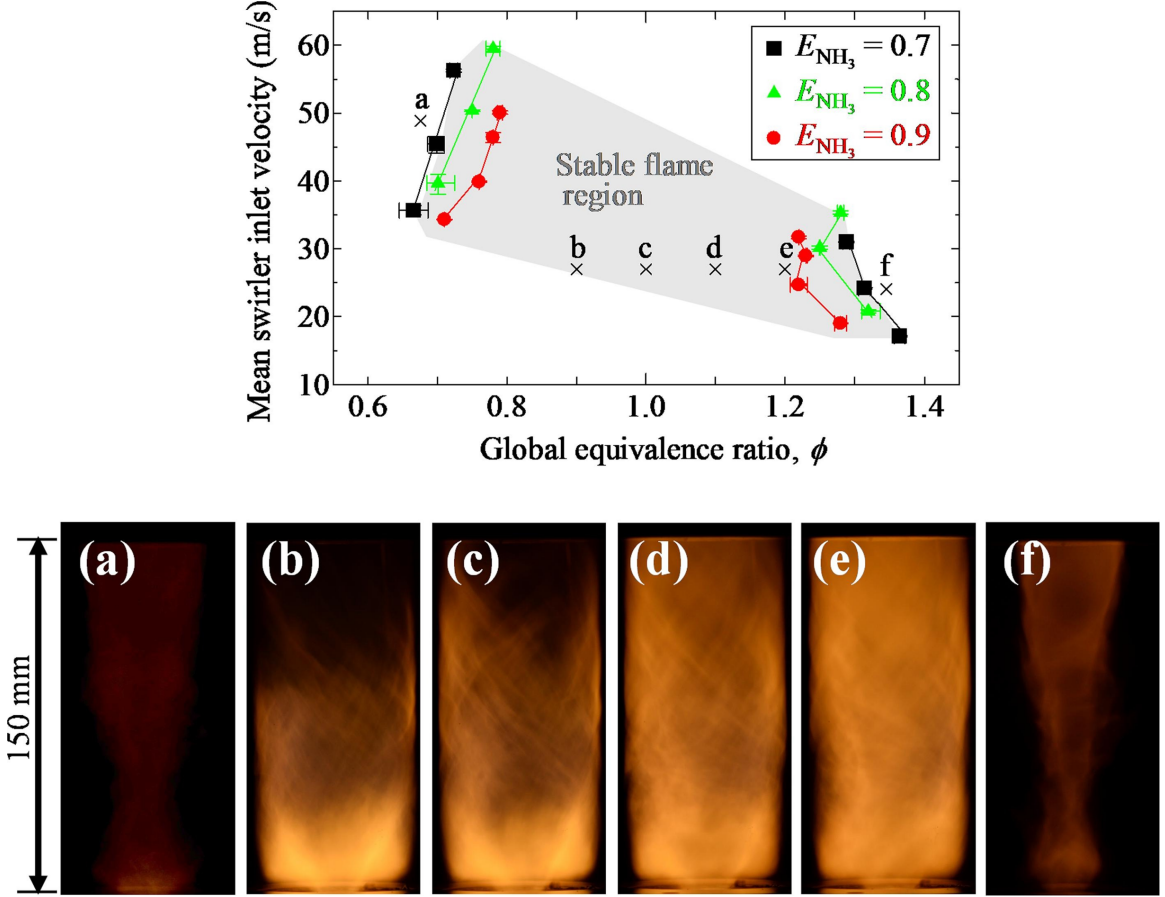


Figure 1.5: Stability region and flame image for spray ammonia co-fired with methane at $E_{\text{NH}_3} = 0.7$ [69].

Okafor et al. [69] also found that the co-combustion of gaseous ammonia and methane in a single-stage combustor produced NO emissions above 5000 ppmv at equivalence ratios of 0.8–1.0. This level was approximately twice that of NH_3 –air combustion and an order of magnitude higher than that of CH_4 –air combustion. At sufficiently fuel-rich conditions, NO_x emissions became negligible, but emissions of unburned NH_3 , H_2 , HCN and CO were significant. The liquid NH_3 – CH_4 flame exhibited a trade-off similar to that of the gaseous mixture: approximately 4000 ppmv NO was measured under lean conditions ($\phi = 0.85$), whereas more than 1000 ppmv NH_3 was measured under rich conditions ($\phi > 1$) [69]. The minimum combined NO and NH_3 emissions were reported at a global equivalence ratio of 1.06 under fuel-rich

conditions, with an ammonia fraction above 0.5 [69, 107]. CO production decreased as the ammonia fraction increased [108]. The trends in NO₂ and HCN were similar to those in NO and NH₃, respectively [69]. These results indicate that two-stage combustion is a promising approach for consuming unburned NH₃ and HCN and controlling emissions from liquid-ammonia-methane combustion [65, 64, 69].

1.5.2 Combustion strategy of gas turbine

Due to the high NO_x emission potential of ammonia-containing fuels, it is necessary to design combustion strategies that can reduce NO_x while maintaining flame stability and acceptable efficiency. Several strategies have been discussed in the literature for application in gas turbine combustors.

1.5.2.1 Swirl combustion

Swirl-stabilised combustion is widely used in gas turbines because the swirling flow creates an internal recirculation zone (IRZ), which enhances mixing, heat recirculation and radical transport (Figure 1.6), thereby stabilising the flame [38, 87]. For ammonia and ammonia-hydrogen/methane flames, swirl burners have been extensively studied in both premixed and non-premixed configurations [42, 41, 92, 108]. The swirl number, inlet velocity and equivalence ratio all affect the size and strength of the recirculation zone and hence the stability limits and emission characteristics [38, 108, 42].

Experiments and numerical simulations have shown that for premixed swirl flames of ammonia-hydrogen-air or ammonia-methane-air, increasing the hydrogen or methane fraction can shift the lean blow-off limit towards lower equivalence ratios and improve flame robustness [42, 41, 108]. However, high swirl can also promote local hot spots and enhance NO_x formation if not properly optimised [38, 17]. As a result, careful design of the swirl level and fuel staging is required.

1.5.2.2 Extremely lean condition

Extremely lean combustion is a potential strategy for ammonia mixtures because it can reduce NO_x emissions without requiring major combustor modifications [23]. Khateeb et al. [42, 41] reported the stability limits and NO emissions of ammonia blended with hydrogen or methane at various pressures. They concluded that elevated pressure broadened the operating range between flashback and lean blow-off [42]. Ammonia-hydrogen flames can also be stabilised under very lean conditions while

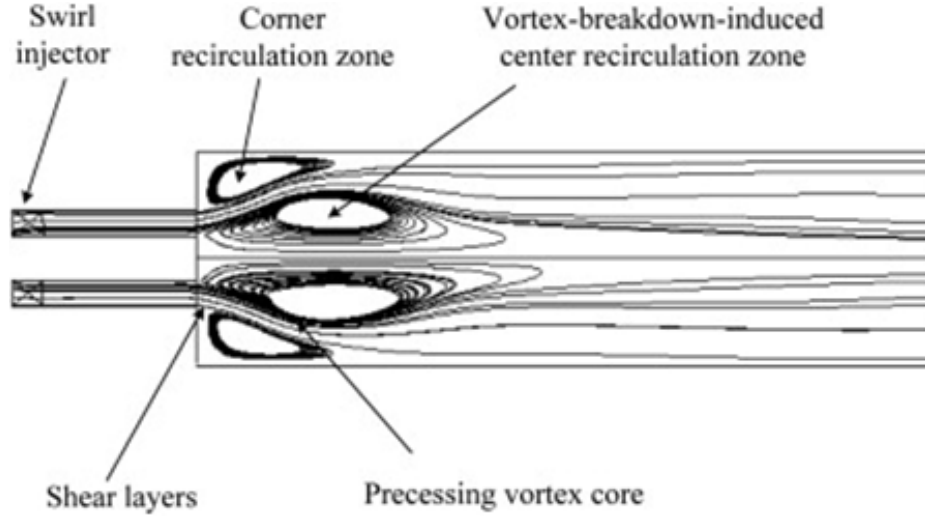


Figure 1.6: Streamlines generated by swirler inside chamber [38].

producing less than 200 ppm NO_x . By contrast, lean pure-ammonia and ammonia-methane flames were unable to achieve both stable combustion and low NO_x emissions [23]. Zhang et al. reported a lower blow-off limit than Khateeb et al., although the corresponding NO_x emissions require further investigation [108].

1.5.2.3 Rich-Quench-Lean two-stage combustion

Rich-Quench-Lean two-stage combustion strategy is designed for the consumption of unburned fuel under fuel-rich conditions as the ammonia-methane flame will produce less NO at an equivalence ratio of around 1.1. There are also reaction routines in the methane ammonia chemical mechanism, which consumes both unburnt NH_3 and NO [65]. Research was carried out on the equivalence ratio, pressure, and geometry of chamber and inlets. The air supplied in the second stage was found to dominate the first stage equivalence ratio, which is highly relative to the final emission[23].

Okafor et al. [66], [64] conducted premixed/non-premixed ammonia/liquid ammonia experiments and numerical simulations with two-stage combustion. Simulation results in Fig. 1.7 demonstrate the NO emissions in the first and second stages and the relationship between the primary equivalence ratio and the NO emissions[66]. It is summarized by Elbaz et al. that slightly fuel-rich conditions ($\phi = 1.1\text{--}1.3$) can reduce NO_x emissions [23]. Okafor et al. [66] simulated the results regarding NO_x emissions of 49 ppm with negligible N_2O and NH_3 emissions for ammonia-methane at 2.5 bar. Pugh et al. [73] reported ammonia/air flame generating NO and NH_3 emissions below 75 ppm, and Rocha et al. [75] found NO and NH_3 emissions below

50 ppm and 4 ppm, respectively. However, the experiment of Okafor et al. [64], did not reach the optimal NO_x emission. The discrepancy was explained by the uneven wall temperature and concluded due to insufficient fuel mixing[64].

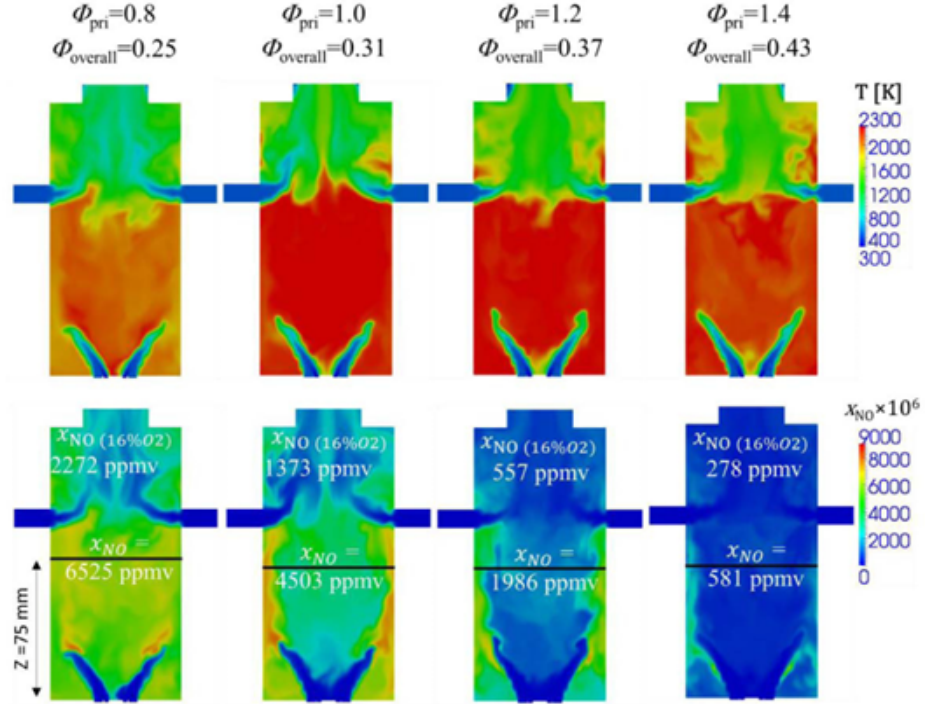


Figure 1.7: A molar fraction of NO with different equivalence ratios in two-stage ammonia-methane spray combustion [66].

1.5.2.4 MILD combustion

Moderate or Intense Low Oxygen Dilution (MILD) combustion also referred to as Flameless combustion, is a combustion strategy that recirculates the exhaust gas to dilute the oxidizer (Figure 1.8). In MILD, the reactants are highly preheated and diluted with exhaust gases such that the temperature rise during combustion is moderate, and oxidation occurs in a distributed regime without visible flame fronts [17]. This regime can significantly reduce NO_x emissions due to lower peak temperatures and more uniform heat release [17, 77].

Recent studies have investigated MILD combustion for ammonia-containing fuels, showing that NO_x emissions can be reduced, but the strong dilution and low oxygen levels further challenge ignition and stability [77, 25, 9]. The combination of MILD concepts with swirl burners and fuel blends (e.g. ammonia–hydrogen–methane) remains a promising but complex approach for future gas turbine applications [35, 8, 72].

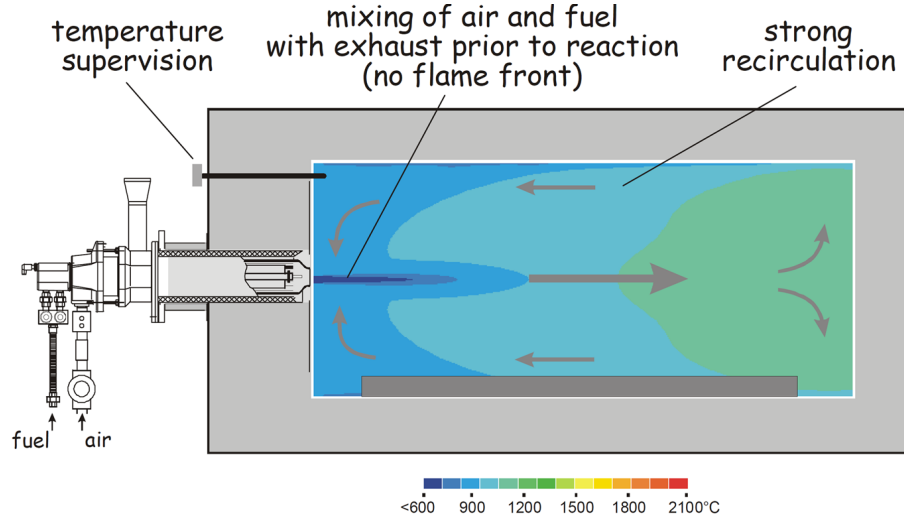


Figure 1.8: Schematic of MILD combustor concept [75].

1.5.2.5 Wet combustion, plasma and magnetic-field-assisted combustion

Wet combustion or humidified gas turbine cycles introduce water or steam into the combustor. The presence of steam can lower flame temperature, modify reaction pathways and thus reduce NO_x emissions, but may also influence stability and efficiency [35, 8]. For ammonia combustion, one-dimensional flame simulations and system studies have examined the effect of water addition on flame structure and emissions, showing potential for NO_x reduction but also risks of incomplete combustion and condensation issues [81, 35, 8, 9].

In addition, plasma-assisted combustion has been proposed to enhance ignition and stabilisation of low-reactivity fuels such as ammonia. Nanosecond pulsed plasma and other non-thermal plasma discharges can generate radicals and active species, thereby promoting chemical reactions at lower bulk temperatures [20, 88]. Experimental studies on plasma-assisted ammonia-air flames have demonstrated simultaneous improvements in stability and reductions in NO_x emissions [20, 88].

Magnetic fields have also been investigated as a means of influencing combustion dynamics and heat transfer. For certain conditions, magnetic fields can affect charged species and flow structures, which might be utilised to control ammonia combustion and emissions [27]. These advanced control strategies are still at an early stage but offer additional leverage for dealing with the challenges of ammonia combustion.

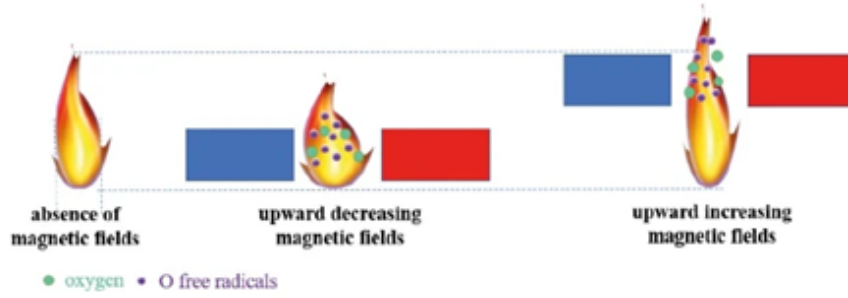


Figure 1.9: The influence of magnetic on flame macrostructure [27].

1.5.3 Chemical kinematic modelling

At low temperatures, ammonia–hydrocarbon chemistry consumes methane mainly through a catalytic cycle involving two reactions: $\text{CH}_3 + \text{NO}_2 = \text{CH}_3\text{O} + \text{NO}$ and $\text{NO} + \text{HO}_2 = \text{NO}_2 + \text{OH}$ [11]. Detailed ammonia kinetics at high temperatures and low pressures have been studied extensively [23], whereas mechanisms for industrial operating conditions still require further development [60]. Recent studies have refined NH_2 recombination reactions at high pressure [30, 83], H_2NO oxidation at low temperature [86], $\text{N}_2\text{O}/\text{NH}_3$ oxidation [46, 36], NH_3 –hydrocarbon interactions [11] and NH_3 –hydrogen chemistry [86, 109].

1.5.4 Turbulence models

In spray swirl combustion, the turbulence model affects the predicted recirculation zones and the interaction of droplets and vapour with the internal flow [43, 53]. Comparative studies show that model performance depends on the quantity and flow region considered. The realizable k – ε model has provided improved predictions of the outer shear layer in some swirl configurations, whereas the renormalisation-group (RNG) k – ε model can better represent strain-sensitive turbulence and scalar mixing in strongly curved flows [76]. These findings do not imply that either model is universally more accurate. Reynolds-averaged Navier–Stokes (RANS) closures remain limited in resolving the unsteady coherent structures of highly swirling flow compared with large-eddy simulation (LES). Reynolds-stress models can improve representation of turbulence anisotropy and internal recirculation, but at greater computational cost and with more demanding convergence behaviour [43].

1.5.5 Spray modelling

Following the definition and scope established in Section 1.2, the spray-modelling literature is considered here with emphasis on how pressure-driven phase change is represented numerically. Theoretical and numerical treatments relevant to flash-boiling spray vaporisation include the models developed by [114, 57, 1, 2, 102, 80]. The vaporization model of one moving droplet developed by Abramzon et al. [1], which includes transient physical property and requires an acceptable computing resources, was utilized for further modelling spray boiling [114]. The superheated boiling condition was researched by Adachi et al. [2] and introduced a correlation of heat transfer coefficient to calculate the intensive evaporation rate of spray flashing. They considered normal convection and diffusion driven vaporization was considered separately. Zuo et al. [114] improved the vaporization model with the flash boiling model to efficiently resolve the spray condition inside a gasoline diesel injection engine. They assumed a constant droplet superheated surface temperature which equalled saturation temperature at local pressure and believed that all energy transferred from the surrounding boils the droplet without heating it. The vapour layer on the droplet surface was considered to suppress heat transfer which decelerates the mass transfer rates from the liquid phase to the gas phase[114]. Xu et al. discovered the correlation between the droplet's saturation pressure to ambient pressure ratio and the diameter of droplets [102]. They distinguished the spray features and divided the pressure ratio interval into three regions namely the initial flashing region, transitional-flashing region, and flare-flashing region. Shen et al. observed the relationship between pressure drop and vortex numerically. They pointed out that due to the high vaporization rate, the fuel gas was distributed unevenly inside a gasoline direct injection engine chamber [80]. Investigation reports on spray properties of ammonia were recently upsurging. Spray experiments of ammonia were carried out by [69, 50, 70]. Okafor et al.[69] discussed that the continuously escalating latent heat of evaporation may disturb the flame stability. The researchers suggested that more evaporation time would help stabilize the fuel rich flame and balance the latent heat of the ammonia vaporization. Pelé et al. [70] compared injection flash boiling sprays of ammonia, gasoline, and ethanol concerning their geometric dimensions and relationships with ambient physical properties. From Fig. 1.10, the ammonia spray showed a narrower and longer shape that differed from the other fuels.

Li et al.[50] investigated the microscope and macroscope structure of ammonia spray under different fuel-chamber conditions. They found the ratio of saturated pressure to ambient pressure as well as the viscosity of fuel strongly connected to

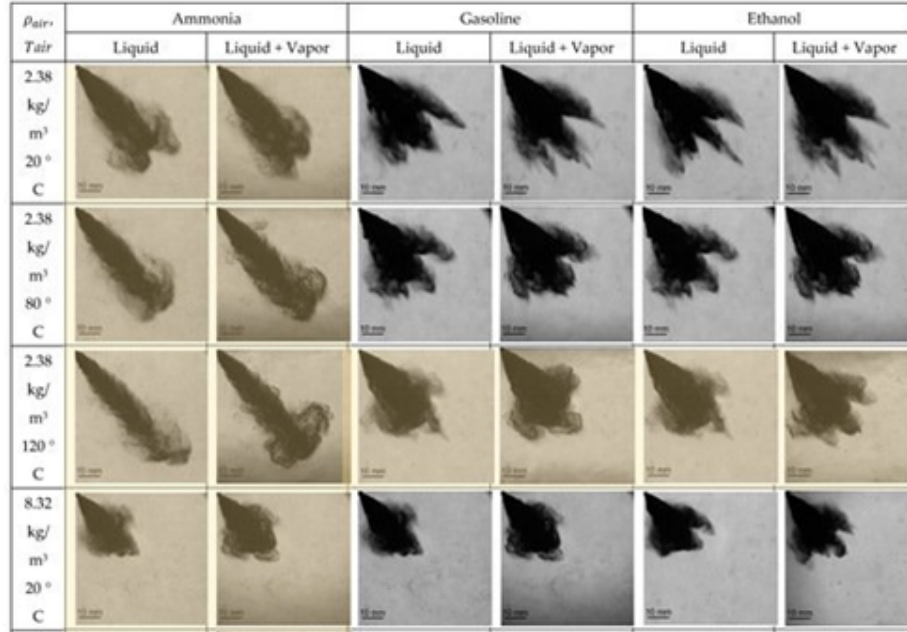


Figure 1.10: Injection morphological characteristics of ammonia gasoline and ethanol under different ambient pressure and temperature. (Flash boiling occurred in yellow figures) [70].

the flashing spray behaviour (Fig. 1.11). Three intervals are divided on the pressure ratio to discriminate the stages of superheated boiling. In the first interval (initial flashing region) the superheated degree and fuel viscosity were controlling the spray behaviour, while in the other two intervals (transitional/flare-flashing region), the ratio of internal viscosity dissipation to the surface tension energy was governing instead [50]. They explained that the spray angle expansion was caused by vortex and pressure reduction.

1.5.6 Summary of literature

The clean combustion of ammonia mixture is a challenging and attractive topic. The selection of second fuel requires different combustion strategies, and it is still under investigation which fuel and strategies are best comprehensively. Methane demonstrates promising performance in promoting low ammonia emission and stable combustion. Zhang et al. [108] studied the co-fired stability limit and the fire image with different global equivalence ratios. They reported the low flame speed, which caused the flame to shape thinner at a high energy fraction of ammonia (Fig 2.4). To enhance this, swirl combustion was chosen for enhancing radical reaction, and optimization can be made to minimize following high NO_x emissions such as the

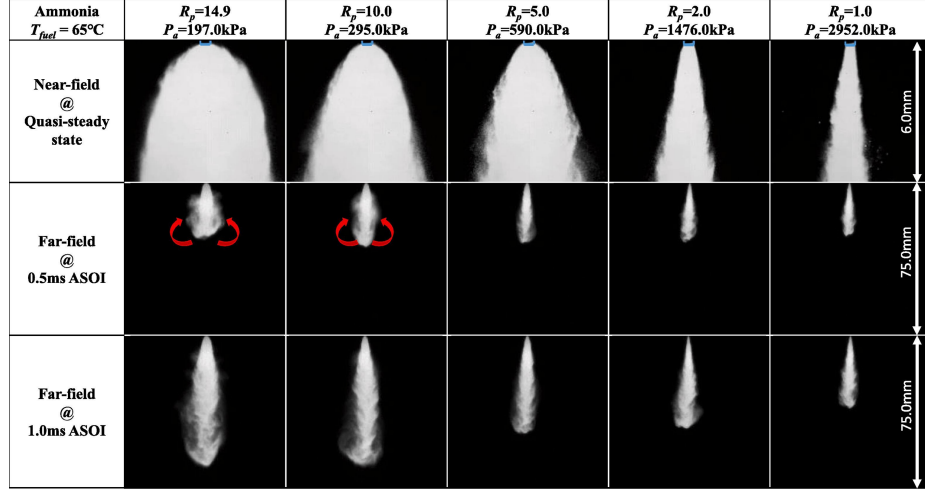


Figure 1.11: Ammonia flash-boiling sprays at different saturation-to-ambient pressure ratios, R_p , and ambient pressures, P_{amb} [3].

Rich–Quench–Lean (RQL) combustion strategy.

In general, Okafor et al. [69] concluded that the liquid ammonia fuel lean combusting with methane can be improved by the high enthalpy oxidizer balancing the latent heat of ammonia evaporation, thus decreasing the discharged N_2O and NH_3 . However, this method encouraged the NO production, so the optimal equivalence ratio lies on the fuel rich side. For the fuel rich side, N_2O was consumed, but HCN and NH_3 were generated intensively due to insufficient residence time and oxidation temperature. Further improvement of emissions was discussed to be the enhancement of higher preheated air temperature and more mixing methane[69].

The heat diffusion from the chamber wall during ammonia combustion was found to be critical to flame stabilization and emission of N_2O and NH_3 [68]. Okafor et al. [64] revealed that, in the first stage of two-stage spray NH_3/CH_4 combustion, inhomogeneous distribution of fuel gas would promote the NO emission at the local area under lean-fuel conditions due to the spray evaporation. The experiment results of inhomogeneous wall temperature distribution from [64] indicate an unstable flow field inside the chamber. Even at the optimal primary equivalence ratio, the large cooling effect of flash boiling and chamber heat diffusion will cause a low reaction rate, leading to inefficient burning and ammonia emissions [64]. Therefore, additional research is necessary to promote the spray distribution and combustion reaction in the first stage by optimizing the internal flow field and fuel spray strategies[9].

The superheated spray is suitable for distributing liquid fuels inside the combustion chamber. However, the long penetration length of ammonia indicates the

developments are still necessary. Different spray nozzles can be tested for better atomization. Other spray characteristics of ammonia are still under discovery including supercritical spray, electro-spray, and ultrasonic atomizing. Kim et al. [44] emphasize that liquid specific heat is critical to ignition delay and latent heat. Consequently, the supercritical spray might be a potential solution. Ammonia would become almost no surface tension and latent heat under supercritical conditions. Furthermore, thermal conductivity and mass diffusivity would be promoted[103].

1.6 Flash-boiling ammonia sprays

The combustor-scale review above shows that ammonia flame stability and emissions depend strongly on atomisation, evaporation and fuel–air mixing. Under the flashing conditions defined in Section 1.2, pressure-driven phase change modifies droplet size, spray angle, penetration and local temperature, thereby establishing the mixture supplied to the reacting flow [93, 50, 70].

The second modelling level in this thesis therefore isolates the external spray and examines whether an Eulerian–Lagrangian framework can reproduce the macroscopic and microscopic behaviour of superheated ammonia. The review first establishes the governing flash-boiling phenomenology and experimental trends, and then evaluates the evaporation, breakup and boundary-condition treatments available for Lagrangian spray simulations.

1.6.1 Evaporation models not used in the present simulations

Several evaporation closures were considered as background when developing the numerical framework but were not used for the ammonia spray cases reported in Case Study II.

The conventional boiling-rate model available in ANSYS Fluent is activated when a droplet reaches its boiling temperature. The corresponding rate of diameter change is

$$\frac{dd_p}{dt} = -\frac{2k_\infty}{\rho_p c_{p\infty} d_p} \left(2 + 0.6\text{Re}^{1/2}\text{Pr}^{1/3}\right) \ln \left[1 + \frac{c_{p\infty}(T_\infty - T_p)}{h_{fg}}\right]. \quad (1.3)$$

This conventional boiling law was not activated in the present simulations.

The classical Frossling model, also described as an extension of the D^2 law, assumes thermodynamic equilibrium at the gas–liquid interface and represents diffusion- and convection-controlled surface evaporation [7]. Its mass evaporation rate is

$$\dot{m}_d = \pi d_d \rho_g D_{i,m} Sh \ln(1 + B_M). \quad (1.4)$$

Although computationally efficient, it neglects the outward vapour flow that modifies the boundary layer at high evaporation rates. The classical Frossling model was not used in the reported ammonia spray cases.

The Abramzon–Sirignano model extends the classical treatment by accounting for the Stefan-flow, or blowing, effect [1]. Correction factors F_T and F_M modify the Nusselt and Sherwood numbers; for example,

$$Sh^* = 2 + \frac{Sh_0 - 2}{F_M}. \quad (1.5)$$

The standalone Abramzon–Sirignano evaporation model was not used in the reported simulations.

