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**Modelling, Simulation, and Life cycle Assessment of a Novel
Sustainable Ammonia Production Process from Food Waste and
Brown Water**

By

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ABSTRACT

Doctor of Philosophy

MODELLING, SIMULATION, AND LIFE CYCLE ASSESSMENT OF A NOVEL SUSTAINABLE AMMONIA PRODUCTION PROCESS FROM FOOD WASTE AND BROWN WATER

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To replace existing high impact ammonia production technologies, a new sustainability-driven waste-based process producing green ammonia with and without urea was devised using life cycle thinking and sustainable design principles, targeting efficiency, carbon emissions, water, and power use competitiveness.

Through this process, food waste and brown water are fed into a two-stage Dark Fermentation (DF) coupled with Anaerobic Digestion (AD)/AD-only bioreactors, resulting in the production of biogas. The biogas is then upgraded into hydrogen through a series of operating stages (emerging membranes) and reacts with nitrogen derived from the migration of air through a membrane in order to produce ammonia. This process is assessed via different scenarios, two hydrogen generating options are paired with four CO₂ fates. For either an AD-centered process or a two-stage process, the resultant CO₂ may be captured and injected, sold to the marketplace, released directly into the atmosphere, or converted to urea. An equation-based modular approach has been devised in Visual Basic for Applications for the new technology and family of configurations. Based on the said model, 72 assessed processes for the cradle-to-gate life cycle assessment model were generated to evaluate the potential efficiency and Greenhouse Gas (GHG) intensity.

Among the assessed technologies, coupling DF with AD and capturing CO₂ for sequestration or later use is most efficient for GHGs, water, and energy, consuming 27% less energy and reducing GHGs by 98% compared to conventional ammonia production. In addition, water consumption is 38% lower than water electrolysis technology. The results indicate that leakage causes nearly all life cycle impacts, demonstrating that failing to prevent leakage undermines the effectiveness of these new technologies. The green ammonia/ammonia+urea process family as designed here can reduce waste and prevent the release of additional CO₂ from ammonia production, while avoiding fossil-based alternatives and decreasing emissions from biogenic waste sources.

Keywords: Green Ammonia; Waste Utilization, Membrane; Carbon Capture, Utilization, and Storage (CCUS); Techno-environmental Assessment; Visual Basic for Applications (VBA); Life Cycle Assessment (LCA)

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Declaration of Authorship

I, Homa Ghavam, declare that the thesis entitled:

MODELLING, SIMULATION, AND LIFE CYCLE ASSESSMENT OF A NOVEL SUSTAINABLE AMMONIA PRODUCTION PROCESS FROM FOOD WASTE AND BROWN WATER

and the work presented in the thesis is both my own, and has been generated by me as the result of my own original research. I confirm that:

- this work was done wholly or mainly while in candidature for a research degree at this University;
- where any part of this thesis has previously been submitted for a degree or any other qualification at this University or any other institution, this has been clearly stated;
- where I have consulted the published work of others, this is always clearly attributed;
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- with the exception of such quotations, this thesis is entirely my own work;
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- parts of this work have been published:

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Signed: Homa Ghavam.....

Date: 06/06/2022.....

List of Abbreviations and Nomenclature

ACES	Advanced Cost and Energy Saving
ADB	Anaerobic Digestion Bioreactor
AEM	Anion Exchange Membrane
AFOLU	Agriculture, Forestry and Other Land-Use
ATR	Auto-thermal Reforming
AWARE	Available Water Remaining
BOD	Biological Oxygen Demand
BW	Brown Water
CapEx	Capital expenditures
CARB	California Air Resource Board
CCS	Carbon Capture and Sequestration
CCU	Carbon Capture and Utilization
CCUS	Carbon Capture, Utilization, and Storage
CML	Institute of Environmental Sciences, University of Leiden, The Netherlands
COD	Chemical Oxygen Demand
COMP	Compressor
COND	Condenser
CSTR	Continuous Stirred Tank Reactor
DFB	Dark Fermentation Bioreactor
DI	Deionized
EMS	Electrochemical Membrane Separation
EPA	Environmental Protection Agency
ESI	Electronic Supplementary Information
FAO	Food and Agriculture Organization
FU	Functional Unit
FW	Food Waste
GHG	Greenhouse Gas
GLO	Global
GWI	Global Warming Impact
GWP	Global Warming Potential
H-B	Haber Bosch
HEX	Heat Exchanger
HHV	High Heating Value
HRT	Hydraulic Retention Time
HTE	High Temperature Electrolysis
HW	Human Waste
IPCC	Intergovernmental Panel on Climate Change
IGCC	Integrated Gasification Combined Cycle
IRL	Integration Readiness Level
ITM	Ion Transport Membrane
KN	Knudsen Number
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCT	Life Cycle Thinking
LHV	Low Heating Value
MEC	Microbial Electrolysis Cell
MFC	Microbial Fuel Cell
MFI	Micro Filtration Index
MOO	Multi Objective Optimization
MTR	Membrane Technology and Research
MSW	Municipal Solid Waste
NASA	National Aeronautics and Space Administration