The Langmuir–Knudsen model treats the gas–liquid interface as a non-equilibrium Knudsen layer and evaluates a molecular-kinetic mass flux using the Hertz–Knudsen–Schrage relation:

$$\dot{m}_d = \pi d_d^2 \alpha \frac{1}{\sqrt{2\pi R_{gas}}} \left(\frac{P_{sat}(T_d)}{\sqrt{T_d}} - \frac{P_\infty}{\sqrt{T_\infty}} \right), \quad (1.6)$$

where α is the accommodation coefficient. This model was also not activated in the present simulations. The evaporation closure actually used is specified once in the Methodology.

1.7 Lagrangian modelling of flashing ammonia sprays

1.7.1 Fundamentals of Flash-Boiling Sprays

Building on the terminology established in Section 1.2, this subsection focuses on the observable spray consequences of flashing. Nucleation and bubble growth can produce rapid fragmentation, radial expansion and cooling of both the dispersed phase and the surrounding gas. Although the present thesis concerns ammonia, studies of other volatile fluids provide useful evidence for these generic features.

Zhou et al. [113] investigated R404A flashing sprays using OpenFOAM and reported agreement with experimental spray morphology and droplet diameter distributions. The R404A spray showed a rapid radial expansion and a large cone angle near the nozzle exit due to explosive flashing atomization, followed by a more contractive spray profile further downstream. The droplet diameter decreased sharply close to the nozzle and then approached a nearly constant value of around $9 \mu\text{m}$. The droplet velocity first accelerated after injection and then gradually decreased because

of aerodynamic drag. The droplet temperature also experienced a very fast reduction near the nozzle and later continued to decrease at a lower rate until reaching a minimum. A relatively warm core with higher droplet temperatures remained inside the spray.

Zhou et al.[113] also demonstrated how ambient pressure controls the intensity of flashing. Lower ambient pressure led to more explosive atomization, higher droplet velocities, and shorter penetration distances than at higher pressures, whereas the mean droplet diameter was only weakly affected. These results established a clear physical picture: flash boiling is strongest in the near-nozzle region where superheat is large, and it weakens downstream as vaporisation and strong cooling reduce the temperature. This generic behaviour provides a useful baseline for understanding flashing sprays of liquid ammonia, which share key features such as rapid radial expansion, strong cooling, and pronounced sensitivity to ambient pressure.

1.7.2 Experimental Characterisation of Liquid Ammonia Sprays

Ammonia contains no carbon, but it has a low normal boiling point and a high latent heat of vaporisation. These properties mean that liquid ammonia can become superheated when injected into a sufficiently low pressure environment. Experimental characterisation of ammonia sprays is therefore needed to quantify spray morphology and droplet statistics and to provide validation data for numerical models.

1.7.2.1 Macroscopic morphology and environmental effects

Liu et al. [55] examined the influence of preheated swirling air on liquid-ammonia sprays in a swirl combustor. Their work was motivated by gas-turbine applications, in which swirl and air preheating are widely used to enhance vaporisation and stabilise flames. Using an optically accessible combustor, they analysed spray morphology in terms of penetration, cone angle and visible liquid volume. Increasing the air-preheat temperature significantly changed the macroscopic spray shape. Higher air temperatures accelerated droplet heating and evaporation, reducing the visible liquid volume and, under some conditions, shortening the axial penetration. The spray also became more dispersed because stronger two-phase interactions promoted secondary breakup. Preheated swirling air improved local fuel–air mixing and reduced ignition difficulty by helping the spray reach flammable vapour concentrations more quickly near the injector. However, these benefits depended on the balance among air temperature, swirl intensity and ambient pressure, which determined whether the droplets reached flash-boiling conditions [55].

Yang et al. [104] investigated the high-pressure direct injection of ammonia through combined experimental and numerical studies of superheated and subcooled sprays in a constant-volume vessel. Using diffuse back-illumination (DBI) imaging at injection pressures of up to 70 MPa, they observed distinct differences between the two thermodynamic states. Flash boiling substantially inhibited the initial penetration of the superheated spray, resulting in a lower initial tip velocity than in the subcooled case. The subcooled spray decelerated rapidly before reaching a more stable penetration regime, whereas the tip velocity of the superheated spray first increased and then decreased. The superheated sprays also exhibited pronounced radial expansion and dilute peripheral regions driven by vapour expansion and intense phase change. Complementary LES indicated that the combination of a Frossling evaporation model and an explicit flash-boiling submodel provided the best agreement with the measured penetration and spray shape. The simulations revealed a severe temperature reduction in the spray core under superheated conditions, reflecting the high latent heat of ammonia. Yang et al. also reported a counter-intuitive trend: the final Sauter mean diameter could be larger for superheated sprays than for subcooled sprays because the smallest droplets vaporised rapidly and disappeared from the measured liquid population.

Together, these studies show that the macroscopic morphology of liquid ammonia sprays is highly sensitive to ambient and operating conditions. Preheated swirling air, injection pressure, and the degree of superheat control penetration, cone angle, and visible liquid volume. The combined evidence suggests that flash boiling tends to reduce axial penetration, increase radial expansion, and induce strong local cooling, while also producing non-trivial trends in observed droplet size.

1.7.2.2 Microscopic characteristics

While macroscopic images reveal the global shape of ammonia sprays, combustor design and model development also require detailed information on droplet statistics. Liu et al.[56] addressed this by performing a microscopic characterisation of liquid ammonia sprays under a range of flash-boiling intensities in a controlled chamber. They used advanced diagnostics to measure droplet-size distributions, Sauter mean diameters and droplet number densities as functions of space and time. Different regimes, including non-flashing, transitional flashing and flare flashing, were classified using reduced pressure or degree of superheat.

Their results showed that reduced pressure had a strong impact on microscopic spray properties. Liu et al. used the reduced-pressure convention $P_r = P_{\text{amb}}/P_{\text{sat}} =$

R_p^{-1} , rather than the superheat ratio defined in Eq. (1.1). Under intense flash-boiling conditions, for example, at $P_r \leq 0.3$, the spray produced much higher droplet number densities and significantly smaller Sauter mean diameters (SMDs), on the order of $15 \mu\text{m}$. In contrast, non-flashing cases exhibited larger SMDs and lower number densities. The size distributions also became multimodal in flash-boiling regimes, indicating the coexistence of very small child droplets generated by bubble-driven fragmentation and coarser primary droplets. This multimodality has important implications for evaporation time scales and local equivalence ratios, since very small droplets vaporise quickly, while larger droplets persist longer.

Liu et al. [56] reported that fragmentation was strongest near the injector and in the early stages of spray development. Downstream, small fragments evaporated rapidly, which altered both the local droplet field and the surrounding gas composition over short distances. These microscopic observations confirm that ammonia flash boiling sprays cannot be described by a simple shift in average droplet size. Instead, they involve complex spatial and temporal evolution of droplet populations that must be captured in models aiming to predict ignition, flame propagation, and pollutant formation.

1.7.3 Challenges in Numerical Modelling of Ammonia Sprays

Most spray models implemented in engine CFD codes were originally developed and calibrated for hydrocarbon fuels. They rely on aerodynamic breakup mechanisms and classical evaporation correlations such as the Frossling model. The experimental findings for ammonia, however, indicate that flash boiling, strong internal bubble growth, and intense cooling play a dominant role, especially near the nozzle. This raises the question of whether conventional Lagrangian spray models can reproduce ammonia spray behaviour across flashing and non-flashing regimes.

Zhang et al.[110] addressed this issue in a numerical study of liquid ammonia direct injection under engine relevant conditions. They showed that current Lagrangian spray models can reproduce ammonia spray characteristics reasonably well under non-flashing conditions. However, under strong flash boiling, the numerical predictions deviated significantly from measurements. Their simulations identified a region of strong flash boiling near the nozzle, with its intensity decreasing downstream as the spray cooled the surrounding gas. Zhang et al.[110] introduced an initial superheat degree, defined as the ratio of ambient pressure to saturation vapour pressure at the initial fuel temperature, to delineate the boundaries between different vaporisation regimes. They concluded that flash boiling models, which account only for enhanced

evaporation, are not sufficient. To reproduce ammonia fuel/air mixing accurately, a more realistic flash boiling model must include thermal breakup mechanisms in addition to evaporation promotion.

An et al.[4] conducted a complementary numerical investigation using LES coupled with an Eulerian-Lagrangian spray representation. They compared several phase change sub-models, and assessed their performance for liquid ammonia flash sprays. Models and parameters calibrated for hydrocarbon fuels systematically mispredicted ammonia behaviour: they tended to overestimate the persistence of the liquid phase and underestimate the intensity of flashing driven fragmentation. Extensions that incorporated non-equilibrium phase change and accounted for rapid breakup improved qualitative agreement with observed spray morphology when ammonia specific relaxation time scales were used, but quantitative agreement still required further tuning and validation.

An et al.[4] also highlighted the strong sensitivity of spray structure to injection superheat and ambient pressure. Small changes in these parameters were sufficient to shift the spray from a dense liquid core structure to a highly fragmented plume characteristic of flash boiling. At the same time, the validation of models was constrained by the limited availability of detailed experimental data for ammonia, especially near the nozzle, where multi bubble interactions and heterogeneous nucleation on injector walls are difficult to resolve. These findings indicate that reusing hydrocarbon based models is inadequate and that ammonia specific breakup and phase change descriptions are needed.

1.7.4 Advances in Breakup and Phase Change Modelling

In response to the limitations identified above, recent research has developed new breakup and evaporation models that explicitly target flash boiling conditions. Two complementary lines of work can be distinguished. One line focuses on representing thermal breakup driven by bubble growth inside droplets. The other emphasises non-equilibrium evaporation and the construction of unified modelling frameworks that remain valid from highly flashing to purely evaporative conditions.

1.7.4.1 Thermal breakup and bubble-growth models

A general Lagrangian Particle Tracking (LPT) study on flash boiling sprays proposed a dedicated 'droplet shattering' model to represent breakup driven by internal nucleation and rapid bubble growth, as opposed to classical aerodynamic instabilities [71].

Within an Eulerian-Lagrangian framework with two-way coupling, the authors implemented standard turbulence, breakup, and collision models, and then introduced a specific flash boiling sub-model that generates child parcels with additional radial velocity components when thermal breakup occurs. This modification was essential to capture the explosive nature of flash boiling. The model successfully reproduced plume curving, inter plume interaction, and the characteristic spray collapse observed in multi hole injector experiments with superheated *n*-pentane and gasoline. The agreement with measured penetration and downstream SMDs showed that the thermal breakup mechanism largely controlled the final droplet size distribution, making the downstream SMD almost independent of the initial droplet size. At the same time, the study pointed out several limitations, such as the lack of direct measurements of droplet radial velocities in dense near nozzle regions and the absence of explicit modelling of under-expanded jet behaviour and shock waves, which may be important in extreme flashing cases.

Building on similar physical ideas but focusing on ammonia, Song et al.[85] developed a flash boiling breakup model in which droplet fragmentation is driven by the thermal growth of multiple bubbles. Their approach is formulated within an Euler-Lagrange framework and is grounded in the Rayleigh-Plesset equation and classical nucleation theory. The model was validated against experimental data for single hole liquid ammonia sprays and demonstrated a strong capability to capture transcritical spray features. Song et al.[85] showed that a decrease in the ambient pressure gradient increases the bubble nucleation rate inside droplets, which in turn promotes frequent breakup events. This mechanism leads to reduced spray tip penetration, larger spray cone angles, and smaller Sauter Mean Diameters. Their results support the view that, under ammonia flash boiling conditions, bubble induced thermal breakup rather than aerodynamic shear is the dominant atomization mechanism.

1.7.4.2 Evaporation and non-equilibrium effects

Accurate modelling of evaporation is particularly important for ammonia because of its high saturation vapour pressure and latent heat. Under flash boiling conditions, the classical Frossling correlation can become numerically unstable when the ambient pressure approaches the saturation pressure, since the driving force for mass transfer becomes infinite. To overcome this problem, Song et al.[85] modified the Frossling model by incorporating the Langmuir-Knudsen (L-K) law. The L-K correction introduces a non-equilibrium term that represents the Knudsen layer at the droplet surface. By doing so, it regularises the mass flux in the limit where $P_g \approx P_{\text{sat}}$ and prevents

the divergence of the evaporation rate. This modification is crucial for maintaining numerical stability during the violent phase transition that accompanies superheated ammonia injection.

Huang et al.[39] examined high pressure ammonia sprays using LES with a specialised flash boiling model and provided further insight into the interaction between evaporation, flow structures, and temperature fields. Their simulations confirmed that ambient pressure strongly influences the fuel superheat and, consequently, the spray morphology. Under flash boiling conditions, they observed an explosive radial expansion and a high initial droplet velocity, followed by rapid velocity decay due to intense phase change and drag. The evaporation source terms were much larger than under non-flashing conditions and induced pronounced local cooling. In non-flashing regimes, in contrast, spray penetration was primarily governed by injection pressure, and radial expansion was more modest.

A distinctive feature of Huang et al. [49] work is the use of Voronoi analysis to study the microscopic spray structure. They showed that regions with strong droplet clustering, indicated by small Voronoi cell areas, coincided with zones of lower gas temperature. This preferential concentration suggests that the spatial organisation of droplets is tightly coupled to evaporation and heat transfer, since clusters of droplets draw heat from the gas more efficiently. Together with the findings of Song et al.[85], these results emphasise that evaporation in ammonia sprays is a highly non-equilibrium process that depends not only on local thermodynamic conditions but also on droplet scale structure and clustering. Models that ignore these couplings are unlikely to predict the correct temperature and vapour fields under flash boiling conditions.

1.7.4.3 Unified modelling approaches

While physics based thermal breakup models provide detailed insight into flash boiling mechanisms, they can be complex to calibrate across a wide range of operating conditions. An alternative strategy is to retain standard frameworks such as the Kelvin-Helmholtz-Rayleigh-Taylor (KHRT) breakup model and to embed flash boiling effects into correlations for model parameters. Zembi et al.[105] followed this route in a Lagrangian CFD study of ammonia sprays. They kept the KHRT structure but introduced a correlation that links the Rayleigh-Taylor breakup parameters and the spray cone angle to the pressure ratio R_p . By calibrating these correlations, they were able to reproduce spray morphology across both highly flashing and purely evaporative conditions using a single model setup. Their simulations also quantified

the strong cooling associated with ammonia’s high latent heat, showing that local gas and droplet temperatures can fall well below the nominal ambient level. This cooling has direct implications for mixture formation and subsequent combustion.

Generally, Song et al.[85] and Zembi et al.[105] illustrate two complementary modelling philosophies. The first emphasises detailed bubble growth physics and explicit thermal breakup, while the second relies on empirical correlations that embed the effects of pressure ratio and superheat into existing breakup models. Both approaches, however, agree that flash boiling cannot be treated as a small correction to hydrocarbon based spray models. Instead, model parameters or underlying mechanisms must explicitly reflect the thermodynamic state of the injected ammonia to achieve predictive accuracy.

1.7.5 Boundary Conditions and Injector Dynamics

In addition to breakup and evaporation sub-models, the specification of boundary conditions and injector geometry plays a crucial role in simulations of flash boiling ammonia sprays. Standard Lagrangian Particle Tracking often simplifies the internal injector flow by excluding detailed nozzle and counterbore geometries and by treating nozzle walls as adiabatic boundaries. Under flare flashing conditions, such simplifications can lead to large discrepancies between predicted and observed spray structures.

Bundred and Leach [15] investigated this issue in the context of Eulerian Lagrangian simulations of ammonia sprays. They showed that conventional boundary treatments fail to reproduce the macroscopic morphology of sprays in intense flash boiling regimes, particularly at low back pressures with reduced pressure around $R_p \approx 0.10$. In these cases, experiments reveal collapsed, bulb like spray shapes with strong radial expansion, whereas standard simulations predict narrow plumes with insufficient radial growth.

To address this discrepancy without resorting to computationally expensive VoF simulations of the internal two phase flow, Bundred and Leach proposed a novel boundary condition strategy. They included the nozzle and counterbore in the computational domain and set the nozzle wall boundaries to an inflow condition at the saturation pressure of ammonia. This treatment allowed vapour generated inside the injector to ‘leak’ into the external flow, thereby mimicking the volumetric expansion that occurs as the superheated liquid flashes at the nozzle exit. The resulting pressure based boundary condition induced additional radial velocity components

and produced wide cone angles and bulb shaped sprays that matched experimental observations under flare flashing conditions.

Their findings suggest that, for superheated ammonia, capturing the pressure interactions at the nozzle exit is as important as choosing an appropriate breakup model. A physically informed boundary condition can represent some of the key effects of internal two phase flow at a fraction of the cost of fully resolved multiphase simulations, and it should therefore be considered in any modelling framework that targets engine relevant conditions.

1.7.6 Literature Summary

The literature reviewed in this chapter summarises flash boiling ammonia sprays from physical fundamentals to advanced numerical models. General studies on volatile working fluids, such as Zhou et al.’s work on R404A, have clarified the basic features of flash boiling: rapid radial expansion near the nozzle, strong cooling, and a downstream transition from highly flashing to more conventional spray behaviour. Experimental investigations of ammonia, including those of Liu et al. (2023, 2025) and Yang et al. (2025), have shown that these phenomena are even more pronounced for liquid ammonia because of its low boiling point and high latent heat. At the macroscopic level, preheated swirling air, injection pressure, and the degree of superheat control penetration, cone angle, and visible liquid volume. At the microscopic level, intense flash boiling produces very small droplets, high number densities, and multimodal size distributions, with fragmentation concentrated near the injector and rapid evaporation of small fragments downstream.

On the modelling side, Zhang et al. (2023) and An et al. (2023) have demonstrated that spray models calibrated for hydrocarbons cannot be directly applied to ammonia. Under non-flashing conditions, conventional Lagrangian spray models may still perform acceptably, but under strong flash boiling they exhibit large errors, often overestimating liquid persistence and underestimating fragmentation. This has motivated the development of thermal breakup models that explicitly represent bubble growth inside droplets, such as the shattering model for multi hole injectors and the multi-bubble breakup model of Song et al. (2025). At the same time, the need to handle non-equilibrium evaporation and numerical stability near saturation conditions has led to modified evaporation laws, including Frossling correlations corrected by the Langmuir-Knudsen formulation. LES studies such as Huang et al. (2023) further emphasise that evaporation source terms, local cooling, and droplet clustering are tightly coupled and must be treated consistently in simulations.

Unified models, exemplified by the KHRT approach with pressure ratio dependent parameters proposed by Zembi et al. (2024), show that it is possible to recover both flash boiling and non-flashing behaviour within a single Lagrangian framework, provided that model parameters explicitly reflect the thermodynamic state. At the same time, work by Bundred and Leach (2025) makes clear that accurate prediction of ammonia sprays also depends on the treatment of injector boundary conditions and internal two phase flow effects. Their saturation pressure based nozzle boundary condition offers a practical way to capture key nozzle exit phenomena without full multiphase resolution.

Despite these advances, several important gaps remain. Most experimental datasets for ammonia originate from constant volume vessels or simplified single hole injectors, whereas actual gas turbine combustors employ complex geometries with strong swirl, recirculation, and highly non-uniform ambient conditions. Existing advanced models for thermal breakup, non-equilibrium evaporation, and pressure sensitive breakup parameters have rarely been integrated and systematically tested in such swirl combustor environments. Furthermore, while microscopic measurements and Voronoi analyses provide rich information on droplet clustering and local cooling, these features have not yet been fully linked to combustor level performance metrics such as ignition delay, flame stabilisation, and emissions.

The present work addresses the need for consistent validation of flashing evaporation treatments and injector boundary conditions by applying an Eulerian–Lagrangian framework to ammonia injection in a constant-volume vessel. This study will employ a flashing evaporation law treatment implemented via user-defined functions. The boundary conditions at the injector will be designed to reflect the pressure and phase change behaviour at the nozzle exit, following the strategy suggested by a recent study on flare flashing [15]. By combining these elements and validating them against available macroscopic and microscopic data, the thesis seeks to provide a more consistent description of liquid ammonia flash sprays under combustor relevant conditions and to clarify model sensitivity to boundary conditions and evaporation law implementation.

1.8 Near-nozzle cavitation and compressibility

1.8.1 Transition from dispersed droplets to resolved near-nozzle flow

The Lagrangian literature reviewed above demonstrates that finite-rate evaporation and droplet cooling are essential for predicting the external ammonia spray. However,

such models prescribe the droplet velocity, size distribution and cone angle at the injector exit and therefore cannot determine how these quantities arise. Under strong flashing conditions, the internal nozzle flow may contain cavitation, metastable liquid and vapour structures whose expansion contributes directly to radial momentum and external spray morphology [97, 21, 24].

The third modelling level in this thesis consequently resolves the liquid and vapour phases within the nozzle and near field. This requires a compressible Eulerian formulation capable of representing internal cavitation, delayed phase change and the low mixture sound speed associated with two-phase flow. Experimental measurements remain indispensable for validation, but the dense and optically inaccessible near-nozzle region makes numerical analysis necessary for examining pressure, phase fraction, Mach number and shock structures [21, 50].

1.8.2 Flash-boiling regimes of liquid ammonia

The thermodynamic definition and pressure-ratio convention used in this thesis are given in Section 1.2. The present subsection focuses instead on ammonia-specific regime transitions. As R_p increases, experimental studies distinguish non-flashing, transitional and flare-flashing behaviour through changes in spray cone angle, penetration, liquid-core persistence and droplet-size distribution [55, 70, 97, 21].

For ammonia, flash-boiling is particularly important because it can significantly enhance atomisation and mixing. Liu et al. [55] investigated single-hole ammonia sprays and identified a critical superheat threshold in terms of a superheat index $SI > 1.5$, beyond which spray collapse occurs. In their flare regime, ammonia exhibits rapid atomisation due to explosive bubble growth, producing fine droplets with Sauter mean diameters below $20\ \mu\text{m}$. In the transition regime, intermittent flash-boiling leads to bimodal droplet size distributions, which illustrates the sensitivity of ammonia to thermodynamic instabilities. Pelé et al. [70] studied ammonia sprays using GDI injectors and reported a “delayed flash-boiling” behaviour, in which a liquid core persists for a relatively long time even when the superheat index is above unity. They attributed this to ammonia’s low boiling point and high critical temperature, which create a wider metastable liquid region compared with typical hydrocarbons. These studies indicate that flash-boiling can both improve atomisation and introduce complex transient structures, depending on how the injection conditions are chosen.

The rapid phase change in a metastable liquid can also give rise to discontinuities in the flow field that manifest as evaporation waves and shock waves. During vigorous flashing, local pressure and density can change abruptly, and this behaviour is often

interpreted as a shock wave in the two-phase mixture [48]. Based on evaporation wave theory, flashing sprays can trigger compressible phenomena such as choked flow and shock-cell structures when the depressurisation is sufficiently rapid [95]. The compressibility of a flashing two-phase mixture differs from that of a single-phase fluid and is often modelled using Wood’s equation for effective sound speed [99]. In such mixtures, the speed of sound can be much lower than in either pure liquid or pure vapour, which makes the flow more prone to choking and shock formation. Choked behaviour and shock waves have been observed in a range of flashing jet studies [95, 12, 47, 34, 101]. Chen et al. [18] emphasised the need to understand the coupling between rapid phase change and shock wave interactions in flashing sprays. However, the choking behaviour at the boundary of flare-flashing regimes, especially for conditions around $R_p \approx 10$, has not been fully resolved because of the very large density gradients and strong compressibility in the near-field region.

For flashing ammonia sprays, these issues are further complicated by the presence of cavitation and by the strong influence of injector geometry. Fang et al. [24] reported a resistance phenomenon under high superheat in a diesel injector at 100 MPa, which they linked to cavitation behaviour at high superheat. Wang et al. [97] found that cavitation in slit nozzles can enhance flash-boiling efficiency by up to 40%, but excessive cavitation at high superheat indices leads to hydraulic flip and spray collapse. Colson et al. [21] observed that nozzle geometry and injection temperature jointly determine whether stable flash-boiling occurs or whether vapor lock and mass-flow reduction take place. In many experiments, researchers have reported characteristic spray shapes such as a “bell” morphology in the near-field and a “feather” structure during the early phase of injection. The physical mechanisms that connect flash-boiling, cavitation, compressibility and these complex morphologies are not yet fully clarified. This gap motivates a more detailed theoretical and numerical investigation of ammonia sprays in regimes where cavitation, flash-boiling and shock formation may all interact.

1.8.3 Theoretical background and physical mechanisms

1.8.3.1 Thermodynamic properties and superheat metrics

The thermodynamic properties of ammonia differ significantly from those of typical hydrocarbon fuels such as gasoline or diesel. Ammonia has a low normal boiling point of about -33°C , a relatively high saturation vapour pressure at ambient temperatures and a high latent heat of vaporisation [70, 94, 10]. These properties imply that liquid

ammonia can easily become superheated when stored or transported under pressure and then expanded into a lower-pressure environment. At the same time, the high latent heat means that evaporation and flash-boiling can cause strong local cooling, which in turn feeds back on the thermodynamic state of the jet and the surrounding gas [55, 24].

The pressure ratio R_p defined in Section 1.2 is the principal superheat measure used in this thesis. Values near unity correspond to weak thermodynamic driving, whereas larger values indicate progressively stronger potential for flashing. Other studies employ related indices to account for different thermodynamic reference states or experimental classifications [59, 55, 70, 97, 21].

Liu et al. [55] expressed the degree of superheat using a superheat index SI and showed that ammonia sprays exhibit a critical threshold at $SI > 1.5$, beyond which spray collapse and strong morphology changes occur. In this regime, the spray angle reduces and droplet coalescence increases, even though the underlying atomisation remains vigorous. Pelé et al. [70] observed that ammonia can remain in a metastable liquid state over a relatively wide range of conditions and documented a delayed flash-boiling behaviour at moderate superheat levels. Colson et al. [21] introduced a Flash-Boiling Number FBN based on injection temperature and identified a threshold $FBN > 0.7$ for stable flash-boiling in their modular nozzle experiments. Fang et al. [24] studied the effect of ambient pressure on ammonia spray penetration and width at high injection pressure and found non-monotonic trends that they linked to the behaviour of cavitation bubbles. These works collectively indicate that the thermodynamic path of ammonia during injection, as described by parameters such as R_p , SI and FBN , strongly controls whether the spray behaves as a non-flashing jet, a transitional flash-boiling jet or a fully developed flare-flashing spray.

1.8.3.2 Internal nozzle flow

Inside the injector, the liquid experiences strong acceleration and pressure drops as it passes through the orifices. When the local pressure falls below the saturation pressure corresponding to the liquid temperature, cavitation can occur. Cavitation bubbles can form at sharp corners, in separated flow regions or within shear layers, and they often serve as nucleation sites for subsequent phase change. In ammonia injectors, cavitation is further promoted by the low viscosity and high saturation vapour pressure of the fuel.

The geometry of the nozzle has a major influence on cavitation behaviour. Parameters such as the orifice length-to-diameter ratio (L/D), the presence of inlet

rounding or contraction, and the overall aspect ratio of the passage control where and how cavitation develops. Wang et al. [97] investigated ammonia flow through two-dimensional slit nozzles and showed that high aspect ratio nozzles can generate elongated cavitation clouds that destabilise the liquid jet and trigger earlier phase transition. They reported that cavitation can enhance flash-boiling efficiency by up to 40%, as measured by the vapour mass fraction at the spray periphery, and that suitably chosen aspect ratios can reduce droplet Sauter mean diameter by about 25% compared with low-aspect-ratio designs. At the same time, they found that excessive cavitation at high superheat indices can induce hydraulic flip, leading to spray collapse and inhomogeneous mixture formation. Colson et al. [21] examined convergent, divergent and straight nozzle geometries and showed that divergent designs can suppress flash-boiling under subcooled conditions but enhance it at superheated states, while straight nozzles are prone to vapour lock at high temperatures.

Fang et al. [24] observed that flashing liquid ammonia in a diesel injector at 100 MPa exhibits a resistance phenomenon at high superheat. They attributed this behaviour to cavitation bubbles forming in the nozzle under extreme superheat conditions. Their work also showed that spray penetration and width do not vary monotonically with ambient pressure when the injection pressure is very high, which suggests that cavitation and compressibility effects are strongly coupled. Li et al. [50] examined near-field and far-field ammonia flashing spray characteristics and reported that nozzle geometry affects the development of both regions, although the underlying internal flow details are difficult to measure directly.

From a modelling point of view, the homogeneous relaxation model (HRM) proposed by Downar-Zapolski et al. [22] provides a useful framework to describe non-equilibrium phase change in such flows. The HRM introduces a phase change rate that is proportional to $(P_{\text{sat}} - P)/\tau_{\text{relax}}$, where τ_{relax} is a relaxation time that depends on local flow conditions. Downar-Zapolski et al. derived analytical solutions for critical mass flow and choked flow conditions in one-dimensional flashing flows and linked the completeness of flashing to geometric factors such as L/D ratio. Later studies adapted this framework for ammonia and extended it to higher-dimensional configurations [29, 28, 58, 97]. These models indicate that cavitation and phase change within the nozzle are governed by both thermodynamic driving forces and the fluid residence time, with the latter determined by the nozzle geometry and flow rate.