NGASE	Natural Gas Assisted Steam Electrolyzer
NREL	National Renewable Energy Laboratory
NRR	Nitrogen Reduction Reaction
NTP	Non-Thermal Plasma
NWW	National Wind Watch
ODE	Ordinary Differential Equation
OFMSW	Organic Fraction of Municipal Solid Waste
OLR	Organic Loading Rate
PEC	Photo-Electrochemical Cells
PEM	Polymer Electrolyte Membrane
PDE	Partial Differential Equation
PSA	Pressure Swing Adsorption
PSE	Process Systems Engineering
PV	Photovoltaic
R&D	Research and Development
RoW	Rest-of-the-World
SCOD	Soluble Chemical Oxygen Demand
SCR	Selective Catalytic Reduction
SNCR	Selective Non-Catalytic Reduction
SDP	Sustainable Design Principles
SGP	Specific Gas Production
SHP	Specific Hydrogen Production
SMP	Soluble Microbial Product
SMR	Steam Methane Reforming
SOEC	Solid Oxide Electrolysis Cell
SOFC	Solid Oxide Fuel Cell
SOFEC	Solid Oxide Fuel Electrolysis Cell
SRL	System Readiness Level
SRT	Solid Retention Time
SSAS	Solid State Ammonia Synthesis
TCOD	Total Chemical Oxygen Demand
TKN	Total Kjeldahl Nitrogen
ToC	Theory of Change
TRL	Technology Readiness Level
TS	Total Solid
UCG	Underground Coal Gasification
USDOE	United States Department of Energy
USEPA	U.S. Environmental Protection Agency
NIST	National Institute of Standards and Technology
VBA	Visual Basic for Applications
VFA	Volatile Fatty Acid
VS	Volatile Solid
VSA	Vacuum Swing Adsorption
WBCSD	World Business Council for Sustainable Development
WECC	Western Electricity Coordinating Council
WGSR	Water Gas Shift Reaction
WVU	West Virginia University
WVURC	West Virginia University Research Corporation
WWT	Waste Water Treatment
WWTP	Waste Water Treatment Plant

Chapter 1

Research Overview

This chapter provides an overview of the importance, applications, and the production processes currently in use for ammonia along with their shortcomings. A brief description of the proposed ammonia production process, its significance, and novelty are discussed. Finally, the research question, aims, and objectives are defined.

This chapter was drafted based on the publications submitted to the International journal of hydrogen energy, *Frontiers in energy research*, and *Journal of cleaner production*:

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Caroline M. Taylor: Conceptual input on the model and contributed to the draft

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Statement of contribution:

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Caroline M. Taylor: Conceptualization, Writing- Reviewing and Editing.

Peter Styring: Supervision, Reviewing and Funding acquisition

1. Introduction

1.1 The importance of fertilizers

By 2050, global food production will need to increase by 70% in order to keep up with the worldwide growth in population (UN, 2015). This population growth puts a burden on the earth's natural resources, such as the depletion of water supplies and simultaneously, will result in higher waste production. As global population grows, nutritional requirements are driving the need for more food production, leading to the demand for more fertilizers, resulting in higher food demands and more food and human waste (HW) generation (Fig. 1.1).



Fig. 1.1: A schematic of food and human waste to green fertilizer loop.

The projected global population along with the total nitrous oxide (N₂O) and methane (CH₄) emissions from human sewage and domestic wastewater from 1990-2030 are shown in Fig. 1.2. The amount of HW necessarily increases proportionally with the global population. The amount of HW has increased by approximately 51% over the course of 40 years, while population growth is approximately 47% over the same time period.

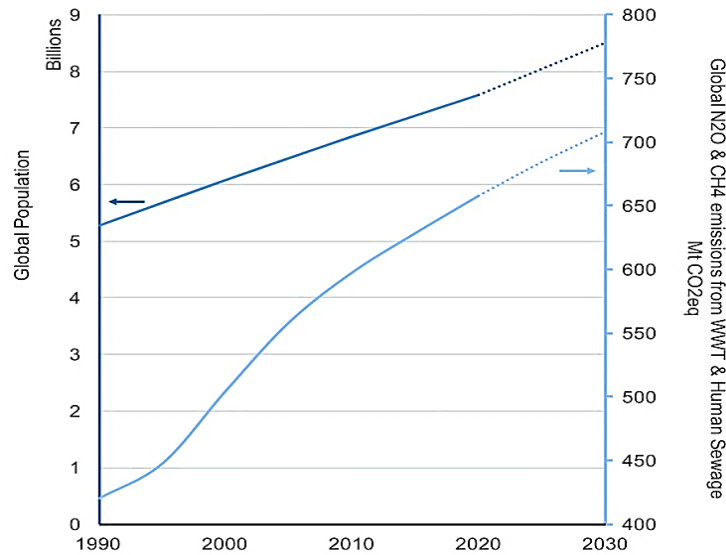


Fig. 1.2: The projected global population along with the total nitrous oxide and methane emissions from human sewage and domestic wastewater in MtCO₂ eq from 1990-2030 (data from USEPA and ICF, 2012; Isaksson et al., 2020).

Commercial fertilizers are used in about 40-60% of global food production with the main feedstock for their production processes being fossil fuels (Roberts, 2009). Alexandratos and Bruinsma (2012) projected that fertilizer usage will increase proportionally to the population growth in the period 1960-2050. Furthermore, they estimated that fertilizer usage will increase by approximately 25% from 210 million tonnes (Mt) in 2020 to 262 Mt in 2050.

The three main types of fertilizer are nitrogen (N), phosphorus (P), and potassium (K) (Choi et al., 2013). The projected global supply of each fertilizer from 2016-2022 shows that, N-based fertilizers have the highest production rate compared to phosphorus and potassium (Fig. 1.3).

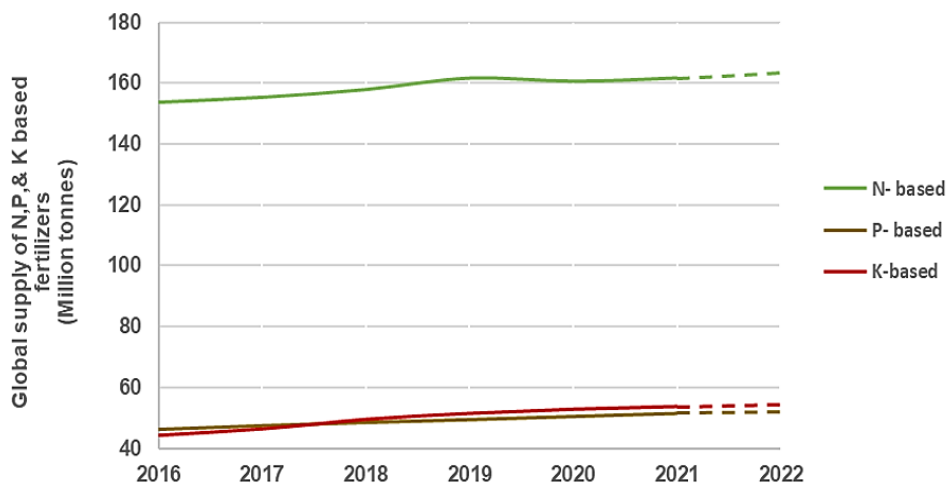


Fig. 1.3: The projected global production rate for N, P, K-based fertilizers from 2016-2022 (FAO, 2019).

The increase in global market demand for N-based fertilizers keeps pace with global population growth and this trend is projected to continue. Global population is set to increase by about 14% over the course of 6 years; while global nitrogen fertilizer demand has increased nearly 6% over the same time period (Fig. 1.4).