1.8.3.3 External spray dynamics

Once the fluid exits the nozzle, it expands into the ambient environment. For high injection pressures and large pressure ratios, the jet is often under-expanded at the exit, meaning that the static pressure of the fluid is higher than the ambient pressure. Under-expanded jets are known to develop complex shock-cell structures as the flow adjusts to the surrounding conditions. In flash-boiling sprays, this expansion occurs in a two-phase mixture whose properties differ from those of either pure liquid or pure vapour.

The compressibility of two-phase mixtures is often described using Wood’s equation, which gives an effective sound speed that can be much lower than in single-phase flows. This low sound speed makes the mixture more susceptible to choking and shock formation. Studies of flashing jets have shown that rapid depressurisation can lead to the formation of evaporation waves, Mach disks and shock diamonds [95, 12, 47]. Guo et al. [33, 32, 34] numerically investigated under-expanded and flash-boiling jets in multi-hole GDI systems. Their simulations focused on jet development, jet-to-jet interactions and spray collapse mechanisms. They found that phase change and inertial forces jointly shape the shock-cell structure and the conditions under which spray collapse occurs. Parameters such as relaxation time, expansion ratio and the relative strength of phase change and inertial effects determine the behaviour of flashing jets and the formation of shock waves.

Gärtner et al. [29, 28] carried out numerical and experimental studies of flashing cryogenic jets and provided further insight into compressible two-phase jet behaviour. By coupling HRM with a real-fluid equation of state, they were able to resolve shock diamonds and Mach disk structures in superheated nitrogen and ammonia jets. Their large-eddy simulations revealed helical instabilities that enhance air entrainment and documented the transition between under-expanded and over-expanded regimes. Lyras et al. [58] developed a numerical framework for subcooled and superheated jets under thermodynamic non-equilibrium conditions, capturing the interaction between rapid phase change and shock waves. Wang et al. [97] implemented a compressible volume-of-fluid solver in OpenFOAM to study nozzle aspect ratio effects on ammonia flash-boiling. Their simulations showed that high-aspect-ratio designs can promote annular flow patterns and that shock waves in these nozzles create local supercooling zones, which may accelerate material fatigue.

These theoretical and numerical results indicate that external spray dynamics in flashing ammonia jets are governed by a combination of expansion, phase change, cavitation remnants and compressibility. Shock waves and choked regions can modify

the velocity and pressure fields, which in turn influence droplet breakup, evaporation and mixing. Experimental observations of near-field “bell” shapes and early “feather” structures in ammonia sprays [55, 70, 21, 24] suggest that these compressible features play a significant role in shaping the overall morphology. However, the exact coupling between internal cavitation, external shock structures and macroscopic spray shape remains only partially understood. This motivates the detailed numerical investigation presented in this work, which aims to clarify how cavitation, flash-boiling and compressibility interact in ammonia sprays under flare-flashing conditions.

1.8.3.4 Research gap

The experimental and numerical studies reviewed above have greatly improved the understanding of ammonia flash-boiling sprays, but important gaps remain. Most experimental work has concentrated either on external spray morphology or on in-nozzle flow behaviour, without resolving the full chain that links internal cavitation, external shock structures and the observed spray shapes. Liu et al. [55] provided detailed macroscopic and microscopic data for single-hole ammonia sprays under different flash-boiling regimes, and Pelé et al. [70] compared ammonia with gasoline in GDI hardware, highlighting phenomena such as delayed flash-boiling and prolonged liquid cores. Wang et al. [97] and Colson et al. [21] showed that nozzle aspect ratio, contraction ratio and geometry strongly affect cavitation and flash-boiling transitions. Fang et al. [24] reported non-monotonic trends in penetration and spray width at high injection pressures and high superheat, which they associated with cavitation bubbles. However, these works have mainly treated cavitation, flash-boiling and external morphology as separate topics, and have not yet established a unified picture that quantifies how in-nozzle cavitation patterns feed into external shock systems and, in turn, control the development of characteristic spray morphologies.

A second gap concerns the role of internal shock structures and their interaction with momentum transport in flare-flashing ammonia jets. Studies of flashing jets in other fluids have demonstrated that evaporation waves, Mach disks and shock diamonds can form when rapid depressurisation occurs [95, 12, 47]. Gärtner et al. [29, 28] and Lyras et al. [58] have shown, using HRM-based simulations, that shock cells and under-expanded jet structures play a central role in cryogenic and superheated jets. Guo et al. [33, 32, 34] have analysed the interaction between phase change and shock-cell structure in multi-hole GDI systems. Yet, for ammonia in the strong flash-boiling regime, especially at conditions corresponding to large superheat parameters such as $R_p \approx 10$, there is still limited quantitative information on how internal shocks

form in the two-phase mixture, how they interact with cavitation remnants and how they block or redirect momentum along the jet axis. Existing work has tended to focus on either phase-change modelling or on global jet development, rather than on a detailed mapping of shock locations and their impact on the axial and radial momentum balance in flare-flashing ammonia sprays.

A third gap appears when the distinctive “bell” and “feather” spray shapes observed in experiments are considered. Single-hole and multi-hole ammonia sprays often exhibit a near-field “bell” morphology, followed by a more diffuse, “feather-like” structure in the early injection phase [55, 70, 21, 24, 50]. These morphologies are generally described qualitatively and are attributed to a combination of flash-boiling, collapse, jet–jet interaction or hydraulic flip. However, there is still no consistent explanation of these shapes based on the compressible two-phase nature of the flow. In particular, the extent to which low sound speed, choked regions and shock-cell patterns dictate the opening angle and density distribution of the “bell” region, and how these features evolve into “feather” structures downstream, has not been clarified. Without such an explanation, it remains difficult to translate observed morphologies into quantitative design guidelines for nozzle geometry and operating conditions.

On the numerical side, Lagrangian spray models have been widely used in combustion simulations because they are efficient and can be coupled with detailed chemistry [4, 19, 37]. However, current Lagrangian injection models have struggled to reproduce the complex morphologies of flashing ammonia sprays, as highlighted by Shin et al. [82] and by the discrepancies reported in studies that compare simulations with high-speed imaging and droplet statistics. Eulerian two-phase methods coupled with HRM, such as those used by Downar-Zapolski et al. [22], Gärtner et al. [29, 28], Guo et al. [33, 32, 34], Lyras et al. [58] and Wang et al. [97], have proven capable of capturing flash-boiling, cavitation and shock waves in other fluids and geometries. Yet, these methods have not been fully exploited to study ammonia in nozzle geometries and operating conditions that are typical of engine-relevant flare-flashing regimes. In particular, there is a lack of studies that calibrate HRM relaxation time scales specifically for ammonia and that systematically explore how nozzle aspect ratio, orifice diameter, injection pressure, ambient pressure and superheat jointly affect cavitation onset, shock formation and external spray shape.

In summary, the current state of research shows strong experimental and numerical foundations, but several key questions remain open. There is no complete coupling chain that links in-nozzle cavitation, external shock structures and observed

spray morphology for ammonia. The internal shock structure and its role in momentum blockage during intense flash-boiling are not yet fully quantified. The origin of characteristic morphologies such as near-field “bell” shapes and early “feather” patterns still lacks a clear explanation grounded in compressible two-phase flow physics. Addressing these gaps requires a numerical framework that can resolve cavitation, flash-boiling and shock waves in a unified way and that can be applied to ammonia-specific conditions and geometries.

1.9 Aim and specific objectives

The aim of this thesis is to develop and critically assess a connected, multiscale numerical description of liquid-ammonia injection, from phase change within and immediately downstream of the nozzle to dispersed-spray evolution and combustor-scale mixing and reaction. The work examines how fuel thermodynamic state, injector and combustor geometry, and the level of multiphase-flow resolution influence predicted spray behaviour and the reliability of subsequent combustion predictions.

This aim is addressed through four specific objectives:

1. to assess a combustor-scale Eulerian–Lagrangian CFD framework for ammonia–methane spray combustion against the available experimental flow-field and liquid-penetration data, and to determine how limitations in conventional injection, breakup and evaporation treatments affect the predicted mixing and reacting fields;
2. to develop and evaluate a Lagrangian description of superheated ammonia sprays incorporating finite-rate, pressure-dependent flashing evaporation, and to quantify its ability to reproduce measured penetration and spray morphology under different injection and ambient conditions;
3. to resolve the internal and near-nozzle liquid–vapour flow using a compressible Eulerian VOF–HRM framework, and to determine how nozzle geometry, operating conditions and the relaxation time scale govern cavitation, metastability, phase change, shock formation and external spray morphology; and
4. to synthesise the three modelling levels, define their respective capabilities and limitations, and establish how detailed near-nozzle physics can inform reduced spray models and the design of ammonia injection and combustion systems.

The first three objectives correspond to the three case studies, progressing from the practical combustor-scale problem towards increasingly resolved descriptions of the spray and nozzle physics. The fourth objective integrates their findings and clarifies how modelling assumptions at one physical scale influence predictions at the next.

1.10 Organisation of the thesis

Chapter 2 presents the three numerical methodologies in the sequence used to address the scale-specific objectives: the combustor-scale reacting-spray model, the Lagrangian flashing-spray model and the Eulerian VOF–HRM model. Chapters 3–5 then present the corresponding case studies. Chapter 3 examines ammonia–methane spray combustion in a swirl combustor; Chapter 4 assesses Lagrangian predictions of ammonia flashing sprays; and Chapter 5 investigates cavitation, relaxation-controlled flashing and compressible near-nozzle structures. The final chapter synthesises the findings, defines the applicability of each framework and identifies priorities for future work.

Chapter 2

Numerical methodology

2.1 Methodological framework

This chapter describes the three numerical methods used in the case studies. The combustor calculation couples turbulent reacting flow with Lagrangian droplets in a swirl combustor. The constant-volume-chamber calculation uses a pressure-dependent, non-equilibrium evaporation model for superheated Lagrangian droplets. The near-nozzle calculation treats the liquid–vapour mixture as a compressible Eulerian field and uses the homogeneous relaxation model to represent cavitation, delayed phase change and shock formation. The methods are presented in the same order as the case studies.

For both Eulerian–Lagrangian formulations, F_x denotes the resultant acceleration produced by any additional particle forces not written explicitly in the drag and gravity terms. It has units of m/s^2 and is zero unless an additional force model is enabled. This definition applies throughout the thesis and is not repeated in the individual case-study methodologies.

2.2 Case Study I: combustor-scale spray combustion methodology

2.2.1 Modelled experimental set-up

This study currently applied the finite-volume method for 3D CFD simulations through ANSYS Fluent 2021 R2. The geometry of the combustor was made on SpaceClaim based on the experimental data from Okafor et al. [69, 64]. Simplifications were made for mesh generation and only the interior of the chamber (Fig. 2.1) was built (Fig.2.2). The liquid ammonia hollow cone spray nozzle has an inner diameter

of 0.28 mm and a spray angle of 90°. The swirler produced a swirl flow with a swirl number of 2.34 which will cause vortex breakdown and back flow on outlet [87]. There are 16 circle methane inlets with a diameter of 1.8 mm positioned at the bottom of preheating area.

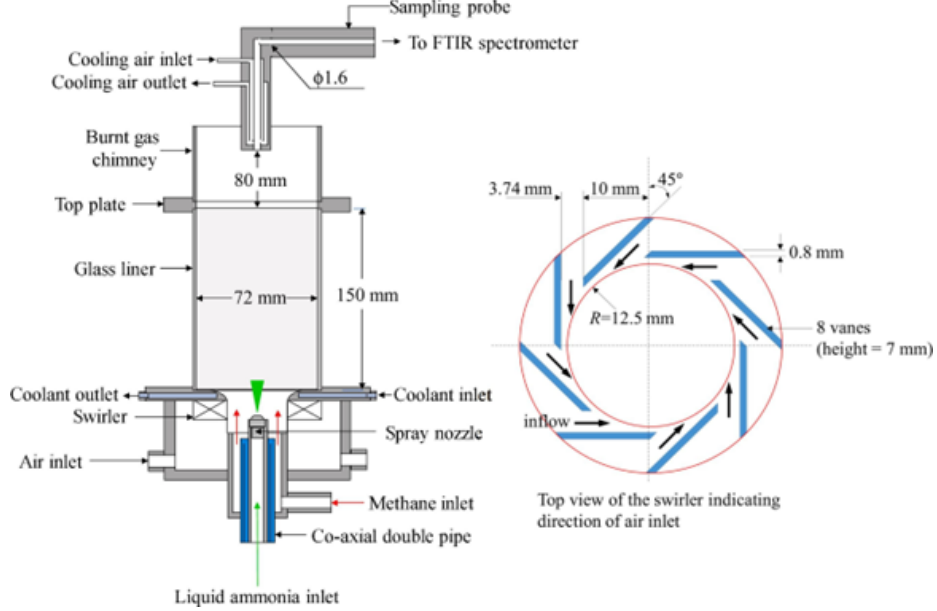


Figure 2.1: Liquid ammonia swirl burner co-firing with methane [69]

The Reynolds-Averaged Navier-Stokes (RANS) turbulence model used in this study is the RNG k - ε model considering the computational time cost. Differing from the standard k - ε model, the RNG k - ε model calculates the Prandtl numbers through semi-analytical relations; it shows more precision at high curvature conditions [76]. Turbulent viscosity in the k - ε model is expressed by turbulent kinetic energy $\bar{k}$ and turbulence energy dissipation rate $\bar{\varepsilon}$ as following:

$$\mu_t = C_\mu \rho \frac{(\bar{k})^2}{\bar{\varepsilon}} \quad (2.1)$$

where C_μ is model constant.

The transport equations for turbulence kinetic energy and turbulence energy dissipation rate are:

$$\frac{\partial}{\partial t} (\rho \bar{k}) + \frac{\partial}{\partial x_i} (\rho \bar{k} \bar{u}_i) = \frac{\partial}{\partial x_j} \left(\alpha_k \mu_{\text{eff}} \frac{\partial \bar{k}}{\partial x_j} \right) + G_k + G_b - \rho \bar{\varepsilon} - Y_M + S_k \quad (2.2)$$

$$\frac{\partial}{\partial t} (\rho \bar{\varepsilon}) + \frac{\partial}{\partial x_i} (\rho \bar{\varepsilon} \bar{u}_i) = \frac{\partial}{\partial x_j} \left(\alpha_\varepsilon \mu_{\text{eff}} \frac{\partial \bar{\varepsilon}}{\partial x_j} \right) + C_{1\varepsilon} \frac{\bar{\varepsilon}}{\bar{k}} (G_k + C_{3\varepsilon} G_b) - C_{2\varepsilon} \rho \frac{\bar{\varepsilon}^2}{\bar{k}} - R_\varepsilon + S_\varepsilon \quad (2.3)$$

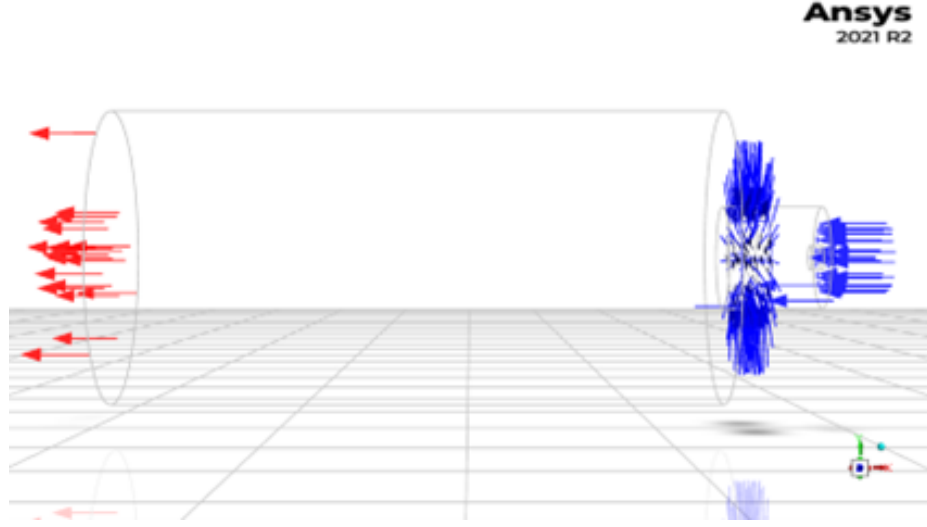


Figure 2.2: 3D model of the interior inside the combustion liner

Among the equations, G_k is the source term due to the mean velocity gradient, G_b is the buoyancy source term, Y_M is the fluctuating dilatation dissipation, and α_k and α_ε are inverse effective Prandtl numbers [7]. The RNG model will calculate a smaller turbulent viscosity than the standard model due to an extra term. The extra term compared to the standard k - ε model is

$$R_\varepsilon = \frac{C_\mu \rho \eta^3 (1 - \eta/\eta_0) \bar{\varepsilon}^2}{(1 + \beta \eta^3) \bar{k}} \quad (2.4)$$

where η_0 and β are constants.

The radiation model chosen in this study is the Discrete Ordinates (DO) radiative heat transfer model which was considered to outperform the P-1 model for spanning the entire range of optical thickness and the ability of multiple rays [43].

2.2.2 Discrete phase model

This study applied the Euler-Lagrangian approach for modelling droplets, which treated the gas phase as a continuum by calculating the N-S equations, while the liquid droplets are tracked as particles through the flow field. It is assumed that the liquid phase is filling a minimal part of the volume regardless of the mass rate fraction [7]. In the acceleration conservation equation, which is:

$$\frac{du_p}{dt} = F_D (u - u_p) + \frac{g_x (\rho_p - \rho)}{\rho_p} + F_x \quad (2.5)$$

where $F_D(u - u_p)$ is the drag acceleration and the common additional-force term F_x is defined in Section 2.1. The drag coefficient per unit particle response time is

$$F_D = \frac{18\mu}{\rho_p d_p^2} \frac{C_D Re}{24} \quad (2.6)$$

where C_D is the drag coefficient that will be modified in the following flash boiling drag force, Re is the relative Reynolds number, u and u_p are the fluid and particle velocity, and d_p is the particle diameter.

Considering the droplet break-up, the KH-RT breakup model was used to model the break-up through the velocity difference between two phases [7]. Liu et al. [53] concluded the relevance between the penetration length and KH-RT breakup model was minimal. It is the turbulence model that determines the momentum transportation between two phases, thus solving the final travel distance of liquid droplets.

2.2.3 Turbulent combustion models

The probability density function (PDF) approach used here is a non-premixed combustion model based on the mixture fraction and its statistical distribution. Thermochemical states are obtained from a precomputed table, commonly under an assumed-chemistry or fast-chemistry closure, rather than by integrating a transport equation for every reacting species [7]. Its principal advantages are robustness and relatively low computational cost. Its disadvantages are the dependence on the presumed PDF and tabulation assumptions and its limited ability to represent finite-rate ignition, local extinction and slow ammonia chemistry. In this study, the PDF solution was therefore used to initialise the reacting flow rather than as the final chemistry model.

The eddy dissipation concept (EDC) couples turbulent mixing with finite-rate chemistry by treating reactions as occurring within small turbulent fine structures. Species source terms are obtained by integrating the imported reaction mechanism under the local thermochemical conditions [7]. Compared with the PDF approach, EDC can represent finite-rate reaction pathways and local species formation, which is important for ammonia oxidation and NO_x chemistry. The trade-offs are substantially greater computational cost, increased stiffness and more difficult convergence. The mechanism employed here was developed by Okafor et al. [65, 67] from the mechanism of Tian et al. [89] and GRI-Mech 3.0. It contains 42 species and 130 reactions and was selected for its demonstrated performance for laminar burning velocity and major-species trends in ammonia-methane flames [65].

Rocha et al. [75] compared ammonia mechanisms at $\phi = 0.9$ and found that the reduced mechanism of Okafor et al. [65] reproduced the trend in NO more successfully than the alternatives considered, although the magnitude was underpredicted by approximately 40%. At $\phi = 1.2$, the tested mechanisms did not reproduce the measured location and magnitude of the maximum NO concentration. NO predictions under rich conditions are therefore interpreted cautiously in this thesis.

2.2.4 Numerical parameter settings

Structured mesh of hexahedrons was built for most of the combustion chamber, while due to the complexity of the inlet area, unstructured tetrahedron mesh was made for the inlet part (Fig.2.3). After the improvement of mesh quality made by Fluent, the mesh orthogonal quality reached 0.18 at minimum.

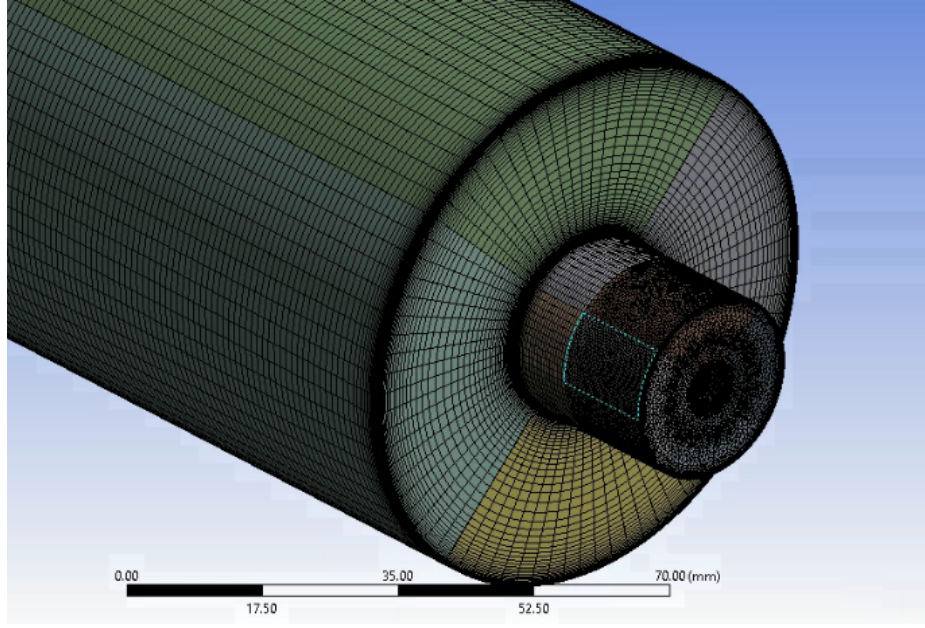


Figure 2.3: 3D model of the interior inside the combustion liner

The boundary conditions for the initial cases are listed in Table 2.1. All the parameters are calculated from the flow rate of liquid ammonia (10 g/min), the heat fraction of ammonia ($E_{\text{NH}_3} = 0.7$), and the global equivalence ratio (1.15).

In the injection settings of the Discrete Phase Model (DPM), the interaction of two phases is considered and liquidous ammonia was injected as particles with 90° solid-cone spray. The injected particle was distributed with a mean diameter of 0.011 mm at the start of the injection.

Table 2.1: Boundary conditions based on Okafor’s experimental liquid-ammonia spray combustor [69].

Boundary	Velocity [m/s]	Mass Flow Rate [kg/s]	Temperature [K]
Air inlet	7.772	1.12×10^{-3}	500
Ammonia inlet	1.1093	1.67×10^{-4}	295
Methane inlet	1.127	2.66×10^{-5}	300

2.3 Case Study II: Lagrangian spray methodology

This chapter employs a Lagrangian Particle Tracking (LPT) approach on ANSYS Fluent 2023R2 to simulate the behaviour of ammonia sprays under flash boiling conditions. The methodology integrates User-Defined Function (UDF) evaporation models tailored for superheated sprays and validates the predictions against the experimental measurements of Li et al. [50]. Key parameters such as ambient pressure, injection pressure, and fuel temperature are systematically varied to assess their influence on spray morphology, droplet size distribution, and penetration length. The computational framework utilises an Eulerian-Lagrangian coupling with two-way interactions to capture the complex multiphase dynamics inherent in flash boiling scenarios. Pressure-dependent boiling models are utilised for changes in boiling point and saturated vapour pressure of superheated liquid.

Turbulence is modelled using the standard k - ε model, with the model constant $C_{\varepsilon 1}$ specified according to the Fluent turbulence-model formulation [7]. The simulations are conducted in a three-dimensional domain representing the spray chamber.

Lagrangian particle tracking is a method using Newton’s second law to track the motion of individual droplets within the spray. The equations of motion for a discrete phase particle in ANSYS Fluent are derived from the force balance on the particle, which is written in a Lagrangian reference frame. This force balance equates the particle inertia with the forces acting on the particle, and can be written (for the x direction in Cartesian coordinates) as:

$$\frac{du_p}{dt} = F_D(u - u_p) + \frac{g_x(\rho_p - \rho)}{\rho_p} + F_x \quad (2.7)$$

where the common additional-force term F_x is defined in Section 2.1, $F_D(u - u_p)$ is the drag acceleration, and

$$F_D = \frac{18\mu}{\rho_p d_p^2} \frac{C_D \text{Re}}{24} \quad (2.8)$$

Here, u is the fluid phase velocity, u_p is the particle velocity, μ is the molecular viscosity of the fluid, ρ is the fluid density, ρ_p is the density of the particle, and d_p is

the particle diameter. Re is the relative Reynolds number, which is defined as

$$Re \equiv \frac{\rho d_p |u_p - u|}{\mu} \quad (2.9)$$

The drag coefficient, C_D , for smooth particles can be taken from

$$C_D = a_1 + \frac{a_2}{Re} + \frac{a_3}{Re^2} \quad (2.10)$$

where a_1 , a_2 , and a_3 are constants that apply over several ranges of Re .

2.3.1 Particle diameter distribution Model

The Rosin-Rammler distribution is used to define the initial droplet size distribution at the injector exit. The cumulative mass fraction $F(d)$ of droplets with diameter less than or equal to d is given by

$$F(d) = 1 - e^{-(d/d_{mean})^n} \quad (2.11)$$

where d_{mean} is the mean diameter and n is the spread parameter that defines the width of the distribution.

2.3.2 Heat and Mass Transfer Models

The heat balance equation for droplet temperature is given by

$$m_p c_p \frac{dT_p}{dt} = h A_p (T_\infty - T_p) + \frac{dm_p}{dt} h_{fg} + A_p \varepsilon_p \sigma (\theta_R^4 - T_p^4) \quad (2.12)$$

where c_p is the droplet heat capacity (J/kg K), T_p is the droplet temperature (K), h is the convective heat-transfer coefficient (W/m² K), T_∞ is the continuous-phase temperature (K), dm_p/dt is the rate of change of particle mass (kg/s; negative during evaporation), h_{fg} is the latent heat (J/kg), ε_p is the particle emissivity (-), σ is the Stefan-Boltzmann constant (5.67×10^{-8} W/m² K⁴), and $\theta_R = (G/4\sigma)^{1/4}$ is the radiation temperature, with G denoting incident radiation.

The convective heat transfer coefficient h is evaluated from the Nusselt number correlation:

$$Nu = \frac{h d_p}{k} = \frac{\ln(1 + B_T)}{B_T} \left(2 + 0.6 Re_d^{1/2} Pr^{1/3} \right) \quad (2.13)$$

where d_p is the particle diameter (m), k is the continuous-phase thermal conductivity (W/m K), Re_d is the droplet Reynolds number (-), and $Pr = c_p \mu / k$ is the continuous-phase Prandtl number (-).

B_T is the Spalding heat transfer number defined as:

$$B_T = \frac{c_{pv}(T_\infty - T_p)}{h_{fg} - \dot{q}_p/\dot{m}_p} \quad (2.14)$$

where $\dot{q}_p$ is the heat transferred to the droplet (W), $\dot{m}_p$ is the particle evaporation rate (kg/s), and c_{pv} is the specific heat of the droplet vapour (J/kg K).

B_T is computed from the Spalding mass number by:

$$B_T = (1 + B_M)^{\frac{1}{Le} \cdot \frac{Sh}{Nu} \cdot \frac{c_{pv}}{c_{pg}}} - 1 \quad (2.15)$$

where $Le = k/(c_{pg}\rho D_{i,m})$ is the Lewis number (-), and c_{pg} is the specific heat of the gas mixture (J/kg K).

For the unity Lewis number and with the further assumption that $c_{pv} = c_{pg}$, the equation reduces to:

$$B_T = B_M \quad (2.16)$$

When temperature differences between droplet and bulk gas are large, transient effects become important. The assumption of uniform droplet temperature and the assumption of emanating vapor in temperature equilibrium with the bulk gas may be questioned. In such conditions, an averaging of the Spalding heat transfer term may produce more realistic results.

$$F_T = 1 - Y_{is}(1 - F_{T_0}) \quad (2.17)$$

where

$$F_{T_0} = \frac{\ln(1 + B_T)}{B_T} \quad (2.18)$$

and Y_{is} is the surface mass fraction of the evaporating species.

2.3.3 Zuo–Adachi evaporation model

The Zuo–Adachi model is the evaporation closure used for all ammonia spray cases reported in this chapter. It combines heat-transfer-driven surface evaporation with an additional flashing contribution caused by droplet superheat [2, 114]. The total droplet mass-loss rate is

$$\dot{m} = \dot{m}_{\text{flash}} + \dot{m}_h. \quad (2.19)$$

The Adachi correlation gives the superheat-driven flashing rate:

$$\dot{m}_{\text{flash}} = \pi d_d^2 \alpha_f \frac{(T_d - T_b)}{h_{fg}}. \quad (2.20)$$

Here, T_d is the droplet temperature, T_b is the local pressure-dependent boiling temperature supplied by Fluent, and h_{fg} is the latent heat of vaporisation. Flashing is therefore driven by the superheat $T_d - T_b$ and ceases when the droplet cools to the local boiling temperature. The empirical flash-evaporation coefficient is

$$\alpha_f = \begin{cases} 0.76(T_d - T_b)^{0.26}, & 0 \leq T_d - T_b < 5, \\ 0.027(T_d - T_b)^{2.33}, & 5 \leq T_d - T_b < 25, \\ 13.8(T_d - T_b)^{0.39}, & 25 \leq T_d - T_b. \end{cases} \quad (2.21)$$

The Zuo formulation accounts for the interaction between flashing and external heat transfer. Vapour generated by flashing produces an outward Stefan flow that thickens the effective gas-side boundary layer and reduces heat transfer from the surrounding gas. The heat-transfer-driven evaporation rate is

$$\dot{m}_h = \pi d_d \frac{\lambda_g Sh}{c_{p,g}} \left(\frac{1}{1 + \dot{m}_{\text{flash}}/\dot{m}_{\text{total}}} \right) \ln \left[1 + B_T \left(1 + \frac{\dot{m}_{\text{flash}}}{\dot{m}_{\text{total}}} \right) \right]. \quad (2.22)$$

Here, $\dot{m}_{\text{total}} = \dot{m}_{\text{flash}} + \dot{m}_h$. The first parenthetical term is the blocking correction: a larger flashing fraction reduces the heat-transfer-driven contribution. Because $\dot{m}_h$ appears implicitly through $\dot{m}_{\text{total}}$, the UDF evaluates the coupled relation iteratively before updating droplet mass, diameter and temperature. The evaporated ammonia and corresponding latent-energy source are then transferred to the continuous phase. Further implementation details are given in Appendix A.

2.3.4 Experimental and computational case setup

The experimental set-up used to parameterise and validate the numerical spray simulations was a constant-volume chamber (CVC) with optical access (up to four windows), in which the ambient static pressure was adjusted to span a broad range of superheat conditions while the ambient temperature was held near 298 K. Liquid ammonia was injected by a modified common-rail solenoid injector fitted with a single straight nozzle hole (0.28 mm, $L/D = 6$). The injection pressure was fixed at 30 MPa, and the injected-fuel temperature was controlled by a heated fuel line and an injector jacket to nominal values of 308, 323, and 338 K (within ± 1 K).

The saturation pressure of ammonia was evaluated using the Antoine equation

$$\log_{10} \left(\frac{P_{\text{sat}}}{\text{bar}} \right) = A - \frac{B}{T + C}, \quad (2.23)$$

where T is in kelvin, $A = 4.86886$, $B = 1113.928$ K, and $C = -10.409$ K. These coefficients are valid over $239.6 \leq T \leq 371.5$ K and therefore cover all injection temperatures considered here [62]. The superheat ratio was calculated using Eq. (1.1),

with P_{amb} equal to the chamber pressure. The chamber pressure was selected according to the required value of R_p . Injection timing was synchronised with imaging and data acquisition (55 ns resolution). Spray structure was measured using DBI: a high-speed camera with a regular lens captured far-field evolution, and the same camera, coupled to a long-distance microscope, captured near-field features. Image segmentation used a threshold of 10% of maximum intensity for both near- and far-field boundaries; near-field analysis focused on the first 3 mm below the nozzle, assuming axisymmetry to infer volume. Macroscopic validation metrics included tip penetration and cone angle, computed consistently from the processed DBI images, with statistics based on five repeat shots [50]. A three-dimensional $75 \times 75 \times 75$ mm computational domain was constructed to represent the constant-volume chamber of Li et al. [50], with the injector centred on the upper wall. The injector exit was represented by a circular orifice of diameter 0.28 mm. No Eulerian carrier-gas inflow was imposed through this boundary; liquid ammonia entered only through the transient Lagrangian DPM injection described below. A pressure outlet with reverse-flow prevention was placed on the opposite boundary to maintain the prescribed chamber pressure, and all remaining chamber walls were adiabatic and no-slip. The carrier gas was initialised at the ambient pressure and temperature listed in Table 2.2. The injected parcels were initialised with the listed droplet temperature and full spray angle. The simulations were run for a total physical time of 0.001 s to capture the

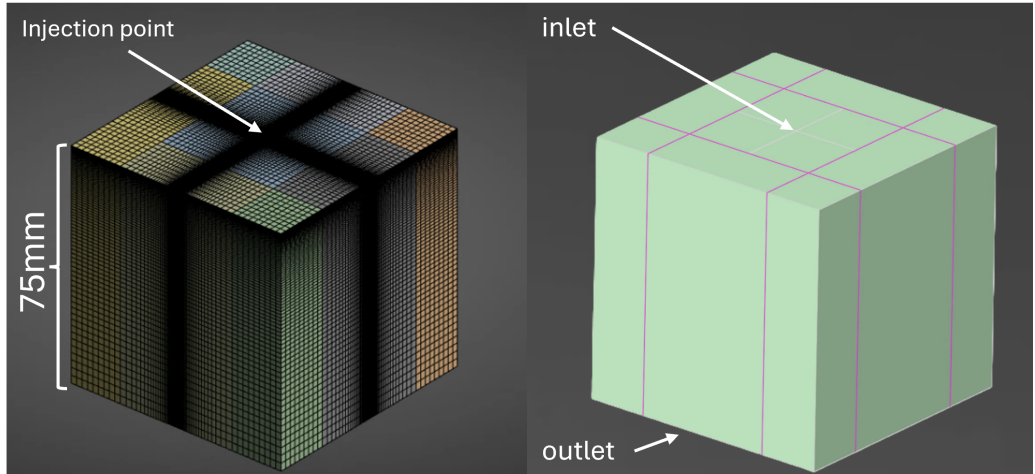


Figure 2.4: The constant volume chamber model and mesh used in the simulations

transient spray development. The mesh was refined near the injector axis to resolve the high velocity and temperature gradients associated with flash boiling. The mesh independence study was conducted to ensure that the results were not sensitive to

grid resolution. A time step of 1×10^{-6} s was employed for both the Eulerian and Lagrangian phases to maintain numerical stability and consistent two-way coupling.

Table 2.2: Initial thermodynamic and DPM conditions for the simulated spray cases.

	Case 1	Case 2	Case 3	Case 4
Ambient Pressure (kPa)	295	134	590	1476
Ambient Temperature (K)	298	298	298	298
Droplet Temperature (K)	338	308	338	338
Spray Angle (degrees)	30	40	25	20
Superheat ratio, R_p	10	10	5	2

Liquid ammonia was introduced at the injector exit using a transient solid-cone Discrete Phase Model (DPM) injection. Parcels were released from $t = 0$ to 1.66×10^{-3} s; therefore, injection remained active throughout the 1 ms simulation window. For the calibrated reference condition (Case 1), the droplet temperature was 338 K, the initial velocity magnitude was 108 m/s, the outer injection radius was 0.121 mm, and the total liquid mass flow rate was 2.662×10^{-3} kg/s. The droplet diameters followed a Rosin–Rammler distribution with a minimum diameter of $3.6 \mu\text{m}$, a maximum diameter of $119 \mu\text{m}$, a mean diameter of $13.8 \mu\text{m}$, a spread parameter of 1.4, and 40 discrete diameter classes. For the other thermodynamic cases, the droplet temperature and cone half-angle were adjusted consistently with the full spray angles listed in Table 2.2; the velocity-calibration procedure is described in the injection-model subsection. The UDF described above updated the parcel mass and temperature and imposed the corresponding ammonia-vapour and latent-heat source terms on the continuous phase.

2.3.5 Mesh independence

To ensure that the simulation results are not influenced by the mesh size, a mesh independence study is conducted. Three different mesh sizes are tested: coarse, medium, and fine. The coarse mesh consists of approximately 605696 cells, the medium mesh has around 907500 cells, and the fine mesh contains about 1749068 cells. The key parameters evaluated for mesh independence is the spray penetration length at 0.0001 s. The results show that the spray penetration length converges as the mesh is refined. As shown in Figure 2.5, the difference in spray penetration length between the medium and fine mesh is less than 5%, indicating that the medium mesh is sufficient for accurate simulations. Therefore, the medium mesh with 907500 cells is selected for all subsequent simulations to balance computational cost and accuracy.

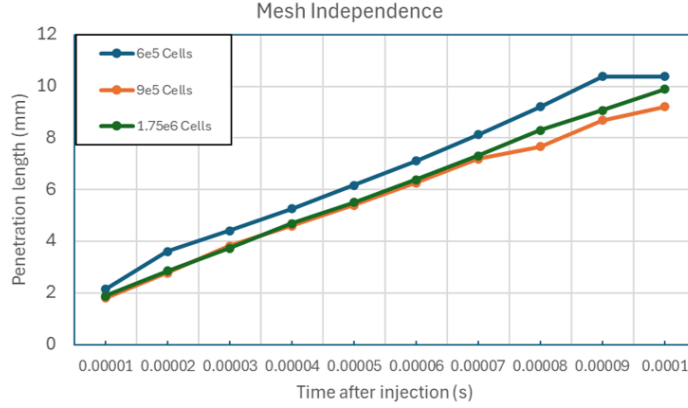


Figure 2.5: Mesh independence study for spray penetration length at 0.0001s

2.3.6 Injection model

The Fluent solid-cone injection model was used to represent the single-hole injector. It requires the mass flow rate, cone half-angle, initial velocity, orifice diameter and droplet-size distribution. The cone half-angle was obtained from the measured full spray angle [50]. Because the experiment reported an injector delivery rate rather than the instantaneous ammonia exit velocity, an equivalent discharge-coefficient approach was used to relate the pressure difference to the initial parcel velocity:

$$v_0 = C_d \sqrt{\frac{2(P_{inj} - P_{amb})}{\rho_{fuel}}} \quad (2.24)$$

where $C_d = \dot{m}/[A\sqrt{2\rho_{fuel}\Delta p}]$, P_{inj} and P_{amb} are the injection and chamber pressures, and ρ_{fuel} is the liquid-ammonia density. An initial value $C_d = 0.242$ was inferred from the reported injector delivery. Applying the full 0.28 mm orifice area gives $v_0 = 78$ m/s for the 338 K, $R_p = 10$ case, but this value underpredicts the measured penetration. The exit velocity was therefore treated as an equivalent boundary parameter that incorporates unresolved contraction and cavitation within the injector. At fixed mass flow rate, the effective flow area was reduced and the velocity was calibrated against the experimental penetration. Table 2.3 records the tested values; this calibration is a modelling limitation because the measured in-nozzle velocity and effective discharge area were not available independently.

The results of the adjusted initial velocity are compared with the experimental spray penetration length in Fig. 2.6. To save the computational cost, all cases listed in the table above are only calculated to 0.0005 s, which is sufficient to capture the spray evolution. Sensitivity analysis shows that under a fixed mass flow rate and constant

Table 2.3: Injection parameters for simulation cases

	Case 5	Case 6	Case 1	Case 7
Initial Velocity (m/s)	78	93	108	123
Mass Flow Rate (10^{-3} kg/s)	2.662	2.662	2.662	2.662
Effective Diameter (mm)	0.280	0.261	0.242	0.227

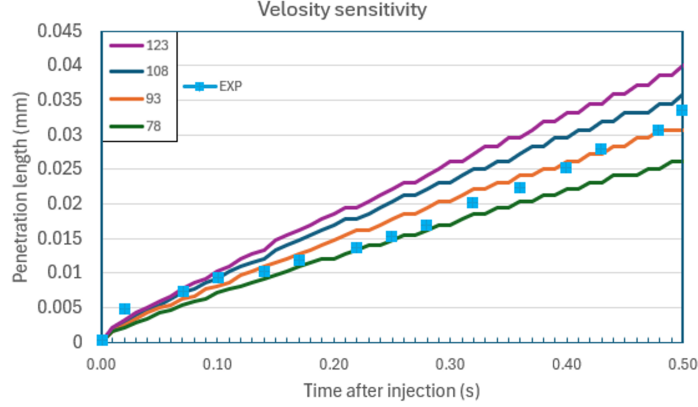


Figure 2.6: Comparison of predicted and measured spray penetration for adjusted initial velocities at $R_p = 10$.

other model parameters, the predicted penetration distance is approximately linearly related to the exit velocity within the examined velocity range. This indicates that under the current model configuration, the early spray behavior is primarily controlled by the exit axial momentum flux $\dot{m}U_0$, while the effective injection cross-section (denoted by d_{eff}) primarily serves to satisfy the closure relation

$$\dot{m} = \rho A_{\text{eff}} U_0, \quad (2.25)$$

and presents a secondary effect on the penetration criterion in this study. Based on this, the exit velocity is treated as an equivalent nozzle boundary parameter, and the inverse problem calibration is performed by minimizing the error of the penetration curve, from which d_{eff} and the equivalent discharge coefficient C_d are back-calculated.

At the moment of $t = 0.0005$ s, linear regression of penetration distance was performed using four groups of exit velocities (78, 93, 108, and 123 m/s), yielding

$$S_{\text{mm}} = 1.6976 + 0.3136 U_0, \quad (2.26)$$

where the slope is $b = 0.3136$ mm/(m/s) (95% confidence interval: 0.2823–0.3448, $R^2 = 0.9989$), indicating an approximately linear response of penetration to exit velocity at this moment. The corresponding dimensionless sensitivity is defined as

$$S = \frac{\partial \ln S}{\partial \ln U_0} \approx \frac{b U_0}{S}, \quad (2.27)$$

which at $U_0 = 108$ m/s equals $S \approx 0.945$ (with slope interval propagation giving 0.851–1.039), showing that the penetration response to velocity approaches a proportional relationship. Based on this slope, if the exit velocity has an uncertainty of ± 5 m/s, the penetration uncertainty can be estimated as $\Delta S \approx \pm 1.57$ mm (approximately ± 1.41 to ± 1.72 mm obtained from slope confidence interval propagation), corresponding to a relative uncertainty of approximately $\pm 4.4\%$ at $S \approx 35.84$ mm.

2.4 Case Study III: Eulerian VOF–HRM methodology

2.4.1 Governing equations

The simulations use the compressible volume-of-fluid (VOF) framework developed by Gärtner et al. [29] in OpenFOAM, coupled with the homogeneous relaxation model (HRM) for finite-rate phase change. Turbulence is represented by the k – ω shear stress transport (SST) model. Reynolds averaging is denoted by an overbar, Favre averaging by a tilde, and Favre fluctuations by a double prime. The Favre-averaged liquid-volume-fraction equation is

$$\frac{\partial(\bar{\rho}_L \tilde{\alpha}_L)}{\partial t} + \nabla \cdot (\bar{\rho}_L \tilde{\alpha}_L \tilde{\mathbf{u}}) + \nabla \cdot (\overline{\rho_L \alpha_L'' \mathbf{u}''}) = \tilde{m}_L. \quad (2.28)$$

Here, $\tilde{m}_L$ is the liquid-phase mass source and is negative during evaporation. The Favre-averaged mixture-momentum equation is

$$\frac{\partial(\bar{\rho} \tilde{\mathbf{u}})}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{\mathbf{u}} \tilde{\mathbf{u}}) = -\nabla \bar{p} + \bar{\rho} \mathbf{g} + \nabla \cdot (\tilde{\boldsymbol{\tau}} + \boldsymbol{\tau}_t), \quad (2.29)$$

where $\tilde{\boldsymbol{\tau}}$ and $\boldsymbol{\tau}_t$ are the molecular and turbulent stress tensors. Separate Favre-averaged sensible-enthalpy equations are solved for the liquid and vapour phases:

$$\begin{aligned} \bar{\rho} \frac{D\tilde{h}_L}{Dt} + \bar{\rho} \frac{D\tilde{K}}{Dt} &= \frac{\partial \bar{p}}{\partial t} + \nabla \cdot (k_{L,\text{EFF}} \nabla \tilde{T}_L) \\ &+ \frac{\bar{\rho}}{\bar{\rho}_L \tilde{\alpha}_L} \tilde{m}_L [h_{SG}(\bar{p}) - \tilde{h}_L], \end{aligned} \quad (2.30)$$

$$\begin{aligned} \bar{\rho} \left(\frac{D\tilde{h}_G}{Dt} \right) + \bar{\rho} \left(\frac{D\tilde{K}}{Dt} \right) &= \frac{\partial \bar{p}}{\partial t} + \nabla \cdot (k_{G,\text{EFF}} \nabla \tilde{T}_G) \\ &+ \frac{\bar{\rho}}{\bar{\rho}_G \tilde{\alpha}_G} \tilde{m}_L [\tilde{h}_G - h_{SG}(\bar{p})]. \end{aligned} \quad (2.31)$$

Here, $\mathbf{u}$, K , h , k_{EFF} , $\mathbf{g}$ and α denote velocity, kinetic energy per unit mass, sensible enthalpy, effective thermal conductivity, gravitational acceleration and phase

volume fraction, respectively. Subscripts L and G denote liquid and vapour, while SL and SG denote saturated-liquid and saturated-vapour properties. Mixture properties without a phase subscript are obtained by volume averaging. The effective thermal conductivity is the sum of molecular and turbulent contributions, with

$$k_t = \rho \frac{\nu_t}{Pr_t} \quad (2.32)$$

where $Pr_t = 1.0$ is the turbulent Prandtl number. The unresolved volume-fraction flux is closed using a gradient-diffusion assumption [5]:

$$\overline{\rho_L \alpha_L'' \mathbf{u}''} = -\bar{\rho}_L \frac{\nu_t}{Sc_t} \nabla \tilde{\alpha}_L, \quad (2.33)$$

where ν_t is the turbulent kinematic viscosity and Sc_t is the turbulent Schmidt number. A linearised pressure–density relation, $\rho = \rho_0 + \psi p$, is used locally. Following the homogeneous-mixture relation described by Brennen [14], the mixture compressibility is

$$\psi = \frac{\partial \rho}{\partial p} = \left(\sum_{i=1}^N \rho_i \alpha_i \right) \left[\sum_{i=1}^N \frac{\alpha_i}{\rho_i} \left(\frac{\partial \rho_i}{\partial \mathbf{p}} \right) \right]. \quad (2.34)$$

The mass and momentum equations formulate the pressure equation,

$$\nabla \cdot \left(\frac{\nabla p}{a_p} \right) - \nabla \cdot \left(\frac{H(\mathbf{u})}{a_p} \right) = \frac{1}{\rho} \frac{D\rho}{Dt} \quad (2.35)$$

The operators $H(\mathbf{u})$ and a_p contain the off-diagonal and diagonal contributions of the discretised momentum equation, respectively. The material derivative of density contains the mixture compressibility expressed in equation (7). The resulting mixture sound speed can be substantially lower than the sound speed of either pure phase at intermediate volume fractions [63], which is central to the near-nozzle shock structure.

The HRM formulation follows the definitions introduced in Section 1.3. The liquid mass source is related to relaxation of the instantaneous vapour mass fraction χ towards the equilibrium value $\bar{\chi}$ by

$$\frac{D\chi}{Dt} = \frac{\bar{\chi} - \chi}{\theta} = -\frac{\tilde{m}_L}{\bar{\rho}}. \quad (2.36)$$

The relaxation time scale is

$$\theta = \theta_0 \alpha_v^{-0.54} \varphi^{-1.76} \quad (2.37)$$

$$\alpha_v = \left(\frac{\rho_L - \rho}{\rho_L - \rho_v} \right) \quad (2.38)$$

$$\varphi = \left(\frac{p_s(T) - p}{p_c - p_s(T)} \right) \quad (2.39)$$

where α_v is the vapour volume fraction, $p_s(T)$ is the saturation pressure, p_c is the critical pressure and θ_0 is the empirical time constant. The exponents and original value of θ_0 were calibrated using flashing-water experiments [22]; their applicability to ammonia is therefore examined through validation and sensitivity analysis in the following sections. In equation (12), p_s stands for saturation pressure and p_c stands for the critical pressure of the fluid.

2.4.2 Numerical setup

The numerical domain is built according to the nozzle geometry and parts of the outside chamber in the experiments of Colson et al. [21]. The inner diameters of the injector and the nozzle orifice are 5mm and 0.21mm, respectively, connected by a 120-degree cone with a rounded corner, whose radius is 0.1 mm at the orifice inlet.

The numerical cases in this paper are built in 2D, including the nozzle inner flow area and part of the outside chamber. In Figure 1, the symmetric domain built outside the nozzle is 17mm in length and 9mm in width, with the symmetric axis at the zero position of the x-axis. Boundary conditions for the inlet, outlets, and walls are also noted in Figure 1. Detailed nozzle geometry information of different cases is listed in Table 1. The injection was simplified to a fixed injection pressure, without considering the effect of needle movement. The instantaneous solutions are calculated in this study, and the following results are compared at 0.01 s. To compare the effect of initial temperature, nozzle L/D ratio and orifice diameter on spray parameters, 5 cases were selected for validation from the experiments of Colson et al.[21]. Additional cases were constructed to examine increased injection pressure and reduced ambient pressure. The initial time step was 6×10^{-9} s, after which an adaptive time step was used. The merged PISO–SIMPLE (PIMPLE) algorithm was applied with three outer corrector iterations per time step. All simulations use an ambient pressure of

Cases	1	2	3	4	5
Injection temperature (K)	270	295	292	291	279
R_p	3.8	9.0	8.2	7.9	5.2
Injection pressure (Pa)	8.7×10^5	1.01×10^6	1.09×10^6	1.01×10^6	9.6×10^5
Nozzle aspect ratio	10	5	10	10	10
Nozzle diameter (mm)	0.21	0.21	0.21	0.15	0.21
θ_0 (s)	1×10^{-7}	1×10^{-4}	3.87×10^{-7}	2×10^{-7}	2×10^{-7}
Flashing stage	Partial flashing	Non- flashing	Fully flashing	Fully flashing	Partial flashing

Table 2.4: Injection conditions and empirical constant for different cases.

1×10^5 Pa and an ambient temperature of 298 K. The time constant θ_0 was adjusted

to 1×10^{-4} s for Case 1 and 1×10^{-7} s for Case 2 following Wang et al. [96]; the original correlation was retained for Case 3. The grid-independence assessment used approximately 37,000, 48,000 and 106,000 cells. The axial and radial liquid-volume-fraction profiles at the nozzle exit changed only slightly between the two finer meshes, while local refinement within the orifice provided improved resolution of the internal field.

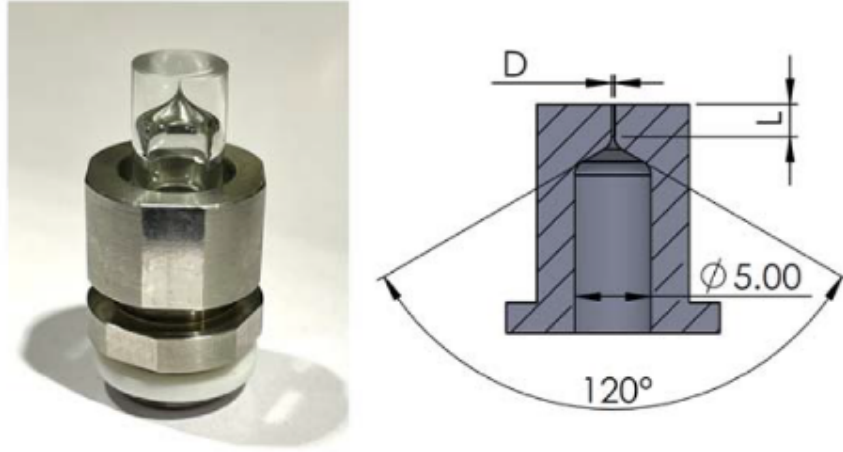


Figure 2.7: Nozzle inner geometry in the experiment of Colson et al.[21].

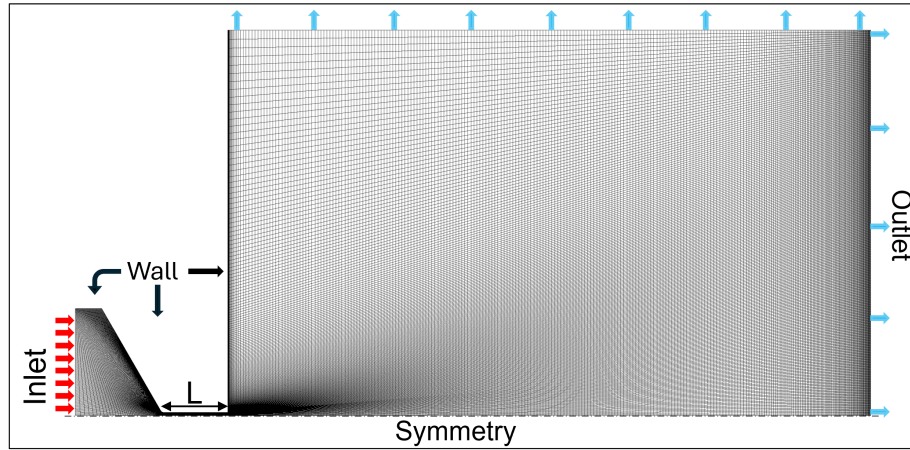


Figure 2.8: Mesh and boundary of the 2D simulation domain (chamber domain length = 17mm).

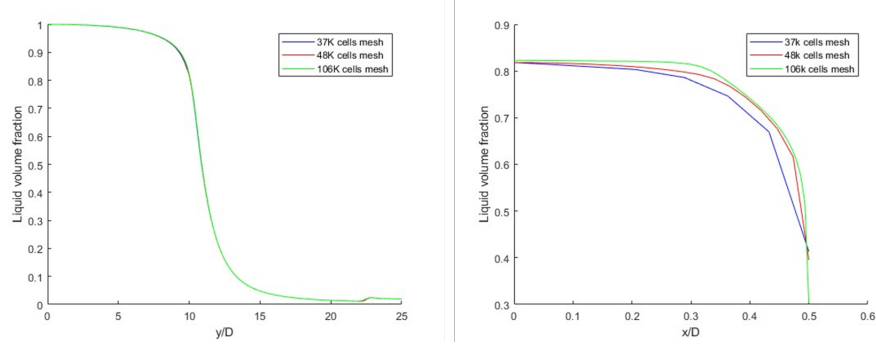


Figure 2.9: Liquid volume fraction profiles at (left) axial position where $x/D = 0$ and (right) radial position where $y/D = 10$ with three different mesh resolutions.

2.5 Relationship between the three modelling levels

The three methods address different spatial scales. The combustor model predicts flow, mixing and reaction but does not resolve the injector interior or the compressible flashing region. The Lagrangian chamber model includes finite-rate droplet evaporation and cooling, although its injection conditions must be prescribed. The VOF-HRM model calculates the internal and near-nozzle phase change that establishes those conditions, but its computational cost restricts it to a smaller domain. These differences define how the results from the three case studies should be compared.

Chapter 3

Case Study I: Ammonia–methane spray combustion in a swirl combustor

This case study applies the combustor-scale framework described in Section 2.2. It assesses the predicted recirculation, spray penetration, temperature and species fields and identifies the limitations of applying conventional spray closures to superheated liquid ammonia. These limitations motivate the dedicated flashing-spray investigations in Chapters 4 and 5.

3.1 Model validation

Validation is restricted to quantities reported in the experimental study of Okafor et al. [69]: the particle-image-velocimetry (PIV) flow field and the measured liquid-spray penetration. Because numerical velocity profiles at the experimental sampling locations are unavailable, the velocity-field validation remains qualitative and does not establish pointwise accuracy in velocity magnitude.

The experimental liquid penetration of approximately 24.5 mm provides a direct quantitative metric. Both numerical approaches predict a penetration of approximately 40 mm. Relative to the experimental value, this corresponds to an overprediction of approximately 63%. The penetration result therefore represents a clear quantitative disagreement rather than successful validation. Table 3.1 summarises the evidence used. Temperature and species fields are excluded from the validation because corresponding quantitative measurements are not available for the simulated case.

Table 3.1: Validation against data reported by Okafor et al. [69].

Quantity	Experimental data	Numerical result	Validation outcome
Mean-flow topology	PIV field at the nearest inlet condition of 8 m/s	PDF and EDC velocity fields at 7.772 m/s	Qualitative comparison; EDC gives the closer topology
Liquid penetration	Approximately 24.5 mm	Approximately 40 mm for both approaches	Approximately 63% overprediction

These comparisons define a limited domain of credibility. The model captures the principal combustor-flow organisation sufficiently well for qualitative analysis of recirculation, but it does not reproduce the measured liquid penetration. The subsequent temperature and species results are consequently discussed as simulation outputs affected by the spray-model error, not as validated predictions.

3.2 Results and discussion

The CFD case was first initialised using the PDF approach until a steady discrete-phase solution was obtained. Because turbulence and species transport were strongly coupled, a detailed chemical mechanism was subsequently introduced through the EDC approach to predict the local reaction and temperature fields. A customised flash-boiling law and modified droplet drag treatment were not included in this combustor-scale model. The results are therefore interpreted as a baseline comparison of the PDF and EDC combustion approaches and as evidence of the spray-model limitations addressed by the dedicated methodologies in Sections 2.3 and 2.4.