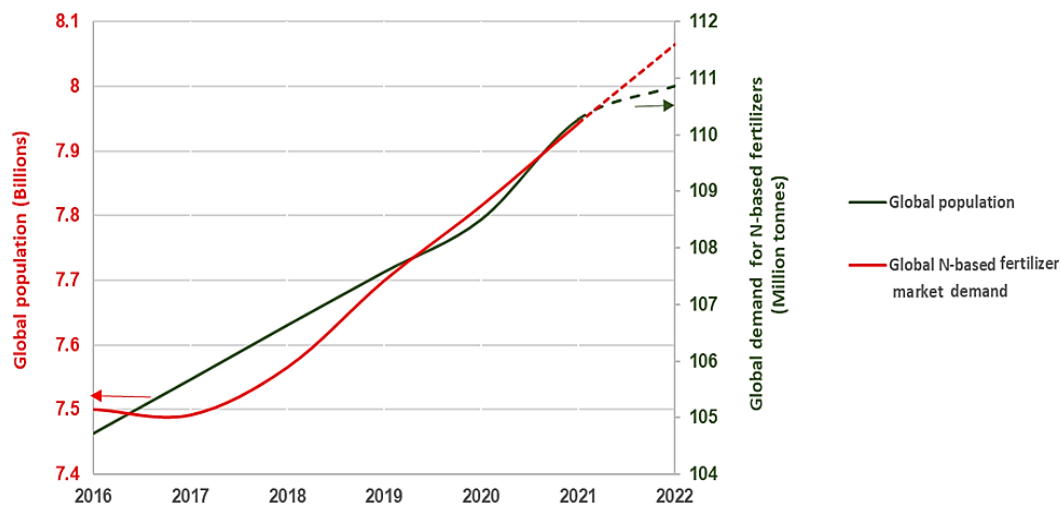


Fig. 1.4: Projected growth of global population and nutrient N demand from 2016-2022 (FAO, 2019).

As shown in Fig. 1.5, the increase in the amount of FW keeps pace with nutrient N demand and this trend is projected to continue. FW has increased by 40% over the course of the 34 years; while the nutrient N demand has increased approximately 49% over the same time period.

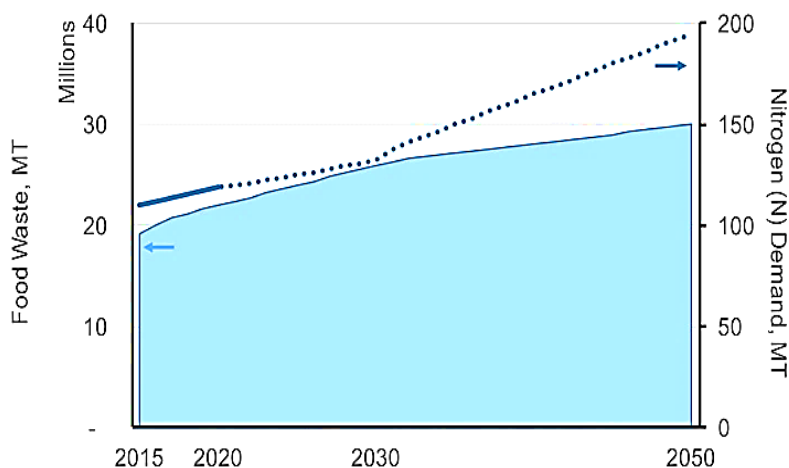
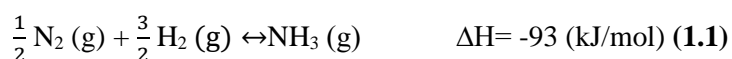


Fig. 1.5: Projected amount of FW and nutrient N demand from 2016-2050 (data from FAO, 2017; Read et al., 2020).

1.1.1 Ammonia as a potential energy carrier

Ammonia (NH_3) is the most produced N-based fertilizer and is the second most produced chemical compound globally (146 million tonnes reported in 2016) after sulfuric acid (H_2SO_4), with fossil fuels being the main feedstock

for its production (CICE, 2016; Ghavam et al., 2021). The exothermic reaction between hydrogen (H₂) and nitrogen (N₂) results in the production of ammonia, via the following chemical (1.1):



Ammonia is both crucial as a fertilizer in the agricultural industry and has promising prospects as an energy carrier (Fig. 1.6). Approximately 89% of the ammonia produced is used as an intermediate chemical for direct production of fertilizers such as urea and only about 11% is traded as ammonia (Jackson et al., 2020).