3.2.1 Velocity profile

From Fig.3.1 the velocity magnitude contours displayed a typical distribution of swirl flow velocity inside the chamber on the plane across the axis. The air from the radial swirler accumulated and accelerated at the inlet preheating zone of the chamber, as the ammonia spray required a large amount of energy to preheat [69]. The swirled air travelled throughout the preheat zone and created a pressure gradient which concentrated the methane fuel and ammonia droplets in the centre of the preheat zone. Then, the flow with fuel and air mixtures rotated and entered the combustion chamber with a large radial velocity. As a result, the flow accelerated and reached the chamber wall, intense flow rate proceeded along the wall. With the decreasing of the radial velocity, the intense velocity magnitude moved apart from the wall, which agrees with the flow pattern from Okafor et al.[69] (Fig.3.2). The velocity magnitude

was reduced to a relatively low value in the flow shear layer between the recirculation zone. Corner flow at the outer recirculation zone was captured in simulations. Along the axis, the swirled flow forward to the outlet created a radial pressure gradient, outside the outlet decay of tangential velocity decreased pressure drop at the central region, which caused a rising pressure along the axis. Hence the reverse flow was generated by the axial pressure gradient [87].

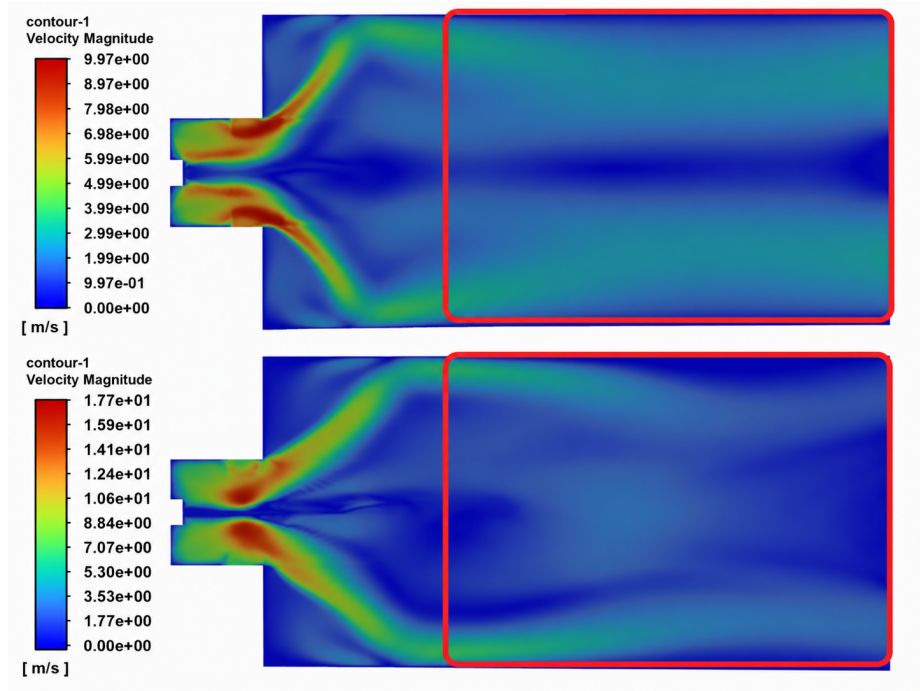


Figure 3.1: Velocity contour of PDF (upper) and EDC (lower) approaches (red frame represents the area consistent with Fig. 3.2)

Both simulations reproduce the principal features expected in a strongly swirling combustor, but the comparison with Fig. 3.2 must be interpreted qualitatively because matched axial and radial velocity profiles were not available. The EDC solution shows a stronger reverse-flow region, clearer shear-layer development and a boundary-layer detachment pattern closer to the experimental PIV field than the PDF solution. Its maximum velocity is approximately twice that predicted by the PDF approach, and its axial velocity is also higher. This difference is consistent with the additional heat release and density change represented by the finite-rate EDC treatment. It does not, by itself, demonstrate that the EDC velocity magnitude is quantitatively accurate; rather, the experimentally observed topology favours the EDC description of the global flow organisation.

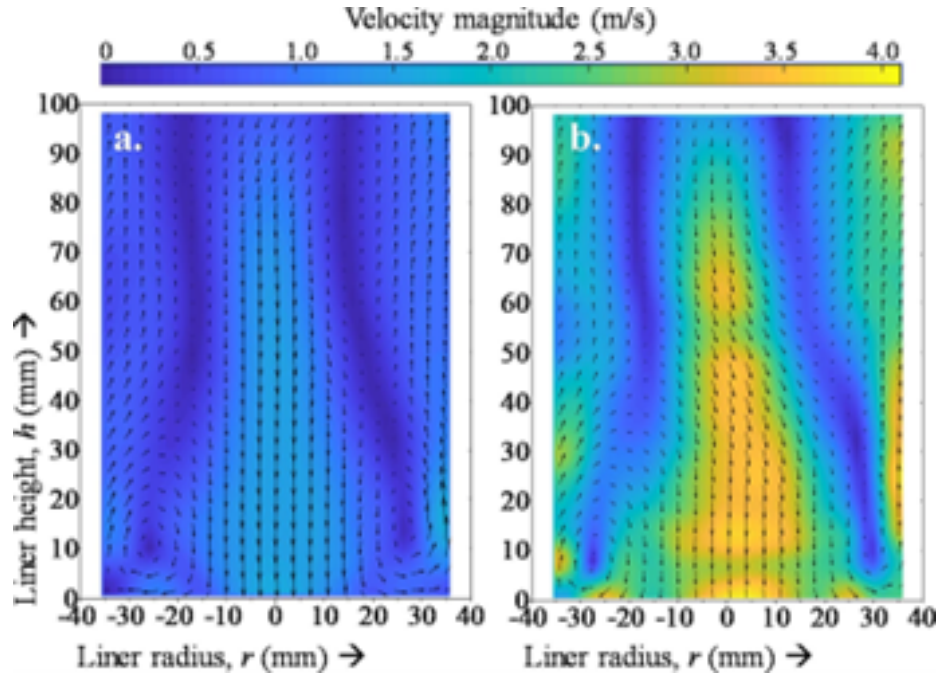


Figure 3.2: Average velocity field measured by particle image velocimetry for 8m/s and 24m/s inlet velocity [69]

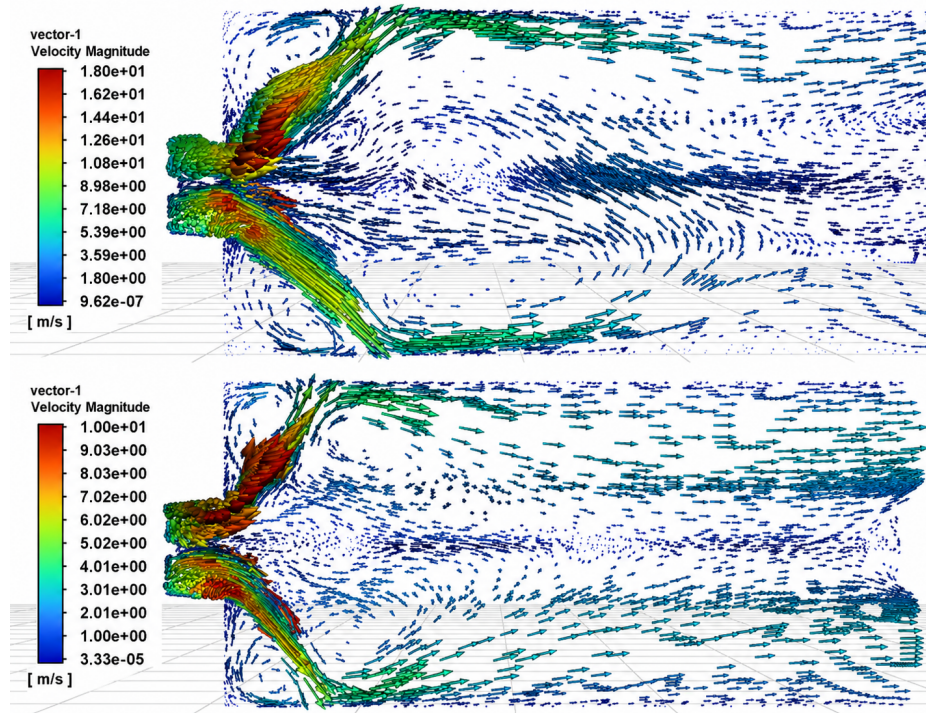


Figure 3.3: Velocity vector on the plane across the axis for PDF(upper) and EDC(lower) approaches

The vector plot in Fig. 3.3, taken on the same plane, provides a more detailed representation of the flow direction. Corner recirculation is evident near the chamber inlet. Two inner recirculation zones are apparent in the PDF solution, whereas one dominant inner recirculation zone occupies the central flow in the EDC solution. Small eddies also appear near the axis in both solutions, possibly because of the DPM momentum source.

The radial velocity of the swirling flow decreases downstream of the main high-velocity region because of radial expansion and combustion-induced acceleration. The pressure gradient drives reverse flow towards the preheat zone and initiates recirculation. Reverse flow from the outlet is evident in the EDC case but is barely visible in the PDF case, indicating a weaker radial motion. Despite the multiple vortices near the centreline in the EDC solution, two principal recirculation zones remain identifiable. Further mesh refinement and parameter assessment are required to resolve the internal flow field more reliably.

Figure 3.4 clarifies the axial flow direction; the plotted orientation is opposite to the positive x direction, so reverse flow is shown in red. In both simulations, the radial swirler divides the inlet flow and produces recirculation towards the main chamber. The numerical liquid penetration is approximately 40 mm, whereas the experiment reports approximately 24.5 mm, terminating near the entrance to the main chamber [69]. As quantified in Table 3.1, this corresponds to an overprediction of approximately 63%. The discrepancy is physically consistent with the omitted flash-boiling process: ammonia injected at 10 bar and 295 K becomes superheated during pressure reduction, and the resulting rapid vaporisation and expansion shorten the visible liquid penetration. The conventional evaporation and KH–RT treatments retain liquid droplets for too long and do not generate the additional radial expansion associated with flashing. The penetration error therefore provides direct evidence that matching the gas-phase recirculation alone is insufficient for validating the coupled spray calculation.

Overall, the EDC approach predicts stronger reverse flow than the PDF approach because heat release and the associated acceleration strengthen the pressure gradients that sustain recirculation. The direction and approximate location of this reverse flow are consistent with the experimental velocity field [69]. However, without velocity profiles at identical sampling locations, this agreement validates the presence and topology of recirculation rather than its magnitude.

Calculated from the given mass flow rate (10 g/min) and heat fraction of ammonia, the mass flow rate of methane is 2.66×10^{-5} kg/min. Thus, the velocity of the methane

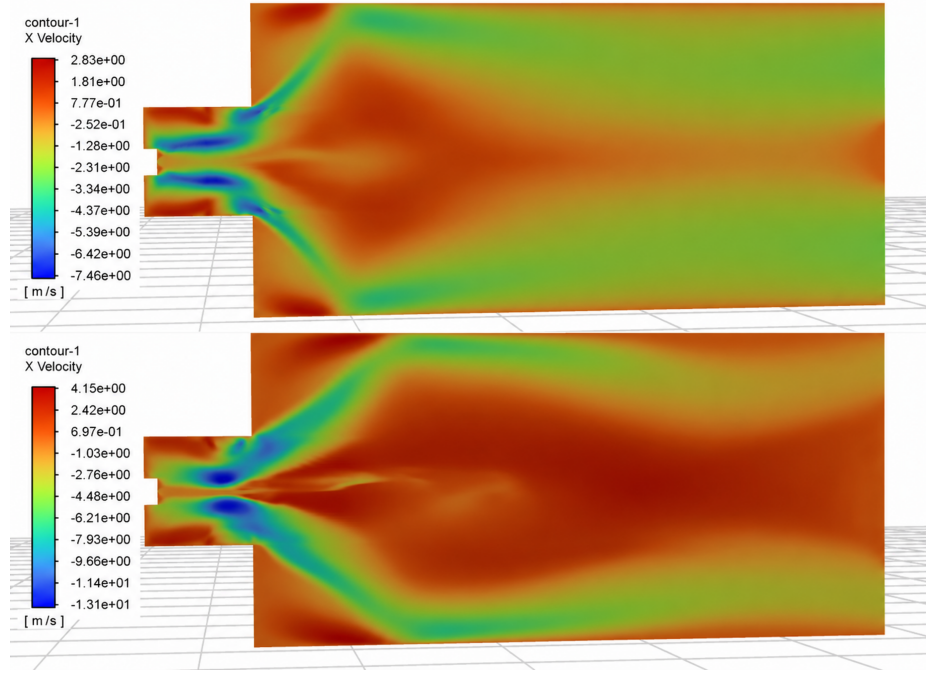


Figure 3.4: The component of velocity on x-axis for PDF(upper) and EDC(lower) approaches

inlet is 1.1093 m/s considering constant density. The swirl air flow is much stronger than the methane flow when compared the value of the air inlet (7.772 m/s) to the velocity of methane. According to Fig.3.5, showing streamlines from the methane inlet, the methane flow was dominated by the preheated swirl air. The axial velocity of methane was negligible compared to the radial velocity of air. Hence, methane flow swirled with the air immediately after entering the domain. A high concentration of methane was found surrounding the liquid spray of ammonia, mixing with evaporated ammonia. The experiment did not observe that part of the methane burnt at the preheated zone heating the spray. No fuel recirculation was found in the simulated cases.

3.2.2 Discrete phase profile

The particle tracks in Fig. 3.6 show that the nominal 90° hollow-cone injection contracts into a narrow, elongated liquid core under the action of the central swirling flow. Both numerical approaches predict a penetration of approximately 40 mm, compared with 24.5 mm experimentally [69]. The similarity of the PDF and EDC penetration values indicates that changing the combustion closure does not correct the liquid-phase error. Instead, the result points to the common DPM injection, breakup and

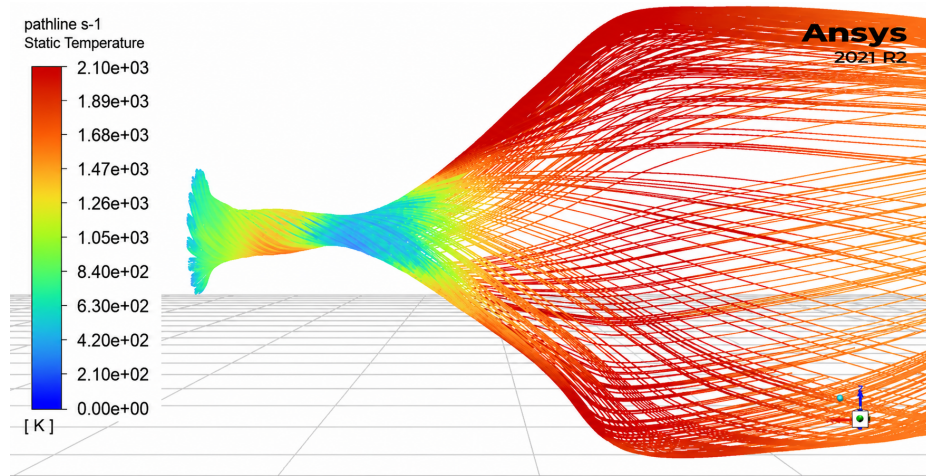


Figure 3.5: Streamlines coloured by temperature for EDC approaches

evaporation assumptions. Experimental studies of superheated ammonia identify the condition as flare flashing, in which bubble growth, rapid phase change and internal energy conversion strongly affect the initial spray expansion [50]. Because these mechanisms are absent here, the simulated droplets retain excessive axial momentum and liquid lifetime. The predicted narrow core should therefore be interpreted as a model artefact that also explains the downstream concentration of ammonia vapour.

The discrete-phase results consequently provide a failed-but-informative validation outcome. They demonstrate that the surrounding swirl field can redirect the injected parcels, but they do not reproduce the experimentally observed disappearance of the liquid phase. This distinction is important because apparently plausible parcel trajectories do not establish that evaporation rate, droplet size evolution or vapour release location are accurate.

3.2.3 Temperature profile

Figure 3.7 shows a marked dependence of the simulated temperature field on the combustion closure. The PDF solution confines reaction to a thin methane–air mixing layer, whereas the EDC solution predicts hot products and radicals recirculating towards the inlet. No experimental temperature measurements are available for this comparison, and the EDC temperature solution did not reach full convergence. The temperature contours are therefore used only to examine differences between the two numerical treatments and are not included in the model validation.

The cold axial region is coupled to the excessive liquid penetration identified above. Droplets that survive too far downstream continue to absorb sensible and

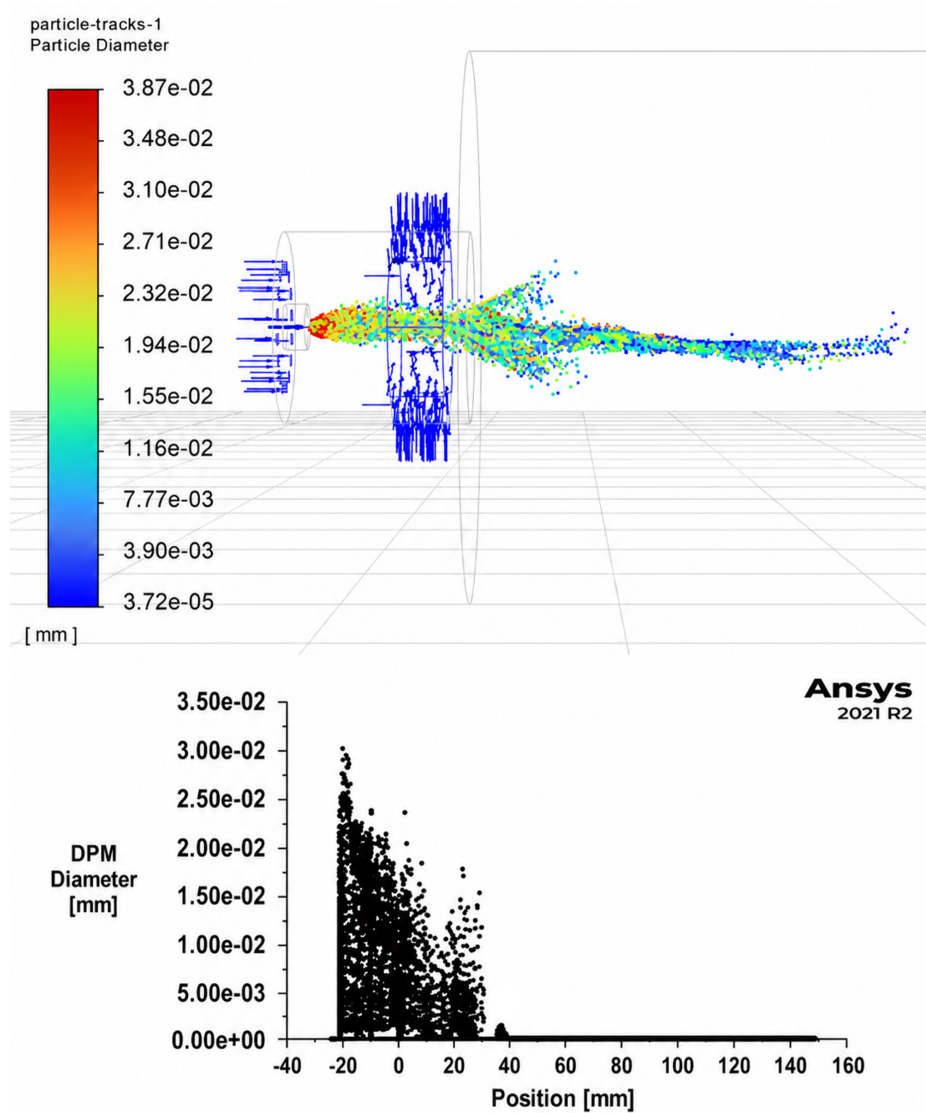


Figure 3.6: (a) DPM particle tracks coloured on particle diameter; (b) particle diameter regarding x-axis for EDC approaches

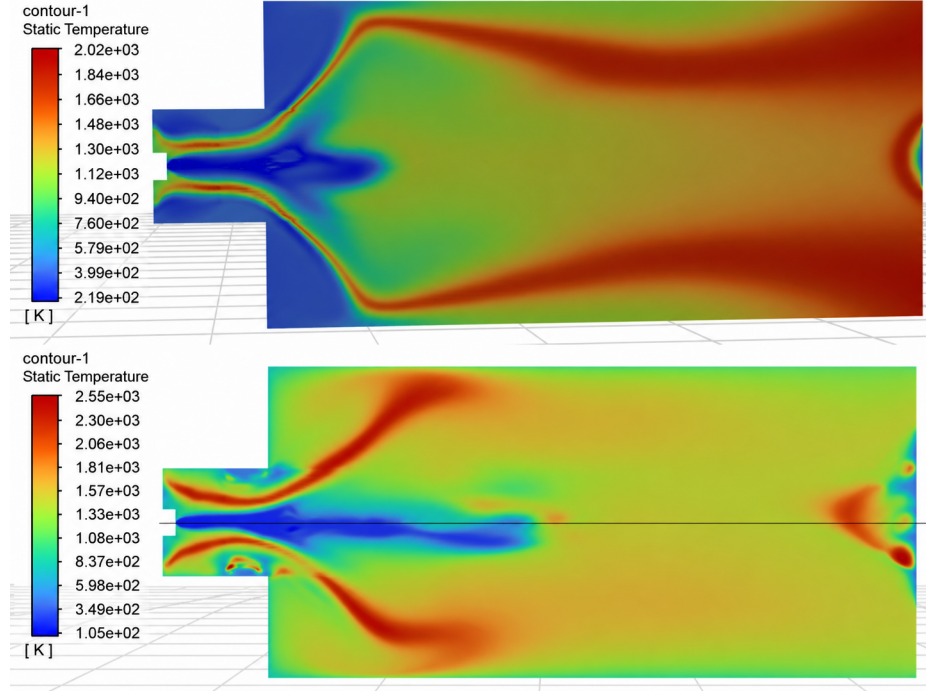


Figure 3.7: Temperature profile on the plane across the axis for PDF (upper) and EDC (lower) approaches

latent heat along the centreline, while delayed vapour release limits premixing with the hot swirling air. Consequently, part of the predicted temperature non-uniformity is a propagated spray-model error rather than an independent combustion-model result. The high outlet temperature is consistent with delayed oxidation of fuel-rich products, but quantitative assessment of this behaviour would require converged energy and species fields together with measured temperatures or exhaust compositions.

3.2.4 Species profile

In Fig.3.8, various species distribution can be observed in EDC approach results. CH_4 was burning rapidly at the preheating zone, while NH_3 evaporated until the reacting zone. The mixing of two fuels was behaving poorly in current cases due to the low vaporizing rate of the liquid phase. $\text{O}/\text{H}/\text{OH}$ radicals reacted with CH_4 creating radical pools and preheating temperature for ammonia. Through the mechanism file, the featured reaction $\text{CH}_3 + \text{NO}_2 = \text{CH}_3\text{O} + \text{NO}$ was not considered, but only $\text{NO} + \text{HO}_2 \rightarrow \text{NO}_2 + \text{OH}$ in the reduced mechanism [65, 23]. The four C/N interaction reactions of the utilized mechanism were $\text{CH}_3 + \text{NO} \rightarrow \text{HCN} + \text{H}_2\text{O}$, $\text{CH} + \text{N}_2 \rightarrow \text{HCN} + \text{N}$, $\text{CH} + \text{NO} \rightarrow \text{HCN} + \text{O}$, and $\text{HCN} + \text{O} \rightarrow \text{NH} + \text{CO}$. The HCN

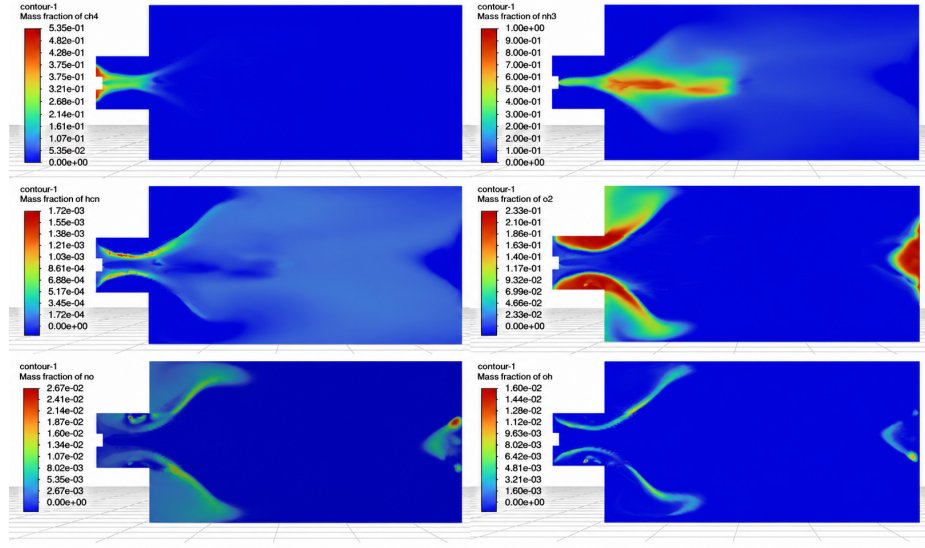


Figure 3.8: $\text{CH}_4/\text{NH}_3/\text{HCN}/\text{O}_2/\text{NO}/\text{OH}$ mass fraction distribution on cross-axis plane for EDC approaches

contour in Fig. 3.8 shows a low mass fraction in the reaction zone. The O_2 mass-fraction field provides an indication of the local equivalence ratio: lean conditions occur in the corner flow and where the fuel and air streams intersect in the preheat zone. The predicted NO distribution is therefore consistent with the fuel-lean regions discussed by Zhang et al. [109]. Regions of high OH concentration also correspond closely to regions of high NO concentration, consistent with the positive sensitivity of NO formation to the reaction $\text{H} + \text{O}_2 = \text{O} + \text{OH}$ [23].

No experimental species measurements are used to validate the fields in Fig. 3.8. The contours are discussed only to interpret the internal behaviour of the numerical model. The coincidence of OH -rich regions with NO formation follows the temperature-sensitive oxidation pathways represented by the reduced mechanism, while HCN formation in locally fuel-rich regions follows the included C/N reactions. The mechanism itself has been reported to underpredict NO by approximately 40% near $\phi = 0.9$ and to misrepresent the NO maximum under richer conditions [75]. Uncertainty is further increased by incomplete convergence and by the overpredicted liquid penetration, which shifts the local equivalence-ratio field and hence the predicted NH_3 , HCN and NO distributions. These contours identify modelled reaction zones and coupling mechanisms but cannot be used to claim accurate emission levels.

3.2.5 Integrated discussion and uncertainty assessment

Taken together, the experimental comparisons reveal two different validation outcomes. The mean gas-flow structure shows qualitative agreement sufficient to identify the main recirculation zones and distinguish the PDF and EDC responses, whereas the liquid-spray behaviour fails the quantitative penetration test. Temperature and species are outside the validation scope and remain dependent on both the predicted flow and the inaccurate liquid-spray behaviour. Consequently, qualitative agreement in the PIV comparison cannot be used as evidence that the complete reacting-spray model is validated.

The comparison between the PDF and EDC cases is nevertheless informative. The EDC treatment substantially changes heat release, gas acceleration and recirculation, while both cases retain a similar liquid penetration. This separation indicates that the excessive penetration is not primarily caused by the combustion closure. It originates from assumptions shared by both cases: the prescribed droplet size and cone angle, conventional KH–RT breakup, equilibrium-type evaporation behaviour and the absence of flash-induced radial momentum. Conversely, differences in the downstream temperature and species fields can be attributed to an interaction between the combustion closure and the common error in vapour delivery.

The principal error begins with the underprediction of flashing, which produces an excessive liquid lifetime and axial penetration. Vapour release is consequently delayed and concentrated along the centreline, biasing the local equivalence ratio and evaporative cooling. These errors then propagate to the predicted temperature, radical concentrations and emissions, increasing the uncertainty associated with the reacting-flow results. This causal chain explains why improving only the chemical mechanism or turbulence parameters would not be sufficient. A more accurate chemistry model would still react with an incorrectly distributed fuel field, while local mesh refinement would not recover the missing thermodynamic mechanism responsible for rapid flashing and spray expansion.

Other numerical uncertainties remain relevant. The minimum mesh orthogonal quality of 0.18 and the absence of a dedicated mesh-independence assessment for this combustor case reduce confidence in small vortices, shear-layer thickness and local scalar gradients. Incomplete convergence of the EDC energy and species equations further limits comparisons of peak values. These limitations are less likely to explain the full 63% penetration error because both combustion approaches produce a similar penetration despite markedly different reacting-flow fields. They may, however, affect

the detailed recirculation topology and the locations of predicted temperature and species maxima.

The resulting domain of credibility is therefore deliberately limited. The model is suitable for identifying the principal combustor flow paths, examining qualitative coupling between swirl and fuel delivery, and diagnosing which missing spray processes dominate the disagreement. It is not yet suitable for predicting absolute liquid penetration, evaporation completion, peak temperature or exhaust emissions. Establishing that broader predictive capability would require, at minimum, a mesh and time-step sensitivity study, converged reacting solutions, implementation of the flashing-evaporation treatment developed in Case Study II, and quantitative comparison with velocity profiles, temperature measurements and outlet species data.

3.3 Conclusion & Future Work

Based on the experimental configuration, this case study developed CFD simulations of ammonia–methane co-firing in a gas-turbine combustor. It established the combustor geometry, hybrid mesh, and a coupled CFD framework comprising turbulence, DPM and EDC combustion models. Flash-boiling evaporation was not included at this modelling level; this limitation provides the direct link to the Lagrangian and Eulerian flashing-spray studies presented in Chapters 4 and 5. The principal conclusions are as follows:

- The RNG k – ε framework reproduces the principal recirculation and shear-layer topology observed experimentally. The EDC solution gives closer qualitative agreement than the PDF solution, but the absence of matched velocity profiles prevents quantitative validation of velocity magnitude and recirculation strength.
- Liquid penetration is overpredicted by approximately 63%, from 24.5 mm experimentally to approximately 40 mm numerically. Because this error is similar for the PDF and EDC approaches, it is attributed primarily to their common DPM injection and evaporation treatment rather than to the combustion closure.
- Temperature and species fields are excluded from validation because corresponding experimental measurements are not available for the simulated case. They are retained only for discussion of the numerical model and remain affected by incomplete convergence, chemical-mechanism uncertainty and the inaccurate vapour-release distribution.

The overpredicted liquid penetration and concentrated ammonia distribution demonstrate that combustor-scale predictions depend strongly on the representation of superheated injection. Chapter 4 therefore examines finite-rate flashing evaporation within a Lagrangian framework, while Chapter 5 resolves cavitation and compressible phase change using the VOF–HRM approach. Together, these subsequent case studies address the principal spray-physics limitations identified here.

Chapter 4

Case Study II: Lagrangian modelling of ammonia flashing sprays

This case study applies the Eulerian–Lagrangian methodology described in Section 2.3. It evaluates spray penetration, morphology, droplet statistics and thermal fields across a range of superheat conditions, while also examining the consequences of prescribing the injection state at the nozzle exit.

4.1 Results and discussion

4.1.1 Comparison of penetration with the experimental results

The simulation results obtained with the modified evaporation laws are compared with the experimental measurements of Li et al. [50]. Figure 4.1 shows the spray-tip penetration during the first 1 ms. Here, penetration is defined as the axial distance from the nozzle exit to the furthest point of the 10% intensity contour extracted from the simulated field, consistent with the 10% threshold used in the experimental image processing [50]. This comparison carries methodological uncertainty because the experimental “intensity” is an optical signal and does not uniquely correspond to liquid volume fraction or vapour mass fraction, particularly in the dense near-nozzle region under strong flashing [70, 50]. Using the same threshold in the simulation and experiment nevertheless enables an equivalent macroscopic comparison.

In the simulations, penetration increases monotonically with time. In contrast, Li et al. [50] reported a high initial tip velocity, followed by mild deceleration between

approximately 0.05 ms and 0.3 ms and re-acceleration after 0.3 ms. The initial high-velocity stage is associated with start-of-injection transients in the internal nozzle flow, during which the effective discharge conditions evolve rapidly and cavitation or vapour blockage develops with a delay; these processes depend on injector geometry and operating conditions [97, 21, 24]. The present Eulerian–Lagrangian setup prescribes a constant injection velocity at the boundary and cannot reproduce this transient momentum delivery at the beginning of injection [50].

The deceleration phase observed in the experiment aligns with the onset of intense flash boiling and two phase compressibility effects. Rapid phase change reduces mixture density, enhances radial expansion, and modifies interfacial momentum exchange, which decreases the axial momentum available for tip advancement [59, 48]. Evaporation waves and shock related structures have been reported in rapidly depressurised flashing jets and can alter the near-field pressure gradient and velocity field that govern penetration [95, 12, 47]. These wave dynamics mechanisms are not resolved in a point particle Lagrangian framework coupled to an incompressible carrier-phase description [48, 95]. The mismatch in beginning of penetration curvature is therefore attributed primarily to missing near-nozzle compressible two phase physics rather than to parameter choices alone.

For the superheated cases $R_p = 2, 5$ and 10 at $T_{\text{inj}} = 338$ K, Fig. 4.1 shows that the predicted penetration lies within the reported experimental uncertainty [50]. For $T_{\text{inj}} = 308$ K, penetration is slightly overpredicted. This bias is associated with uncertainty in the momentum boundary condition at the lower temperature and ambient pressure, because the injection velocity was not independently measured or recalibrated for this condition [50]. The prescribed droplet-size distribution also affects inertia and evaporation time scales and can shift penetration under otherwise similar macroscopic conditions [4]. Microscopic measurements show that characteristic diameters and distribution widths vary with operating conditions [56]. The 308 K discrepancy is therefore treated as combined sensitivity to the injection momentum and size-distribution specification, rather than as evidence of an evaporation-rate error alone.

4.1.2 Rosin–Rammler distribution parameters

Because the particle-history output is parcel-based, unweighted statistics represent the distribution of computational parcels rather than that of physical droplets. This study therefore computes droplet-number-weighted statistics using the particle number in parcel (PNIP), and mass-weighted statistics using the parcel mass. These

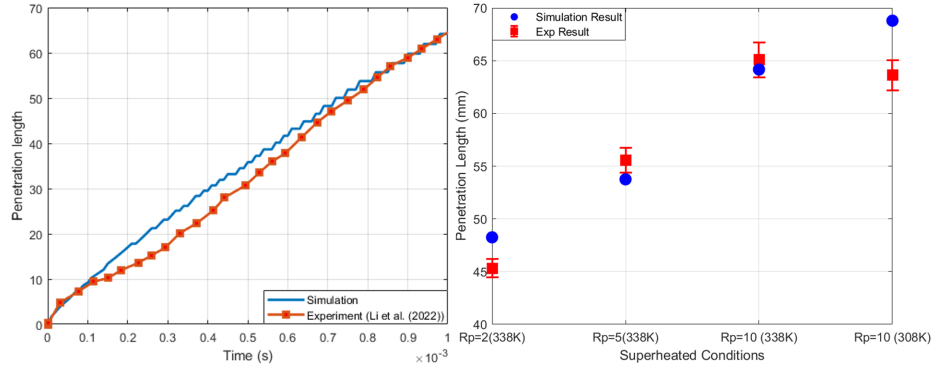


Figure 4.1: Comparison of measured and predicted spray penetration after the start of injection (ASOI) under different superheat conditions.

weights provide physically meaningful diameter distributions and derived metrics, including D_{v10} , D_{v50} , D_{v90} and D_{32} . Figure 4.2 shows substantial differences between the unweighted and PNIP-weighted histograms, demonstrating that weighted post-processing is required for droplet-scale interpretation.

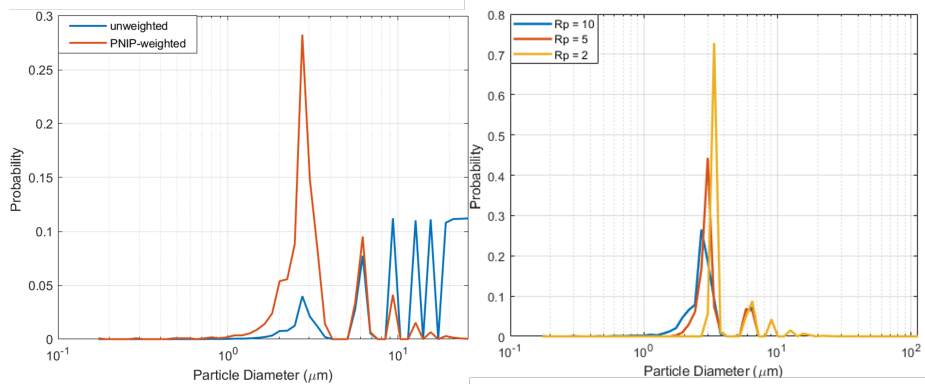


Figure 4.2: Comparison of unweighted and PNIP-weighted droplet-size probability distributions at $T_{inj} = 338$ K and $R_p = 10$, and PNIP-weighted distributions for different values of R_p .

Previous numerical studies on ammonia sprays have shown that the initial droplet size distribution significantly influences the spray characteristics under flash boiling conditions[4]. They found that the shape parameter exerts the most pronounced influence on the spray morphology of superheated liquid ammonia[56]. When the characteristic diameter is small, the calculated penetration distance is greater. The shape parameter exhibits a positive correlation with penetration distance. As the shape parameter increases, the peak of the particle size distribution shifts towards larger diameters and becomes more concentrated. Overall, spray penetration increases with enhanced shape parameter. The influence of the maximum particle diameter is

comparatively weaker. Under the current settings, most droplets are relatively small, thus the upper limit of maximum diameter contributes little to spray morphology.

For the present Eulerian–Lagrangian modelling strategy, penetration-based validation alone cannot uniquely constrain the injected particle-size distribution. Different combinations of Rosin–Rammler parameters may reproduce similar penetration histories while implying different droplet inertia, evaporation rates and two-way-coupling source distributions. Although the present operating conditions ($T_{\text{inj}} = 338$ K and $P_{\text{inj}} = 30$ MPa) differ from those of Liu et al. [56] ($T_{\text{inj}} = 300$ K and $P_{\text{inj}} = 40$ MPa), their reported parameter ranges provide useful bounds for assessing the plausibility of the prescribed distribution. The shape parameter used here is substantially smaller than the experimentally inferred range, producing a broader diameter distribution with a heavier large-droplet tail and potentially greater penetration because of the higher inertia of the surviving droplets.

The right-hand panel of Figure 4.2 compares the size distributions at different values of R_p . The evaporation model captures the shift of the modal diameter towards smaller values as the degree of superheat increases, consistent with the experimental observations [56]. However, it does not reproduce the measured changes in distribution width. This discrepancy is consistent with using fixed Rosin–Rammler injection parameters, whereas microscopic measurements indicate that both the characteristic diameter and spread parameter vary with operating conditions [56]. Quantitative validation of the predicted droplet distribution will therefore require injection parameters obtained under matched operating conditions.

4.1.3 Comparison between different superheated conditions

Figure 4.3 compares the spray morphology at $t = 0.001$ s for (a) $R_p = 10$, (b) $R_p = 5$ and (c) $R_p = 2$. The Rosin–Rammler injection parameters are identical in all cases; the differences are therefore attributed mainly to the thermodynamic driving force for flashing. The spray narrows as R_p decreases. At $R_p = 10$, the plume has the greatest radial spread and the most diffuse outer boundary. At $R_p = 5$, its radial extent decreases, indicating weaker flash-induced expansion. At $R_p = 2$, the spray most closely resembles a single-phase jet: the apparent cone angle is smallest, the boundary is sharpest and the core is most strongly aligned with the centreline. The accompanying increase in ambient pressure also reduces axial penetration.

The systematic narrowing with decreasing R_p reflects the reduction in flash-boiling intensity as the superheat driving force decreases. At higher R_p , early nucleation and rapid vapour growth increase radial velocity and widen the plume. As R_p approaches

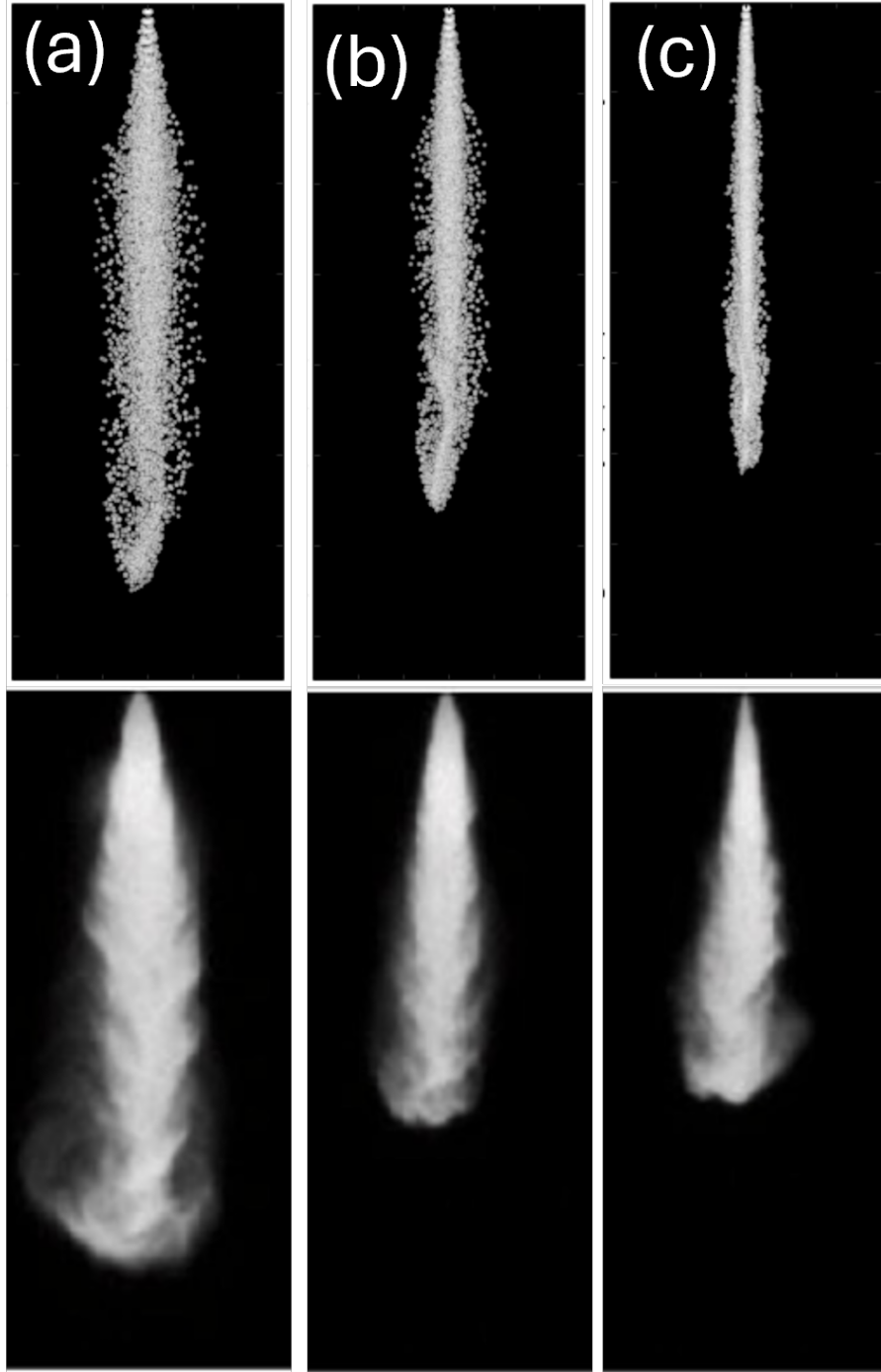


Figure 4.3: Comparison of numerical spray morphology (top) for $R_p =$ (a) 10, (b) 5, and (c) 2 with the corresponding experimental images from Li et al. (bottom) at $t = 0.001$ s under the same operating conditions [50].

unity, phase change weakens and the flow becomes increasingly governed by the imposed injection momentum. The simulated spray-angle trend does not reproduce the non-monotonic variation reported by Li et al. [50]. This discrepancy is consistent with the omission of compressible two-phase near-nozzle physics, which can strongly affect the spray angle under flash-boiling conditions [48, 95]. In the simulations, small droplets surround the main spray core because they are readily dispersed by the gas flow and rapidly lose momentum through drag. Their absence from the experimental images may partly reflect the spatial resolution and threshold used in the optical processing [50]. The simulated tip is also sharper than the rounded experimental envelope. This difference indicates that the prescribed injection distribution and the absence of a dedicated flash-induced breakup treatment do not fully represent formation of the experimental spray tip.

4.1.4 Particle size distribution analysis

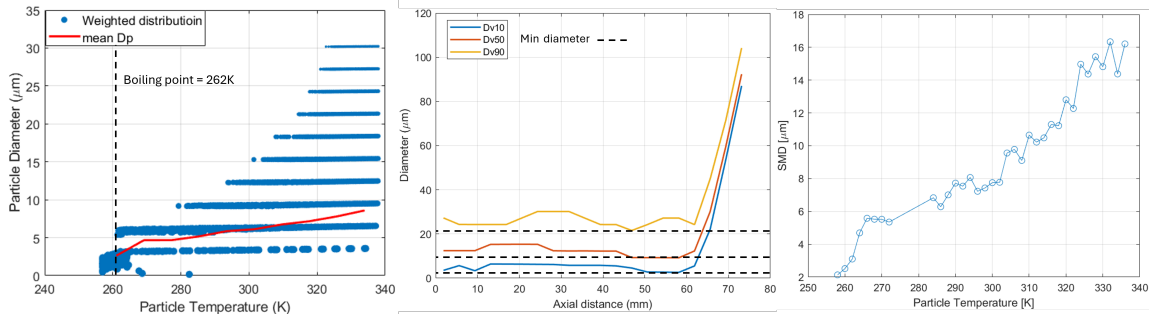


Figure 4.4: (a) Droplet temperature–diameter distribution, (b) Sauter mean diameter as a function of temperature and (c) axial distributions of D_{v10} , D_{v50} and D_{v90} for $T_{\text{inj}} = 338$ K and $R_p = 10$.

Figure 4.4 shows the relationship between droplet temperature T_p and diameter D_p . The curve is calculated using droplet number weighting based on the PNIP, where each parcel is weighted by the number of physical droplets it represents.

The PNIP-weighted D_p – T_p distribution shows a monotonic increase in conditional mean diameter with temperature. This suggests that higher-temperature droplets have larger diameters. However, D_p – T_p is a conditional statistic influenced by sampling and survivorship. Small droplets evaporate rapidly or fall below tracking thresholds, whereas larger droplets persist for longer. The high-temperature subset is therefore biased towards larger, longer-lived droplets, producing a positive D_p – T_p correlation even though individual droplets shrink.

This interpretation aligns with the axial evolution of volume based percentile diameters. Over 0-30 mm, $Dv_{10}/Dv_{50}/Dv_{90} = 6.28/12.45/24.30 \mu\text{m}$. Over 30-50 mm, these decrease to $5.78/12.26/21.31 \mu\text{m}$, and over 50-75 mm they further reduce to $2.72/9.28/21.31 \mu\text{m}$. The decrease in Dv_{10} and Dv_{50} indicates net size reduction, while the constant Dv_{90} beyond 30 mm reflects the persistence of a large droplet tail. Shrinking median diameters combined with a stable upper percentile are consistent with a survivorship biased $D_p T_p$.

The D_p - T_p map also shows horizontal bands, indicating discrete diameter classes. This pattern arises from parcel-based injection, in which a Rosin-Rammler distribution is represented by a finite number of sampled diameters. Consequently, the appearance of the scatter plot depends on the sampling density. Comparisons between evaporation models should therefore use weighted density maps or percentile diameters (Dv_{10} - Dv_{90}) rather than unweighted point clouds. These effects explain why a trend produced by a Zuo-type model may resemble behaviour attributed to Langmuir-Knudsen regularisation. A monotonic D_p - T_p relationship can arise from the preferential loss of small droplets and discrete sampling without any change to the interfacial mass-flux formulation.

The SMD increases with droplet temperature more rapidly than the arithmetic mean radius, indicating that the temperature size distribution evolves primarily via changes in the large droplet tail rather than through a uniform shift of the entire distribution. This suggests that a small fraction of high inertia droplets disproportionately contributes to surface-area-weighted statistics at higher temperatures, consistent with survivorship bias under flashing dominating conditions.

Figure 4.5 shows the axial evolution of particle Sauter mean diameter (SMD), mean velocity and mean temperature. Panels (a), (d) and (g) show that the SMD initially increases and subsequently decreases in all three cases. The initial increase is attributed to preferential evaporation of smaller droplets, which reduces their number and shifts the mean of the surviving population towards larger diameters. Farther downstream, evaporation of the larger droplets produces a decrease in SMD. Unlike simulations with explicit flash-induced breakup, the present evaporation-dominated model therefore predicts an initial statistical increase rather than physical droplet growth. Near the downstream boundary, the surviving high-inertia droplets dominate the sampled size statistics and cause a further rise in SMD.

Panels (b), (e) and (h) show that the mean droplet velocity decreases downstream in all three cases because aerodynamic drag removes particle momentum. The similar deceleration rates are consistent with the broadly similar SMD distributions. Panels

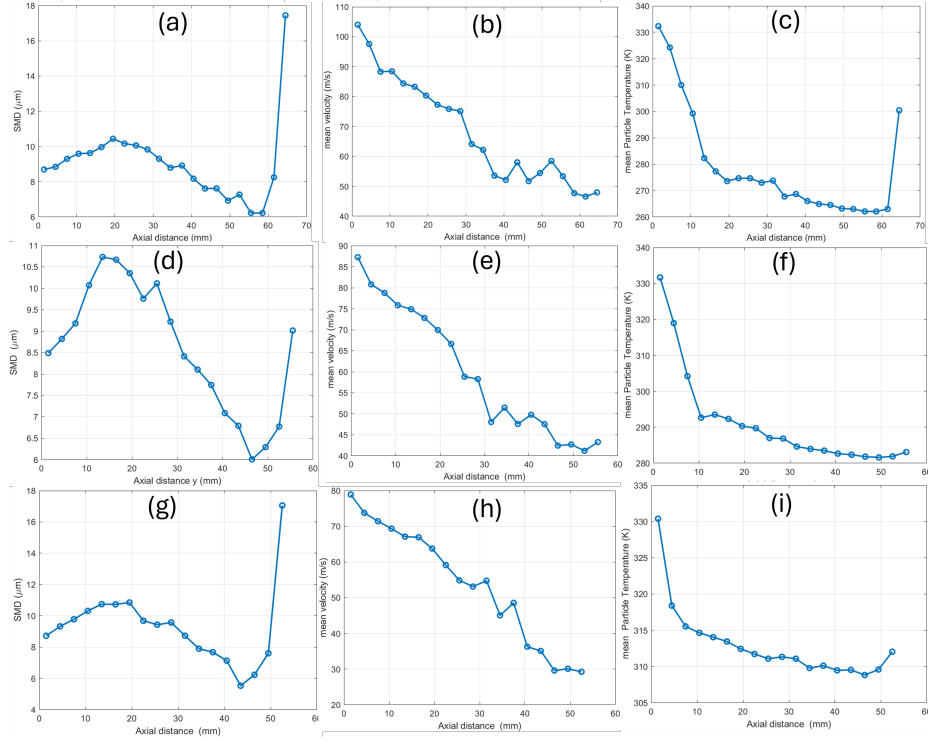


Figure 4.5: Axial evolution of (a), (d) and (g) particle Sauter mean diameter; (b), (e) and (h) mean velocity; and (c), (f) and (i) mean temperature for $R_p = 10, 5$ and 2 .

(c), (f) and (i) show a corresponding reduction in mean droplet temperature. Initially, convection and flashing evaporation act simultaneously; flashing then dominates as the droplets cool; finally, after the thermodynamic driving force has weakened, the remaining droplets exchange heat more slowly with the ambient gas. This staged behaviour is consistent with the finite-rate flashing treatment used in the simulations.

4.1.5 Spray continuous field analysis

Figure 4.6 shows side-view temperature fields for different superheat conditions at $t = 0.001$ s. The maximum temperature occurs near the nozzle exit, where the injected droplets have their highest sensible enthalpy, whereas the strongest cooling occurs farther downstream. Cases (a) and (b) share $R_p = 10$ but differ in T_{inj} and P_{amb} ; their comparison therefore includes the effects of absolute pressure, gas density and thermal buffering as well as the pressure ratio. The higher injection temperature produces a larger high-temperature region around the spray core. Comparing cases (a), (c) and (d), the low-temperature region shrinks as the degree of superheat decreases. The predicted temperature field therefore varies systematically with R_p . Local low-temperature regions are observed along the liquid core because of intense droplet

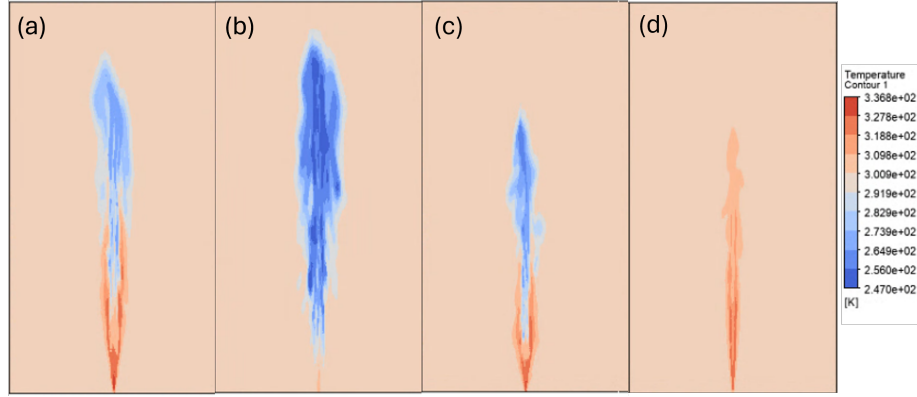


Figure 4.6: Comparison of spray temperature fields under different superheat conditions: (a) $T_{\text{inj}} = 338$ K and $R_p = 10$; (b) $T_{\text{inj}} = 308$ K and $R_p = 10$; (c) $T_{\text{inj}} = 338$ K and $R_p = 5$; and (d) $T_{\text{inj}} = 338$ K and $R_p = 2$.

evaporation near the centreline.

Cooling begins near the centreline and extends radially outwards. This differs from An et al. [4], who reported a relatively warm Eulerian core surrounded by a flash-induced low-temperature region. The discrepancy may arise from differences in the evaporation-model implementation and the prescribed Rosin–Rammner droplet-size distribution.

4.2 Conclusion

In this numerical study, the spray and thermal characteristics of flash-boiling liquid-ammonia sprays were investigated using an Eulerian–Lagrangian framework in ANSYS Fluent. The simulations accounted for droplet transport and breakup and employed a non-equilibrium evaporation model to represent coupled heat and mass transfer under flashing conditions. The predicted spray morphology and tip penetration showed reasonable agreement with experimental measurements across a range of superheat conditions, supporting the validity of the numerical framework at the macroscopic level.

The simulated ammonia sprays exhibited characteristic flashing behaviour, including rapid radial expansion and large cone angles after discharge into a low-pressure environment. The model captured intense phase change and the associated cooling, with the temperature reduction beginning near the spray centreline and extending radially outwards. In contrast to previous studies using the Zuo model, which reported a high-temperature Eulerian core surrounded by a flash-induced low-temperature re-

gion, the present results show localised low-temperature zones along the liquid core, indicating that strong evaporation is concentrated near the centreline. This discrepancy highlights the sensitivity of the predicted thermal fields to the implementation of the evaporation model and the prescribed Rosin–Rammeler injection distribution.

The assessment of the superheat ratio (R_p) indicates that the thermal field is strongly governed by the thermodynamic state. As the superheat driving force decreases, the low-temperature region surrounding the spray core contracts. Under higher-superheat conditions, more vigorous flashing promotes atomisation and distributes cooling over a wider region. Accordingly, the droplet-velocity and size statistics vary with the thermodynamic conditions, while evaporation governs the downstream evolution of the dispersed phase.

In summary, the implemented non-equilibrium evaporation treatment reproduces key macroscopic and microscopic features of flashing ammonia sprays, including the characteristic central low-temperature distribution. Future work will extend this framework to combustor-relevant geometries with strong swirl and detailed chemical kinetics to quantify ignition delay and NO_x formation in practical gas-turbine environments.

Chapter 5

Case Study III: Cavitation and compressible flash boiling near the nozzle

This case study applies the compressible Eulerian VOF–HRM methodology described in Section 2.4. It resolves the internal and near-nozzle liquid–vapour flow in order to connect nozzle geometry and relaxation-controlled phase change with shock formation, momentum redistribution and the characteristic morphology of flare-flashing ammonia sprays.

5.1 Results and discussion

5.1.1 Validation

Colson et al. [21] measured ammonia sprays over a range of superheat conditions and nozzle length-to-diameter ratios. Their case 1 was non-flashing, cases 2 and 5 were transitional, and cases 3 and 4 were fully flashing. In the simulations, the spray boundary was identified from the maximum gradient of liquid mass fraction. Figure 4 compares the resulting numerical and experimental spray angles. Previous HRM calculations required values of θ_0 between 1×10^{-7} and 1×10^{-4} s to improve angle predictions under different regimes [96]; the present work therefore includes a sensitivity study for cases 4 and 5. As shown in Figure 5, the response to θ_0 is strongest for the 0.15 mm nozzle of case 4 and for the transitional-flashing condition of case 5. The baseline HRM correlation was developed principally for fully flashing high-pressure flows [29], which explains why case 3, with the highest injection pressure and fuel temperature, gives the closest prediction without further adjustment. A value of $\theta_0 = 2 \times 10^{-7}$ s gives the closest near-field angles for cases 4 and 5, although

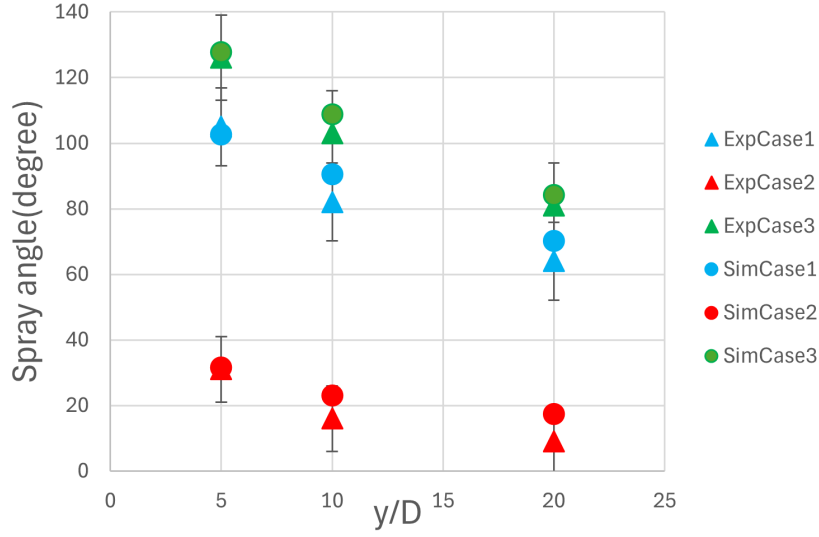


Figure 5.1: Spray angle validation at normalised axial position (5,10, and 20 times of nozzle diameter) compared with experimental results from Colson et al.[11] for cases 1 to 3.

agreement is not exact. The lateral angle remains underpredicted, plausibly because aerodynamic breakup is not represented. The comparison indicates that the original relaxation correlation is less transferable to non-flashing, transitional and very small-orifice conditions than to fully developed flare flashing [22]. Accordingly, θ_0 is treated as a calibrated model parameter rather than a universal ammonia constant.