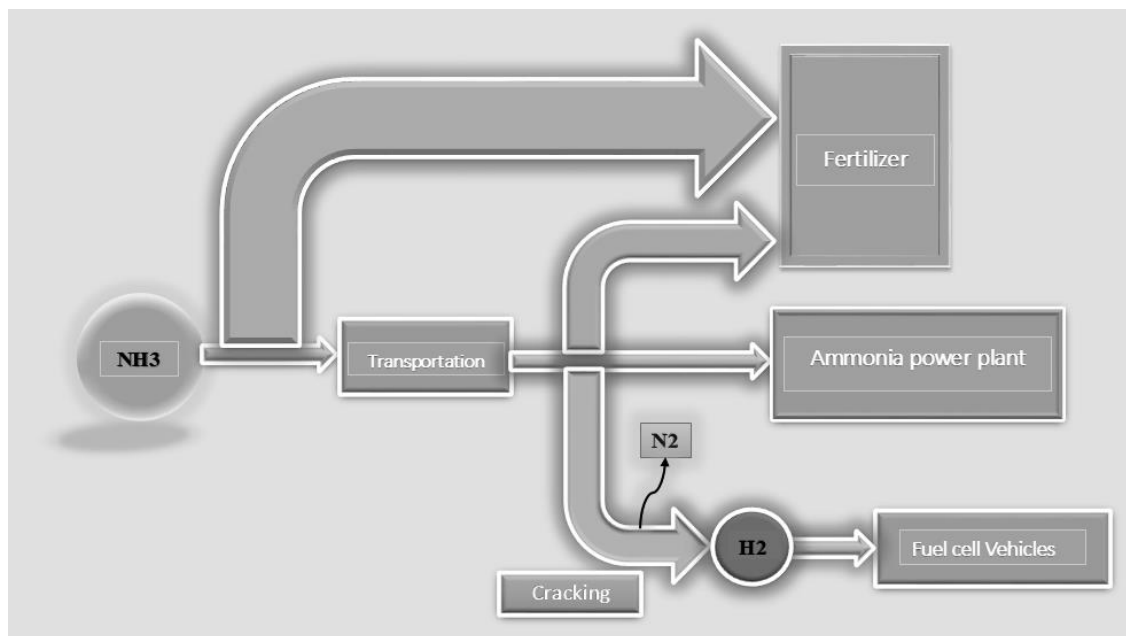


Fig. 1.6: Different applications of ammonia (Service, 2018).

Industrially, ammonia can also be utilized in a wide range of applications, from the production of polyimides and nitric acid, to its use as an energy carrier for energy storage and transportation (CICE, 2016). Ammonia consists of 17.6 weight percent (wt%) hydrogen, showing that this chemical compound is an indirect hydrogen storage (Michael, Alhajji and Demirel, 2015). Ammonia's energy density is 4.32 kWh/L, which is similar to methanol (CH₃OH), and approximately double that of liquid hydrogen (Soloveichik, 2017a). Philibert (2018) points out that liquefying hydrogen is more difficult when compared to ammonia, since ammonia liquefies at -33.4°C and at atmospheric pressure: Hydrogen has to be liquefied by chilling to temperatures lower than -253°C. One of the main challenges of utilizing hydrogen as an energy carrier is the difficulty of transporting and storing it without dissipating, and therefore being unavailable for its intended end use. Another challenge related to this dissipation is its safety during transportation and storage. Yet another challenge associated with hydrogen, used as an energy carrier, is its low energy density and difficulty in handling (Nordvang, 2017). This is due to the volumetric energy density in liquid anhydrous ammonia (10.1 MJ/L) which is approximately 1.5 times higher than of liquid hydrogen as shown in Table 1.1. From a safety point of view, ammonia gas is lighter than air, so in case of leakage ammonia rapidly dissipates into the atmosphere. However, unlike hydrogen, ammonia is not typically explosive, it is a hazardous chemical and it must be handled with care, due to its causticity and toxicity (Brown, 2018). Due to the above-mentioned factors, ammonia is seen as a practical energy vector for hydrogen.

Table 1.1: Energy content of various fuels in liquid state (Giddey, Badwal, and Kulkarni, 2013).