5.1.2 Distribution of spray parameters

Figure 6 gives a comprehensive description of the spray parameters. For the flashing sprays, a first acceleration and depression happen inside the nozzle, which gives the liquid fuel momentum and bubble nucleation. Then the spray has a second depression outside the nozzle, while the liquid phases undergo a flashing evaporation, expanding the spray angle and evaporating quickly. The liquid phase quickly breaks down into small droplets outside the orifice exit. Then, the accelerating droplets cool down and stop flashing due to high latent heat. The normal shock wave formed inside the spray hinders the central mixture momentum, thus the spray near-field morphology became a ‘bell’ shape. For cases where the nozzle L/R ratio is 5 and 10, the spray exhibited a different flashing stage between non-flashing and flare flashing. For two different nozzle diameters, the spray expanded less in volume. For other initial temperatures (case 1 and case 3), the spray follows the transition flashing behaviour and flare flashing behaviour. Generally, the morphology is similar to the experimental results

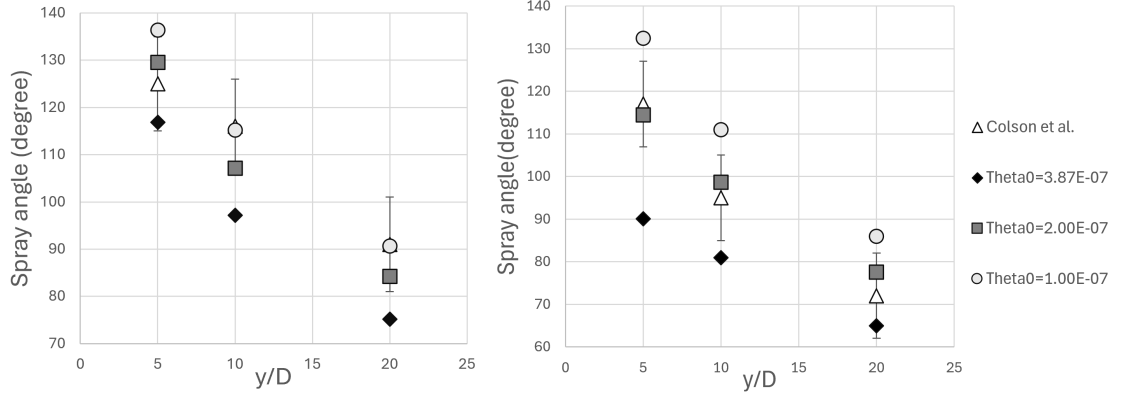


Figure 5.2: The influence of the empirical flashing time constant in Downar-Zapolski [22] HRM model on the spray angle for cases 4 (left) and 5 (right), validated with Colson's results[21].

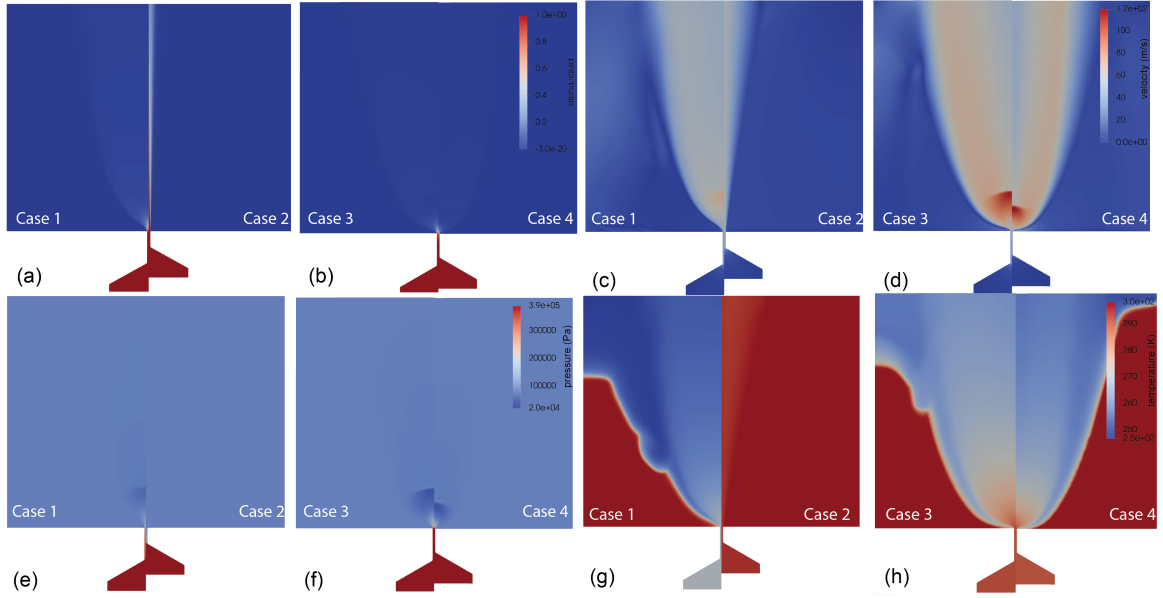


Figure 5.3: Distribution of (a-b) liquid volume fraction (c-d) velocity (e-f) pressure (g-h) temperature for different L/D ratios: case 1 $R_p = 3.8, L/D = 10$ to case 2 $R_p = 9.0, L/D = 5$, and different diameters: case 3 $R_p = 8.2, D = 0.21$ to case 4 $R_p = 7.9, D = 0.15$.

in Colson et al. [21]. The temperature field shows that the liquid phase cools down near the boiling point at the spray edge during the flashing process. Surprisingly, the temperature is higher for case 3 due to a higher initial temperature, which indicates a more violent flashing evaporation. This is also consistent with the higher void fraction found in case 3.

According to equation (9), the flash boiling evaporation time scale constant $/\theta_0$ is partially determined by local pressure. During the flash boiling, the expansion stimulates the evaporation through local static pressure, while the evaporation causes the expansion. The liquid and vapour mixture will eventually cool down to its boiling point or meet the local sound speed.

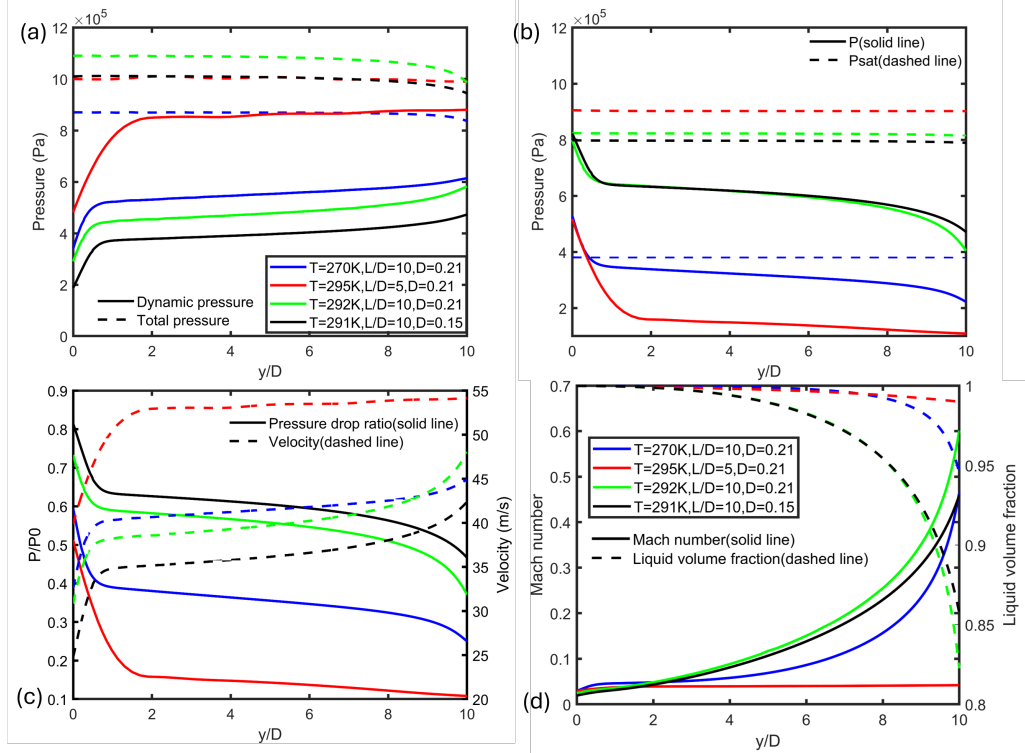


Figure 5.4: Parameters plotted over the nozzle axis: (a) Total pressure and Dynamic pressure, (b) Static pressure and Saturation vapour pressure, (c) Velocity and pressure drop ratio, (d) Mach number and liquid volume fraction.

5.1.3 The influence of superheated and nozzle parameters

5.1.3.1 In-nozzle axis distribution

An analysis of the internal nozzle flow is essential to understand the initial conditions that govern downstream spray development. Figure 7(a-c) presents the axial profiles

of key flow parameters inside the nozzle for all simulated cases. The pressure profiles in Fig. 7(a-b) reveal that for the flashing cases (1, 3, and 4), the static pressure drops below the corresponding saturation vapour pressure. This indicates that the liquid ammonia enters a metastable state within the nozzle orifice, a prerequisite for flash boiling. The observation that the total pressure is approximately the sum of the static and dynamic pressures for a significant portion of the nozzle length suggests the flow remains largely incompressible before the onset of significant phase change. However, for cases 1, 3, and 4, the decrease in total pressure near the nozzle outlet indicates the beginning of two-phase compressible flow. In contrast, the profiles for case 2 with lower L/D are consistent with single-phase, non-flashing behaviour. It is considered by the authors that for the shorter nozzle orifice, due to the hydraulic flip caused by cavitation inside the nozzle, which stabilised the in-nozzle flow leading to less turbulence interaction and less nucleation of small bubble. Therefore, the whole flashing process did not happen like a 'shaken soda water', instead, followed the heterogeneous nucleation process which have a mild vaporisation rate. Notably, even when the static pressure is below the vapour pressure, significant flash boiling does not occur within the nozzle orifice for cases 1, 3, and 4. This phenomenon, where phase change is suppressed, aligns with experimental findings by Wang et al. [97]. They proposed that bubble growth is hindered by in-layer forces, turbulence, and the physical constraints imposed by surrounding bubbles within the confined orifice.

The degree of in-nozzle phase change is strongly influenced by both the nozzle geometry (L/D ratio) and the operating conditions (R_p , injection pressure). The axial profiles of liquid volume fraction, Mach number, and velocity are presented in Fig. 7(c-d). The calculation of the two-phase Mach number required different approaches depending on the flow regime: for the flashing cases (1, 3, and 4), the model is based on Nguyen [63], which is a function of volume fraction, phase density, and the adiabatic sonic velocity for each phase. For case 2, a volume-fraction-averaged sound speed was found to be more suitable. A comparison between case 2 and case 3, which have similar R_p values, shows that evaporation is negligible in case 2. This is attributed to its low L/D ratio (≈ 5), which limits the residence time for bubble nucleation and growth, a conclusion supported by the work of Wu et al. [100]. Consequently, the characteristic two-stage depressurisation of superheated sprays does not occur in case 2. In addition to the aspect ratio, the nozzle diameter itself is influential. Our results show that, unlike a single-phase jet, a larger diameter can cause a more significant pressure loss at the nozzle inlet, leading to a higher outlet volume flow rate; this feature is also observed experimentally by Zhong et al. [111]. Furthermore,

a comparison between the void fraction plots of cases 4 and 3, which share the same R_p and L/D and are simulated with different time scale constants in the HRM model, reveals that the evaporation time constant can be the key difference between flashing sprays in different nozzle diameters.

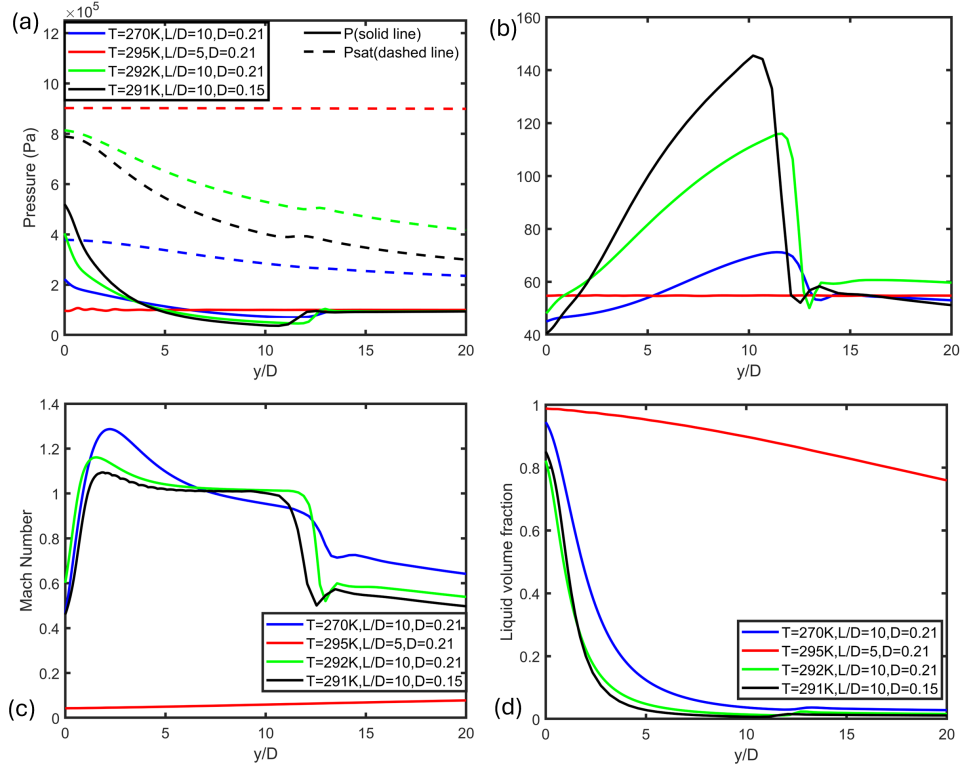


Figure 5.5: Parameters plotted on axial line outside the nozzle: (a) Static pressure and ammonia saturation pressure, (b) Velocity, (c) Mach number, (d) Liquid volume fraction.

5.1.3.2 Out-nozzle axial distribution

Upon exiting the nozzle, the mixture, which was established to be subsonic, undergoes a dramatic transformation in the near-field region as shown by the axial profiles in Figure 8. The flashing cases (1, 3, and 4) experience a vigorous depressurisation process as the fluid expands into the low-pressure ambient environment (Fig. 8(a)). This rapid expansion, fuelled by the intense phase change, converts thermal energy into kinetic energy, accelerating the axial flow significantly (Fig. 8(b)). The combination of this thermal acceleration and the initial exit momentum causes the mixture to exceed the local speed of sound, forming a characteristic under-expanded supersonic jet. This supersonic region, where the static pressure falls well below the ambient

back pressure, is visible for the flashing cases, extending from approximately 4D to 13D downstream.

The subsonic exit condition confirms that the flare flashing jet is not choked at the orifice. Instead, we propose that the flow is hydrodynamically ‘choked’ by a stationary shock wave that forms downstream. This shock wave is evidenced by the abrupt pressure rise and the corresponding sharp deceleration of the flow shown in Fig. 8(c-d). After passing through this shock, the mixture becomes subsonic again, and the pressure begins to recover towards the ambient level. This downstream shock structure, rather than the physical nozzle throat, is what ultimately limits the mass flow rate for the flare flashing regime under these conditions. This mechanism explains the lower-than-expected outlet velocity in cases like case 3, where intense flashing might otherwise be expected to produce even higher speeds.

A comparison of the cases in Figure 8 provides further support for this mechanism. While under similar injection conditions, case 4 accelerates more rapidly and reaches a higher peak velocity than case 3. It is speculated that with a smaller nozzle diameter, the pressure gradient between the nozzle upstream and nozzle orifice is smaller. In contrast, the gradient between the nozzle exit and the ambient environment is steeper, resulting in more intense bubble breakup and evaporation immediately upstream of the shock wave, a finding consistent with Zhong et al. [111]. For the partial flashing spray (case 1), the vaporisation process is slower, providing less energy for expansion and resulting in a weaker acceleration. Notably, while the pre-shock velocities differ significantly across the cases, the post-shock velocities at the centre converge to a similar magnitude, suggesting the shock wave acts as a primary determinant of the subsequent downstream spray centre momentum. This can be explained by the similar injection pressure and ambient conditions in the current cases.

In the near-nozzle region, the expanding and evaporating two-phase mixture can lead to the formation of a normal shock, resulting in a sharp axial velocity reduction downstream. While the axial flow experiences this significant deceleration, the radial velocity, primarily driven by the expansive forces of flash boiling, typically does not reach the local speed of sound at low superheat degrees (low R_p) during flare flashing. Consequently, the central axial velocity of the spray after the shock wave becomes lower than the surrounding flow, contributing to a wider spray angle in the near field. This phenomenon also accounts for the characteristic vortex structures observed during the flare flash boiling stage. The temporal evolution of these large vortices, alongside the lateral shrinking of the single spray liquid plume observed in morphology studies, is governed by the velocity and pressure differentials between the

central and radial mixture flows during flare flashing. Furthermore, experimental results indicate that, consistent with findings by Zhong et al. [111], the presence of the two-phase shock indeed hinders axial momentum transmission. However, the radial velocity does not attain the same Mach number. This complex interplay results in a "feather-shaped" spray morphology, characterised by initial expansion followed by vortex formation and subsequent spray shrinking. At high superheat degrees (high R_p), the surrounding flow exhibits greater displacement, either travelling axially or creating a recirculating area. It is also observed that a reduction in ambient pressure does not further increase the flare flash boiling tip speed [24], owing to choking occurring within the spray centre. In contrast to flare flashing, partial flashing sprays exhibit a higher axial velocity, indicating a less compressible two-phase mixture. However, Case 1 under partial flashing conditions demonstrated a higher Mach number both upstream and downstream of the shock. This is attributed to the lower fuel temperature leading to a reduced local speed of sound (Figure 8). In the model utilised in this study, the influence of decreased sound speed on the Mach number was found to be more significant than differences in local flow velocity, highlighting a critical aspect for model refinement.

For case 2 in Figure 9, the flashing process is barely happening, while surface evaporation is dominating. For the other cases, the effect of superheat degrees can be observed, where case 1 evaporates much more slowly than the others. During the travelling of the spray, the evaporation rate slowly dropped when the evaporation is generally stabilising. Over the selected axial position, the temperature reduction is the highest for case 4, due to the high superheat degree and small nozzle diameter. This also indicates that a small nozzle diameter can induce a more violent nucleation process, enhancing the more intense bubble breakup and evaporation process mentioned earlier. The axial temperature profile in Figure 9 provides additional thermodynamic evidence for the shock structure. During the initial expansion, the mixture temperature decreases sharply due to the latent heat of evaporation. However, as the flow traverses the shock wave, it is rapidly compressed, causing the local temperature to increase slightly due to compressive heating before continuing its gradual decrease. This distinct temperature rise precisely at the location of the pressure jump and velocity drop offers evidence for the existence and location of the two-phase shock wave. The lateral distribution of temperature for case 1, 3, and 4 is shaped like a 'W' similar to Wang et al. [96]'s simulation result and verified in Zhou et al. [112] experimental measurement of flashing temperature field. It is worth noting that temperature values here are mixture temperatures therefore influenced by the droplet temperature except

for the outside diluted part. This explains the 'W' shape in the lateral plot: in the centre of the spray, droplets are surrounded by saturated cold vapour, which slows down the process of evaporation. Meanwhile, on the edge of the spray, droplets are having a great shearing movement and also turbulence mixing with the ambient gas. The droplet surface would have a larger temperature and vapour pressure difference compared with the ambient conditions. Furthermore, the secondary breakup effect can increase the droplet surface area, causing the temperature to be significantly lower than the centre.

Previous study on shape of the flashing spray [12], demonstrates a characteristic radial velocity distribution where the highest velocities are concentrated at the jet's periphery, similar to observations in cases 3 and 4 in Fig. 6. This peripheral velocity emphasis was also reported by Wu et al. [100] at $R_p = 10$ for flashing sprays. They noted that the spray structure resembled that of a pressure-swirl atomiser, characterised by higher radial droplet velocities at the periphery than at the centre, and a negative pressure zone in the core that induces a circulated flow. In this study, this characteristic is attributed to the resistance generated by the two-phase compression shock wave at the spray centre. Experimentally, at low R_p conditions, visualising this shock wave is challenging using methods like schlieren or Diffuse Backlight Illumination (DBI). This difficulty arises because the dense liquid-gas mixture within the spray plume obscures the shock wave. Although the underlying atomization physics differ fundamentally, the observed congruence in flow patterns corroborates the theory of an internal normal shock wave within the spray.

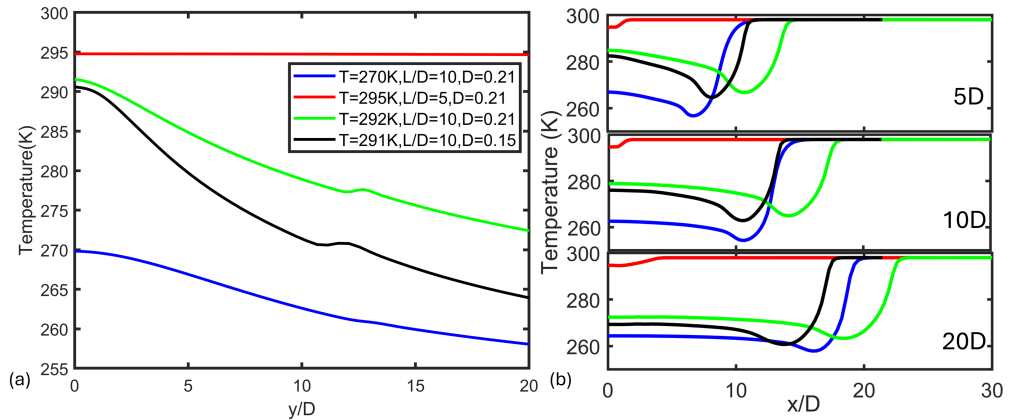


Figure 5.6: Temperature profile of spray parameters outside nozzle at axial location (left) and lateral location on 5D, 10D and 20D locations (right)

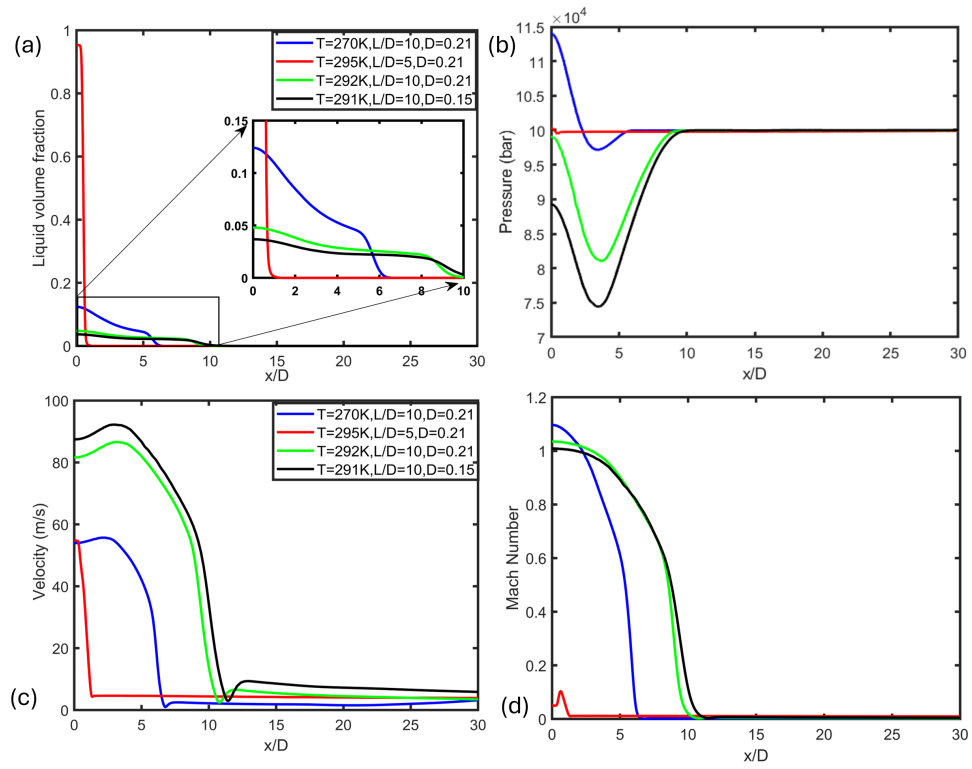


Figure 5.7: Radial profile of spray parameters outside nozzle at 5D (a)liquid volume fraction, (b)pressure, (c)velocity, (d) Mach number.

5.1.3.3 Out-nozzle radial distributions

Figure 10 to 12 present the radial distributions of velocity, pressure, liquid volume fraction, and Mach number at downstream locations of 5D, 10D, and 20D, respectively. At the 5D location (Figure 10), the analysis reveals that the evaporation process is not yet fully initiated for Case 1, as evidenced by a significant liquid core. In contrast, the liquid volume fraction for Cases 3 and 4 is already below 0.1. For all three flashing conditions, the liquid volume fraction is highest at the centerline, a finding that is consistent with the Oblique Evaporation Wave (OEW) theory, which posits that the spray maintains a conical liquid core where an abrupt phase change occurs at the oblique boundary [6]. The extended liquid core observed in Case 1, compared to Cases 3 and 4, is attributed to its lower pressure ratio (R_p). This is further corroborated by the central pressure in Case 1 being considerably higher than the ambient condition (Figure 10b). Furthermore, Figures 8b and 8c reveal that the velocity is marginally lower and the pressure is higher at the spray's centre compared to the outer flow. This phenomenon is a consequence of the turning angle of the oblique evaporation wave, which results in less flow acceleration at the core at the same axial distance. At this same 5D distance, the Mach number for Cases 1, 3, and 4 approaches unity, with the distribution for Case 1 being more concentrated in the axial direction. In contrast, the pressure and velocity distributions for the non-flashing case resemble those of a conventional subcooled spray, which is characterised by a maximum axial velocity at the centerline.

Further downstream at the 10D location (Figure 11), substantial developments in the spray properties are observed. For the flashing cases, the liquid volume fraction is significantly reduced to less than 5%. Concurrently, the pressure at the centerline for Cases 3 and 4 drops to approximately half of the ambient pressure. This pressure reduction is a direct consequence of the rapid expansion from flash boiling, causing the axial front of the mixture to accelerate more rapidly than the lateral portions of the spray. A marked increase in velocity is noted between the 5D and 10D positions; the flare-flashing cases (3 and 4) accelerate by approximately 30 m/s, while the partial-flashing case (1) increases by only 10 m/s. The radial velocity profile is also inverted compared to the 5D location, with the highest velocity now occurring at the centerline. Notably, Case 4 attains the highest velocity at 10D, despite a lower initial nozzle flow rate, due to enhanced atomization from rapid bubble breakup. As seen in Figure 11(d), the mixture Mach number for all flashing sprays reaches unity at the core, indicating that the flow is sonic. However, unlike the flow in a choked single-phase

nozzle, the Mach number here gradually decreases radially and then drops sharply to below 0.5 after passing through a shock wave.

The radial distribution of the liquid fraction is uniform at the 20D position (Figure 12) located downstream of the shock wave, indicating that the flash evaporation process has ended. The pressure here has recovered to ambient conditions. However, a low-pressure and low-velocity region persists at the centerline. This velocity difference is attributed to compressibility effects as the mixture traverses the shock wave. The low-pressure core can lead to vortex formation and spray contraction after the initial injection period. This behaviour is a primary differentiator between flare-flashing sprays and pressure-swirl sprays, the latter of which typically maintain a higher axial velocity. At 20D location in axial, the centerline velocities are similar across all cases. This is due to the controlled equivalent injector flow velocity and similar initial pressures in the experimental setup. The Mach number at this location stabilises at approximately 0.55 and is distributed uniformly in the radial direction.