Chemicals	Energy content (High Heating Value (HHV))		Energy content (Low Heating Value (LHV))	
	(J/kg) ×10 ⁶	(J/l) ×10 ⁶	(J/kg) ×10 ⁶	(J/l) ×10 ⁶
Liquid hydrogen (H ₂)	141.9	10.1	119.9	8.5
Liquid ammonia (NH ₃)	22.5	15.3	18.6	12.7
Methane (CH ₄)	56.2	23.6	50.0	20.9
Methanol (CH ₃ OH)	22.9	18.2	20.1	15.8
Ethanol (C ₂ H ₅ OH)	29.9	23.6	26.9	21.2

According to Soloveitchik (2017b), ammonia is not only considered a fertilizer but also an energy carrier. In addition, with the global transition from fossil fuels to variable renewable energy sources, such as solar and wind, there is an increasing requirement for energy storage solutions that can cover various timeframes for storing the energy. Of particular interest is the capability to store energy economically for long periods of time without a significant reduction in energy, to transport the stored energy over long distances and to be able to store the energy at terawatt-hour (TWh) scales economically, perhaps only needing to charge and discharge a small number of times over a year (Wilson and Styring, 2017). These are the general characteristics of fossil-fuels and help to explain why these fuels are so ubiquitous. It seems evident that fuels (gaseous, liquid or solid) are particularly useful to satisfy these characteristics and will therefore still be necessary in future energy systems due to the continued need to provide interseasonal storage and traded energy across global supply chains (Wilson and Styring, 2017). In future low-carbon energy systems, these should therefore be regarded as low-carbon fuels, and ammonia as a synthetic fuel that is able to meet these requirements.

1.1.1.1 Importance of sustainable ammonia production

According to the Food and Agricultural Organization (FAO) of the United Nations, the world supply capacity of ammonia was 153,646 thousand tonnes in 2016. In the year 2017, the supply of ammonia increased to 155,253 thousand tonnes and in 2018, it further increased to 157,819 thousand tonnes and it is expected to reach 163,219 thousand tonnes in 2022 (FAO, 2019). Ammonia production technologies currently in use require either a steady supply of Deionized (DI) water in high volumes to operate and/or result in high CO₂ production. Consequently, much effort has been put into seeking the most energy efficient, environmentally benign, and economically viable processes for ammonia synthesis in academic and industrial spheres. The scale of the ammonia market makes development and deployment of more environmentally sustainable production routes particularly important.

1.1.1.2 Environmental implications of fossil-based ammonia production processes

The most commonly utilized ammonia production method is the Haber-Bosch (H-B) process which is produced in large plants with yields of 1,000 to 1,500 t/day (Soloveichik, 2017b). Globally, more than 90% of ammonia is produced from fossil fuels through this method (Hughes et al., 2015; Guerra et al., 2020). The H-B process is generally powered by fossil fuels which function at temperatures in the range of 400-500°C and pressure in the range of 150-300 bar, usually in the presence of an iron (Fe) based catalyst (Garagounis et al., 2014; Wang et al., 2018).

About 96% of the hydrogen required for the production of ammonia via Steam Methane Reforming (SMR) coupled with H-B process is derived from fossil fuels (Parkinson et al., 2018). The remaining 4% is generated from water electrolysis which will include some indirect use of fossil fuels from coal or natural gas electrical generation (Michael, et al., 2015). A typical SMR process produces approximately 9-10 tonnes of carbon dioxide equivalent (CO₂ eq) for each tonne of hydrogen produced (Parkinson et al., 2018).

The downside of H-B technology is the production of high GHG emissions, greater than 2.16 kgCO₂eq/kg NH₃, and high amounts of energy usage surpassing 30×10⁹ J/tonne NH₃ mostly due to high operational conditions (Yoo et al., 2013; Wang et al., 2018). For the production of 1 t of NH₃ through SMR coupled with H-B, 0.66 t H₂O is utilized and 9-10 t CO₂ eq is produced, over its full life cycle (Parkinson et al., 2018). A schematic of ammonia production through SMR coupled with H-B process is shown in Fig. 1.7.

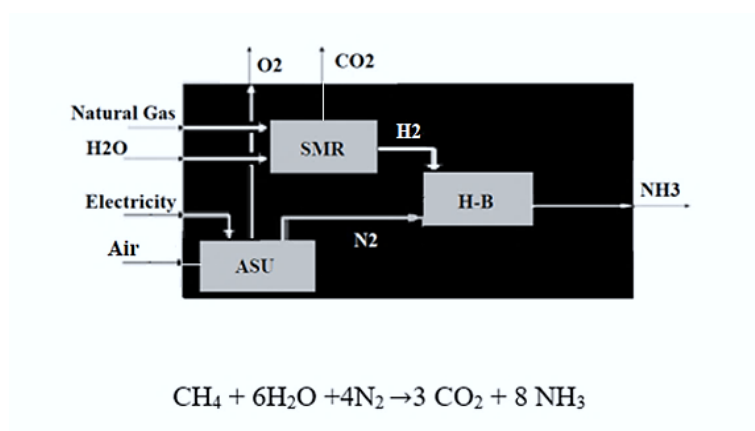


Fig. 1.7: A schematic of SMR coupled with H-B process (Ganley, Holbrook and McKinley, 2007).

Globally, 72% of the hydrogen that can be manufactured for ammonia production is from the SMR process and 26% is derived from coal (IEA, 2012). In 2016, coal-based ammonia made up more than 82% of China's ammonia production (Heffer and Prud'homme, 2016). The largest ammonia producers are: China, India, Russia, and the United States (Fig. 1.8).

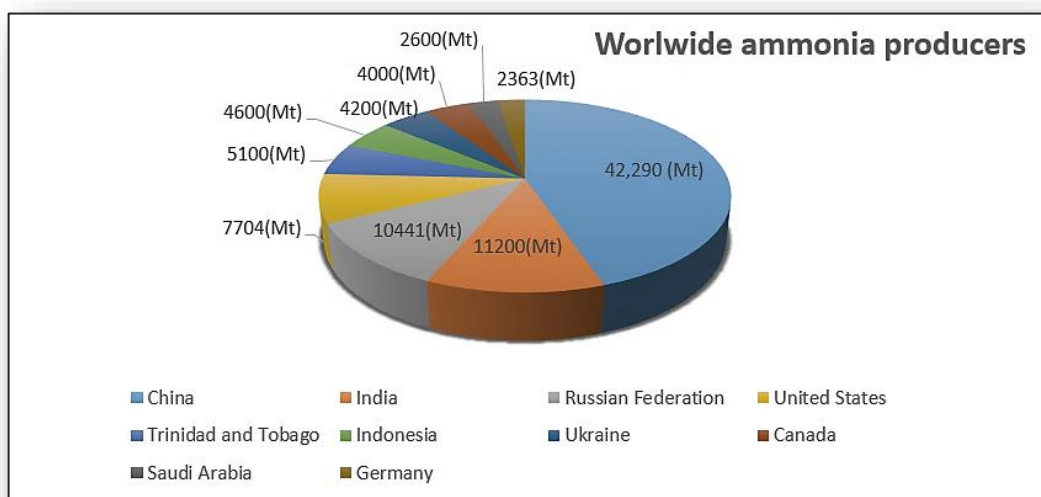


Fig.1.8: Worldwide ammonia producers (Data from, Dincer and Bicer, 2015).

1.1.1.3 The relationship between ammonia manufacturing costs and natural gas prices

Approximately 70-90% of ammonia manufacturing costs from SMR coupled with H-B process are directly tied to the price of natural gas. Fluctuations in the price of ammonia are usually tied to volatility in natural gas prices (Dincer and Bicer, 2015). The price of both natural gas and ammonia have increased in most years, the former from approximately 0.141 \$/m³ in 1975 to 0.53 \$/m³ in 2015, and the latter from 290 \$/ton of NH₃ in 1975 to approximately 850 \$/ton of NH₃ in 2015 and reached its maximum in 2015. Between 2012 -2016, the price of natural gas production decreased globally due to the increase in natural gas production, mainly in the United States.

1.1.1.4 Green ammonia

For sustainable ammonia production, the most widely adopted technology is water electrolysis coupled with H-B powered by renewable technologies such as wind and solar energy also known as green ammonia. In general, a water electrolyzer requires a continuous stream of pretreated water with high purity levels for its operation. Moreover, for production of 1 tonne of hydrogen, 9 tonnes of water is required. For producing 1 t of NH₃ through water electrolysis 1.6 t H₂O is consumed (Will and Lukas, 2018). In 2016, the amount of ammonia produced was reported to be 146 million tonnes globally (Cong et al., 2019). Based on these data, for the production of the same amount of ammonia through water electrolysis, 233.6 million tonnes (233.6 billion liters) of water is required. A schematic of ammonia production through water electrolyzer coupled with H-B process is shown in Fig. 1.9. In a world with greater and greater amounts of deployed lower-carbon renewable generation able to provide the primary electricity for hydrogen electrolysis, this ammonia could be described as green ammonia.