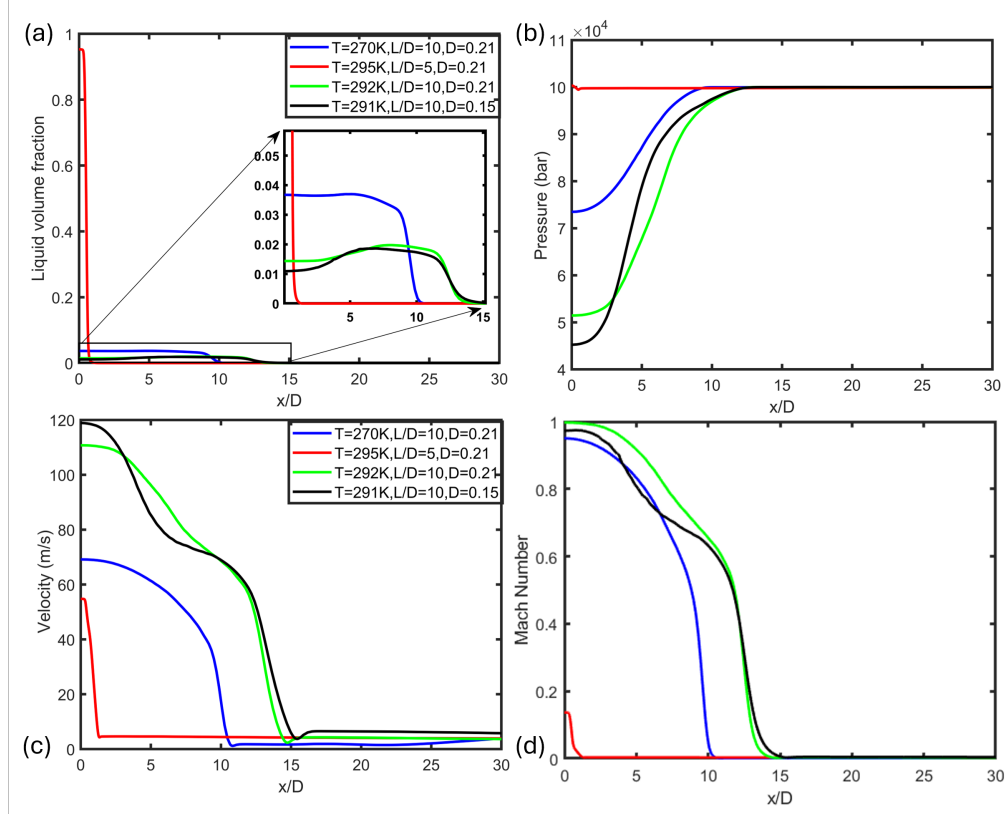


Figure 5.8: Radial profile of spray parameters outside nozzle at 10D (a)liquid volume fraction, (b)pressure, (c)velocity, (d) Mach number.

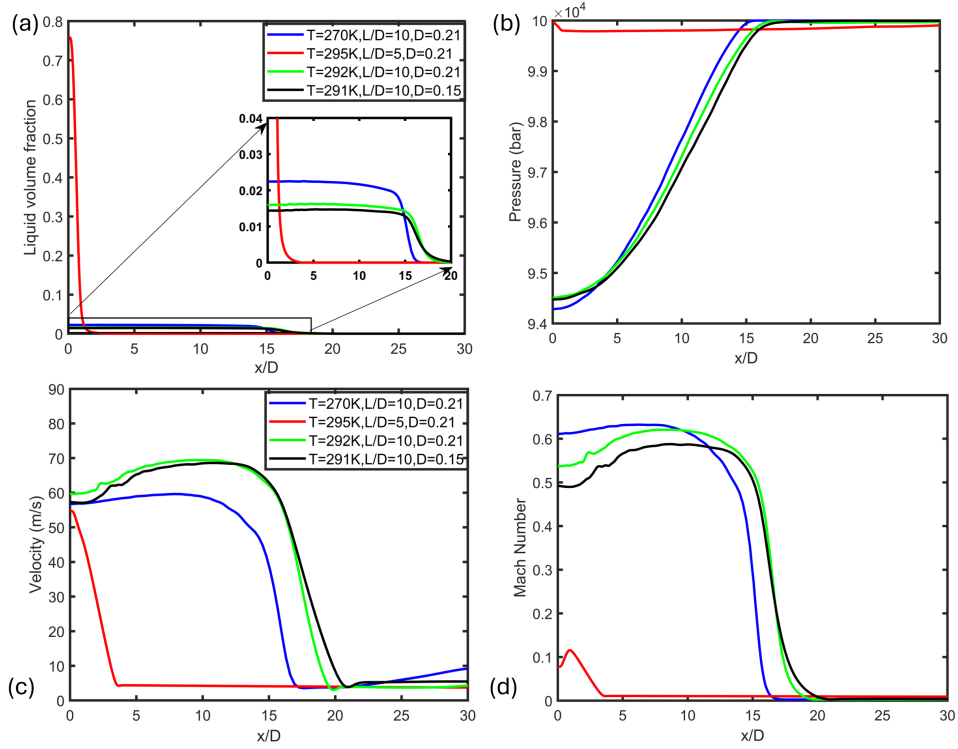


Figure 5.9: Radial profile of spray parameters outside nozzle at 20D (a)liquid volume fraction, (b)pressure, (c)velocity, (d) Mach number.

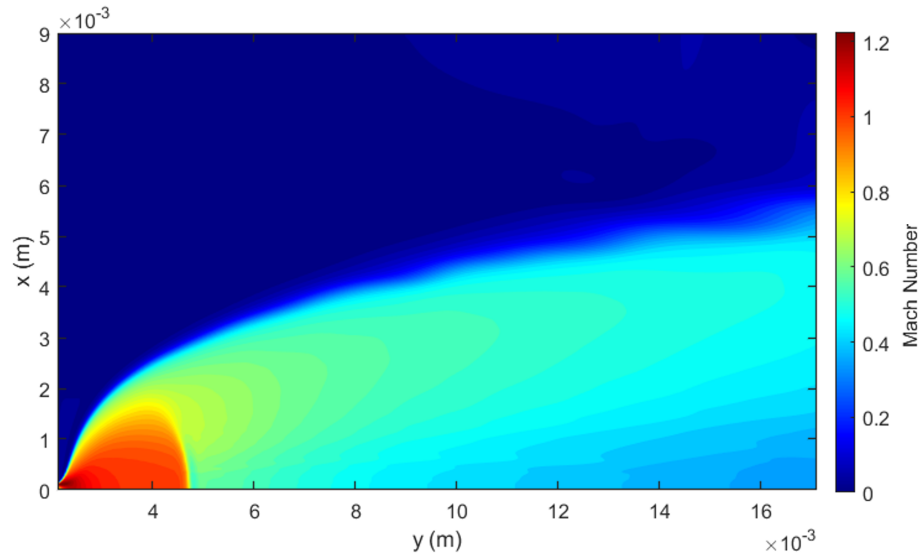


Figure 5.10: Mach number distribution of case 3 based on Wood's equation of mixture sound speed

The link between the internal flow state and the macroscopic spray morphology is visualised explicitly in the two-phase Mach number distribution presented in Figure 13. As established in the analysis of the in-nozzle flow in previous sections, the specific nozzle geometry (L/D) suppresses internal phase change while nucleating bubbles inside the nozzle, delivering a metastable, subsonic liquid jet to the nozzle exit. This subsonic exit condition with highly distributed small bubbles is the critical prerequisite for the external shock structure observed here. Upon exposure to the low-pressure ambient, the metastable liquid undergoes rapid external depressurisation and flash boiling in a homogenous condition through pre-distributed tiny bubbles. Governed by two-phase interface elasticity, the resulting generation of vapour bubbles drastically reduces the local two-phase speed of sound. The homogenous evaporation process drives the flow to supersonic speeds ($Mach > 1$) after the oblique evaporation wave on the liquid core downstream of the orifice. The evaporation wave exceeds the local sound speed and creates a local negative pressure area (compared with ambient pressure) in the supersonic area until it hits the compression shock wave. To restore pressure equilibrium against this high-inertia central core, the stationary shock wave is forced to adapt its topology; the shock front is displaced further downstream along the centerline compared to the edges, resulting in the characteristic arc-shaped geometry rather than a planar front. On the side of this arc-shaped shock, a strong radial velocity component caused by the fast vaporisation cannot reach the local mixture sound speed in their travelling direction due to the variation of phase fraction. Therefore, travelling faster than the spray core after the normal shock wave. It is this shock-induced radial transportation structure that forces the fluid outwards. The difference between outside and inner velocity leads to the 'shrinkage' after the spray tip, which is identified in other experiments and creates the characteristic 'feather-like' spray morphology. Thus, the observed spray structure is verified to be a direct product of the coupling between the subsonic in-nozzle boundary condition and the variable-speed-of-sound gas dynamics in the near field.

5.1.3.4 Analysis of spray dynamics

The distinct effects of injection pressure, initial temperature, and ambient pressure were further investigated by comparing variations against the baseline Case 3 (Figure 13). Increasing the injection pressure (3.00 MPa) postpones the onset of flash boiling, consistent with previous findings [52], resulting in a higher liquid volume fraction downstream of the nozzle. This delayed phase change suggests that the mass

Cases	6	7	8
Injection temperature (K)	292	292	300
R_p	10.5	8.3	10.6
Injection pressure (Pa)	1.09×10^6	3.00×10^6	1.09×10^6
Ambient pressure (Bar)	0.79	1	1
Nozzle diameter (mm)	0.21	0.21	0.21
θ_0 (s)	3.87×10^{-7}	3.87×10^{-7}	3.87×10^{-7}

Table 5.1: Boundary condition of additional cases with L/D ratio 10 and nozzle diameter 0.21mm.

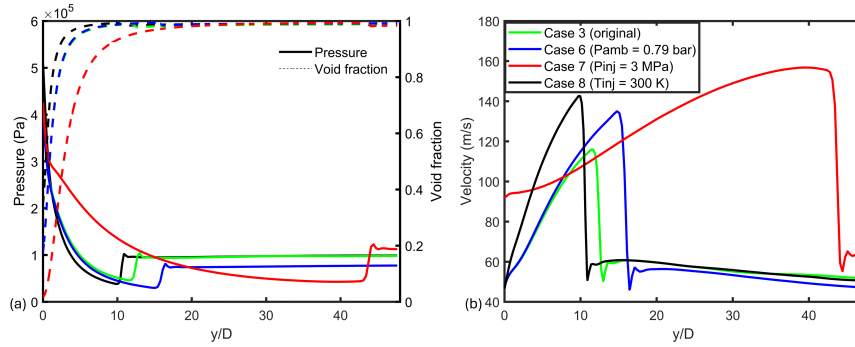


Figure 5.11: Pressure, void fraction, and velocity for cases 6 to 8 compared with case 3.

flow rate in flare flashing is governed by a mechanism distinct from conventional nozzle choking. Conversely, elevating the initial fuel temperature (300 K) accelerates evaporation and increases spray velocity in the initial expansion region, which aligns with observations of increased in-nozzle bubble formation [97]. Interestingly, lowering the ambient pressure (0.79 Bar) to achieve a superheat degree equivalent to the high-temperature case did not yield similar behaviour. Instead, the spray characteristics mirrored the baseline Case 3 until encountering a shock wave at a different position. This comparison demonstrates that the shock wave's location is critically dependent on the pressure differential between the injection and ambient conditions, rather than on the initial fuel temperature alone, consistent with the observation in Zhang et al.[106].

The results of this study demonstrate that the structure of a flashing ammonia spray is dictated by a complex interplay between fluid thermodynamics and nozzle geometry. The HRM time scale constant, which was calibrated to match near-field spray angles at multiple downstream locations (5D, 10D, and 20D), appears to be physically correlated with the bubble nucleation process. Generally, a narrower nozzle diameter was found to promote bubble nucleation, while a shorter aspect ratio (L/D)

nozzle suppressed it. This suppression of in-nozzle nucleation prevents the formation of a strong external shock wave, allowing the metastable liquid to exit the orifice at a higher velocity. The influence of operating conditions on the spray structure is multifaceted. Increasing the injection pressure primarily contributes to the spray’s kinetic energy and penetration, rather than promoting in-nozzle phase change due to the finite time scale of the process. Conversely, while ambient pressure directly influences the position and structure of the downstream shock wave, it has a negligible effect on the internal nozzle flow. The initial fuel temperature governs the overall flashing intensity but has a less direct influence on the shock wave itself compared to other parameters. In summary, this work establishes that the near-field shock wave is the vital, controlling element of the ammonia flashing spray structure. This shock can be precisely manipulated not only by the fuel’s thermodynamic state and ambient conditions but, critically, also by the nozzle geometry, offering a new degree of control over spray atomization and mixing.

5.2 Conclusion

This study investigated numerically using a two-dimensional CFD model coupled with the Homogeneous Relaxation Model (HRM) to reveal the complex physical mechanisms governing the structure of ammonia flash boiling sprays. The influence of nozzle geometry (L/D ratio, diameter) and operating conditions (R_p , injection pressure) on both the in-nozzle flow and the near-field spray development was systematically analysed. The key conclusions are as follows:

- Under flare-flashing conditions, the flow remains subsonic ($M \approx 0.3$) within the nozzle orifice. The liquid ammonia enters a metastable state, but significant phase change is suppressed until after the fluid exits the nozzle, a phenomenon consistent with experimental observations.
- The mass flow rate is not limited by sonic choking at the nozzle throat. Instead, the spray is choked by a stationary, two-phase shock wave that forms in the near-field region downstream of the nozzle. The location and strength of this shock are directly dictated by the in-nozzle exit conditions, which are in turn controlled by the nozzle geometry and operating pressures.
- A shorter L/D ratio or a wider nozzle diameter suppresses in-nozzle bubble nucleation, preventing the formation of a strong shock and leading to a higher

velocity, unobstructed liquid core. Conversely, higher injection pressure increases kinetic energy and spray penetration without significantly altering the in-nozzle flashing, while lower ambient pressure primarily moves the shock front downstream.

- The near-field shock wave is the primary mechanism responsible for the spray's large-scale morphology. By inducing a deceleration and creating a pressure reduction at the spray centerline, the shock transforms the flow field. This low-velocity core, relative to the faster periphery, drives the entrainment of ambient gas and establishes a large-scale recirculating vortex, providing a comprehensive explanation for the characteristic "feather-shaped" morphology.

These findings provide a new framework for understanding flare-flashing atomisation. The realisation that a downstream shock structure controls the flow has implications for the design and optimisation of ammonia fuel injection systems. Controlling the location and strength of the shock wave presents a pathway for controlling the spray angle, penetration length, and ultimately, the fuel-air mixing process, which is crucial for efficient and stable combustion. While this 2D study establishes the fundamental mechanism, future work would extend the analysis to three-dimensional simulations to capture asymmetric instabilities and complex turbulent interactions.

Chapter 6

Conclusion and future work

This thesis examines liquid ammonia injection and spray processes that are central to ammonia gas turbines and other practical combustion systems. While ammonia can be produced and transported at scale, its low reactivity and the presence of fuel bound nitrogen impose stringent requirements on mixture preparation. In particular, the fuel must be atomised, vaporised, and mixed rapidly enough to support stable combustion while limiting emissions, especially NO_x and unburned NH_3 . The work therefore focuses on the coupled roles of superheated thermodynamic state, injector/nozzle conditions, and modelling assumptions in shaping spray morphology, penetration, evaporation driven cooling, and the near-nozzle physics that govern downstream mixture formation.

The thesis is organised as a progression from synthesis to methodology and then to application. Chapter 1 integrates the literature on ammonia combustion, dispersed flashing sprays and near-nozzle cavitation into a single research narrative. Chapter 2 presents the three corresponding numerical frameworks and clarifies their assumptions and ranges of applicability. Chapters 3–5 then apply these frameworks at combustor, dispersed-spray and near-nozzle scales, respectively.

Chapter 3 demonstrates why spray physics is a controlling component of ammonia combustion performance. The combustor-scale CFD model reproduces the principal large-scale swirl structures, including recirculation and shear layers, but also exposes an important limitation. When superheated evaporation and near-nozzle flashing are not represented adequately, the liquid core remains overly concentrated, penetration is overpredicted and the implied fuel–air mixing departs from experimental trends. This result establishes the practical motivation for the two subsequent case studies: reliable combustor predictions require improved representation of the phase change and injection processes that determine the initial dispersion and cooling of liquid ammonia.

Chapter 4 investigates these processes using an Eulerian–Lagrangian framework in a constant-volume chamber, with comparisons against available experimental measurements. Agreement in macroscopic penetration is shown to depend strongly on the prescribed delivery of injection momentum. Calibrated boundary conditions provide reasonable penetration histories over the examined times and distances, although early-time curvature and near-field morphology remain sensitive to compressible two-phase physics that is not explicitly resolved by the point-particle formulation. The study also demonstrates that parcel outputs require physically meaningful weighting. Applying droplet-number weighting through PNIP (Particle Number in Parcel) substantially changes the inferred diameter distributions and derived measures such as percentile diameters and Sauter mean diameter. Conditional trends such as $D_p \mid T_p$ may arise partly from survivorship bias because smaller droplets evaporate and leave the sampled liquid population sooner than larger droplets. The case study therefore distinguishes modelled physical trends from sampling effects and identifies injection boundary specification, near-nozzle compressibility and spray-submodel limitations as the main constraints on quantitative predictiveness.

Chapter 5 addresses the near-nozzle physics directly using a compressible Eulerian two-phase approach in which the volume-of-fluid method is coupled with the Homogeneous Relaxation Model. Under flare-flashing conditions, the simulations indicate that the in-nozzle flow can remain subsonic while the liquid becomes metastable, with the most intense phase change occurring after discharge into the low-pressure environment. The results further suggest that the mass-flow limitation and near-field structure cannot be explained solely by sonic choking at the nozzle throat. Instead, a stationary two-phase shock forms downstream and controls centreline momentum and pressure recovery. Shock-induced deceleration, together with the low effective sound speed of the liquid–vapour mixture, reorganises the flow and provides a mechanism for experimentally observed bell-like and feather-like morphologies. Variations in nozzle L/D and diameter alter residence time and bubble nucleation, thereby changing the nozzle-exit state and the location and strength of the downstream shock. Nozzle geometry is consequently identified as a control parameter for flare-flashing morphology through its influence on metastability, phase change and compressible mixture dynamics.

Taken together, the thesis provides a coherent chain of evidence that links combustor requirements to spray and nozzle physics. It clarifies why ammonia combustion performance depends on the coupled effects of phase change, cooling and near-nozzle momentum redistribution, and it demonstrates how different modelling frameworks

reveal different aspects of this coupling. The work also provides practical lessons for modelling and interpreting ammonia sprays: penetration comparisons are strongly affected by the specification of momentum boundary conditions; droplet statistics extracted from parcel data must be weighted to represent physical populations; and, under strong flashing conditions, compressible two-phase structures can control near-field morphology and centreline momentum.

These conclusions should be interpreted with several limitations in mind. The Eulerian–Lagrangian simulations used for chamber-scale comparisons do not explicitly resolve compressible two-phase wave dynamics, which limits their ability to reproduce early-time penetration curvature and some near-field morphological trends when shock and evaporation-wave physics is important. Injection boundary conditions and effective discharge parameters can dominate macroscopic metrics; without independent information on the in-nozzle state, different calibrations may reproduce the same penetration while implying different droplet-scale fields. The compressible VOF–HRM simulations are primarily two-dimensional and focus on nozzle and near-field physics. Extending these simulations to three-dimensional configurations is necessary to quantify asymmetric instabilities and turbulent interactions that may affect the quantitative results.

Overall, the thesis shows that the reliable modelling and design of ammonia injection systems require the thermodynamic state, injector geometry and compressible two-phase effects to be treated as a coupled problem. When these couplings are represented, the near-field spray structure can be interpreted in terms of identifiable physical mechanisms, providing a basis for more predictive simulations and injector-design choices that support stable, low-emission ammonia combustion.

Future work will focus on applying and optimising the flashing-spray model within the current CFD framework. The injection strategy and combustor geometry will be refined and evaluated through systematic numerical studies. The modelling approach will be extended using both Eulerian–Lagrangian and VOF methods for superheated sprays, with careful validation against experimental measurements. The framework will then be applied to combustor-relevant configurations with strong swirl and detailed chemical kinetics to quantify ignition delay and NO_x formation in practical gas-turbine environments. Finally, the two-phase simulations will be extended to three-dimensional configurations to capture asymmetric instabilities and turbulent interactions.

Appendix A

Flash-boiling law User-Defined Function (UDF) (Fluent Discrete Phase Model, DPM)

A.0.1 Scope and structure

The UDF defines a custom DPM law `Flash_Boiling_Law_Fixed` for a single volatile species (ammonia liquid) in an Eulerian–Lagrangian framework. The mass loss rate is written as the sum of two active contributions,

$$\dot{m} = \dot{m}_{\text{flash}} + \dot{m}_{\text{heat}}, \quad (\text{A.1})$$

The law updates parcel mass, diameter, and temperature during tracking. Gas-phase coupling is applied through a separate DPM source routine that adds evaporated mass and species to the gas and removes latent heat from the gas energy equation.

A.0.2 Local gas and particle quantities

For each tracked parcel, the law uses the local continuous-phase state stored in `tp->cphase[0]`:

- Gas temperature T_g , density ρ_g , viscosity μ_g , thermal conductivity k_g , and specific heat $c_{p,g}$.
- Gas velocity $\mathbf{U}_g$ and particle velocity $\mathbf{U}_p$, giving the relative speed

$$U_{\text{rel}} = \|\mathbf{U}_p - \mathbf{U}_g\|. \quad (\text{A.2})$$

- Particle diameter d_p , mass m_p , density ρ_p , and particle heat capacity $c_{p,p}$.

The Reynolds number is computed as

$$Re = \frac{\rho_g U_{\text{rel}} d_p}{\mu_g}, \quad (\text{A.3})$$

and is clamped for correlation evaluation.

The binary diffusivity D_{bin} is taken from Fluent’s material property macro and clamped to a prescribed range.

A.0.3 Baseline transport correlations

The code uses Ranz–Marshall type baseline correlations for Sherwood and Nusselt numbers,

$$Sh_0 = 2 + 0.552 Re^{1/2} Sc^{1/3}, \quad Nu_0 = 2 + 0.552 Re^{1/2} Pr^{1/3}, \quad (\text{A.4})$$

with

$$Sc = \frac{\mu_g}{\rho_g D_{\text{bin}}}, \quad Pr = \frac{c_{p,g} \mu_g}{k_g}. \quad (\text{A.5})$$

These are then modified by blowing/Stefan-flow corrections described in Section A.0.4.

A.0.4 Surface composition and blowing corrections

A.0.4.1 Gas-side vapour mass fraction Y_∞

The bulk vapour mass fraction is read from the local cell species field,

$$Y_\infty = Y_{\text{NH}_3}(\mathbf{x}_p), \quad (\text{A.6})$$

and clamped to $[0, 1]$.

A.0.4.2 Surface equilibrium mass fraction Y_s

The surface equilibrium is evaluated using an Antoine saturation-pressure relation based on the parcel temperature T_p . The code computes $p_{\text{sat}}(T_p)$, then forms the equilibrium mole fraction $x_s = p_{\text{sat}}/p$, with an explicit cap $p_{\text{sat}} \leq 0.999p$ to avoid $x_s > 1$. The mole fraction is converted to a mass fraction Y_s using species molecular weights.

A second “thermo” variant is computed in the code, but the Antoine-based value is used for the subsequent blowing terms in the current implementation.

A.0.4.3 Mass-transfer driving parameter B_M

The mass-transfer parameter is formed from

$$H_M = \ln\left(\frac{1 - Y_\infty}{1 - Y_s}\right), \quad B_M = \exp(H_M) - 1, \quad (\text{A.7})$$

with explicit limits on H_M and B_M to prevent overflow.

A correction factor F_M is computed as a function of H_M and used to reduce the effective Sherwood number.

A.0.4.4 Heat-transfer blowing parameter B_T and RK3 stabilization

The code defines a factor

$$\phi = \frac{(c_{p,p}/c_{p,g})}{Le}, \quad Le = \frac{\alpha_g}{D_{\text{bin}}}, \quad \alpha_g = \frac{k_g}{\rho_g c_{p,g}}, \quad (\text{A.8})$$

with limits on Le and ϕ .

A target heat-transfer blowing parameter is built from B_M and ϕ . Instead of using the target directly, the code iterates over a log-transformed variable

$$H = \ln(1 + B_T), \quad (\text{A.9})$$

towards its target value using a strong-stability-preserving third-order Runge–Kutta (SSP-RK3) routine (`integrate_BT_RK3`). The RK3 loop includes finite checks, clamping and an early-exit convergence test based on relative change.

A.0.4.5 Corrected Sherwood and Nusselt numbers

The corrected transport numbers are computed by blending toward the baseline form,

$$Sh = 2 + \frac{Sh_0 - 2}{\text{CLAMP}(F_M)}, \quad Nu = 2 + \frac{Nu_0 - 2}{\text{CLAMP}(F_T)}, \quad (\text{A.10})$$

where F_T is a function of B_T . If the corrected values become non-finite, the code falls back to the baseline correlations.

A.0.5 Flash-boiling mass loss $\dot{m}_{\text{flash}}$

The boiling temperature T_b is obtained through Fluent’s `DPM_BOILING_TEMPERATURE`. The superheat is defined as

$$\Delta T = T_p - T_b. \quad (\text{A.11})$$

The code applies explicit bounds to ΔT , and applies a logarithmic softening for large positive superheat to reduce stiffness.

A piecewise correlation $\alpha_f(\Delta T)$ is used:

- low superheat: $\alpha_f = 0.760 \Delta T^{0.26}$,
- intermediate: $\alpha_f = 0.027 \Delta T^{2.33}$,
- high: $\alpha_f = 13.800 \Delta T^{0.39}$.

The flash-boiling mass rate is computed for $\Delta T > 0$ as

$$\dot{m}_{\text{flash}} = \alpha_f(\Delta T) A_p \frac{\Delta T}{L(T_b)}, \quad A_p = \pi d_p^2, \quad (\text{A.12})$$

with finite checks and a non-negativity constraint.

A.0.6 Heat-supplied evaporation $\dot{m}_{\text{heat}}$

The heat-supplied evaporation term uses the corrected Nusselt number and local gas properties. The code forms a target rate M_{target} based on a log form in which the available convective enthalpy difference is normalised by latent heat. A dimensionless coupling factor

$$\text{ratio} = 1 + \frac{\dot{m}_{\text{flash}}}{M_{\text{target}}} \quad (\text{A.13})$$

is used (with bounds and a small positive denominator safeguard in the implementation) to represent the interaction between flash vapour generation and convective supply.

The code does not apply M_{target} directly. It integrates an auxiliary relaxation ODE toward the target using an SSP-RK3 procedure (`integrate_mheat_RK3`) over a small number of pseudo-iterations:

$$\frac{d\dot{m}_{\text{heat}}}{d\tau} = M_{\text{target}} - \dot{m}_{\text{heat}}. \quad (\text{A.14})$$

The RK3 loop includes finite checks, clamping, and a relative convergence criterion.

A.0.7 Particle updates and coupling to Fluent

A.0.7.1 Mass and diameter update

The total evaporation rate is

$$\dot{m} = \dot{m}_{\text{flash}} + \dot{m}_{\text{heat}}. \quad (\text{A.15})$$

A per-time-step mass-loss cap is applied so that no more than a fixed fraction of the current particle mass can evaporate within one tracking step. The parcel mass is updated by

$$m_p^{n+1} = m_p^n - \dot{m} \Delta t, \quad (\text{A.16})$$

with protection against negative mass. Diameter is updated assuming constant particle density using Fluent’s volume-to-diameter conversion.

Parcels are removed if mass or diameter falls below Fluent’s configured minimum thresholds.

A.0.7.2 Temperature update

The law applies latent cooling to the parcel using a power form,

$$Q_{\text{lat}} = \dot{m} L(T_b), \quad (\text{A.17})$$

and calls Fluent’s temperature update routine with $-Q_{\text{lat}}$. The particle temperature is then bounded from below and above, including a lower bound tied to T_b (implemented as $T_p \geq T_b - 5$ K with an absolute floor), to prevent numerical drift.

Convective sensible heat exchange is provided to Fluent by setting the linearised heat transfer coefficient-area product,

$$\text{htcA} = hA_p, \quad h = \frac{Nu k_g}{d_p}. \quad (\text{A.18})$$

This allows Fluent’s DPM energy treatment to handle the sensible term consistently within its coupling scheme.

A.0.7.3 Gas-phase source terms

The source routine applies:

- a mass source to the gas phase equal to the evaporated mass rate,
- a species source to the selected vapour species,
- an energy sink equal to $\dot{m}L$ (latent cooling of the gas).

The source term uses a reference latent heat if available, otherwise it evaluates latent heat through Fluent’s material macro.

A.0.8 Law selection (switch functions)

Two switch functions are provided to map regimes to Fluent’s DPM laws using the relative position of T_p to T_b . Both include a threshold around boiling that determines when the custom flash-boiling law is activated. This thresholding can affect where the solution transitions from inert heating/standard vaporization to the flash-boiling branch.

A.0.9 Numerical safeguards and diagnostics

The code contains a consistent set of numerical protections:

1. Range checks and finite checks for gas properties, latent heat, diffusivity, and correlation outputs, with fallback values.
2. Clamping of key intermediate quantities (Re , H_M , B_M , B_T , ΔT , and others).
3. Log-space RK3 integration for B_T to avoid overflow when B_M is large.
4. RK3 relaxation for $\dot{m}_{\text{heat}}$ to avoid stiff explicit updates.
5. A per-step cap on mass loss.
6. Temperature bounds tied to physical limits and T_b .

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