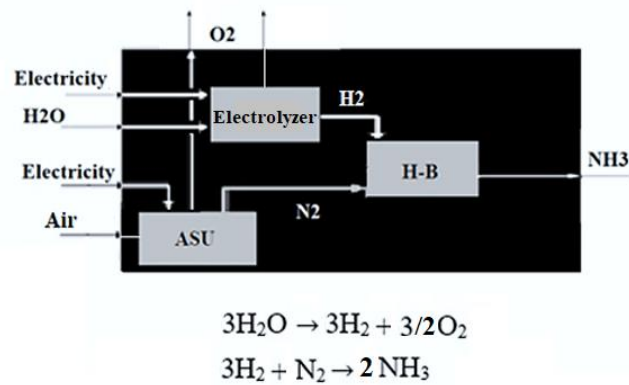


Fig. 1.9: A schematic of water electrolyzer coupled with H-B process
(Ganley, Holbrook and McKinley, 2007).

Environmental implications of high-water consumption for green ammonia production

Many studies have been conducted on sustainable ammonia production and mainly focus on water electrolyzers powered by renewable technologies such as solar and wind. These studies include one conducted by Soloveichk (2017) and a series of different processes that were compiled by Wang et al. (2018), Service (2018), and Hughes et al. (2015). There is a crucial research gap on environmental and economic aspects of sustainability when assessing water consumption in the production of ammonia in these reviews. In order to operate, these processes require a constant water supply while considering the implications of the increasingly severe worldwide water crisis. The critical inputs for electrolysis are electricity and DI water. In general, a water electrolyzer requires pretreated, high purity water for its operation (Mehmeti et al., 2018). Moreover, for production of 1 tonne of hydrogen, 9 tonnes of water is required. The major implications of water consumption in various hydrogen production processes and the effects associated with water on the environment are important factors that have been assessed in the study conducted by Mehmeti et al. (2018) by means of Life Cycle Assessment (LCA). Studies conducted by Alcamo, Flörke and Märker (2007), Distefano and Kelly (2017), Ercin and Hoekstra (2014), and Hoekstra et al. (2011) have shown that there will be a significant increase in water scarcity in the next few decades and this will result in problems for food security, environmental sustainability, and economics. However, it must be noted that water scarcity is dependent on local availability. According to Mehmeti et al. (2018), SMR and water electrolysis cause the most damage to the environment since these processes use high quality water (low-dissolved-solid concentrations/DI water) for operation. Morgan (2013) also conducted a techno-economic feasibility study on an ammonia production plant powered by offshore wind. The study reported that for the production of 300 tonnes of ammonia, 476 tonnes of distilled water is required. The ratio of the treated water required per tonne of ammonia (excluding the water needed for the cooling tower) is approximately 1.6. This figure is also reported by Will and Lukas (2018) when assessing an ammonia production plant using water electrolysis powered by renewable (solar, wind, and hydro) energy. For a 50 tonne/day ammonia production plant, 20 MW power is needed while, 120 MW is required for 300 tonne/day. Based on Will and Lukas's study, the water loss from the cooling towers is said to be in the range of approximately 1-1.5% of the total input water. This shows that for the production of approximately 1 tonne of ammonia, 2.45 tonnes of water is required when taking into account the amount of water loss of cooling towers. While Will and Lukas (2018)

report a portion of the input water is lost through cooling towers, however, when using Available Water Remaining (AWARE) impact assessment method in LCA, the water utilized for cooling towers is counted as 100% loss.

1.1.1.5 A comparison of fossil and non-fossil-based ammonia production technologies currently in use

While a water electrolyzer coupled with renewable technologies as discussed above requires high volumes of water for its operation, the conventional ammonia production process, which is SMR coupled with H-B processes, is also relatively water intensive requiring approximately 0.656 kg of water to produce 1 t of ammonia. However, this figure is lower than the aforementioned methods for ammonia production. Table 1.2 shows that SMR coupled with H-B process is the most carbon intensive technology with 1.8 kg CO₂/t NH₃ compared to the other technology. Water electrolysis is the most water (ca. 1.588 kg H₂O/ tNH₃) and energy (ca. 12,000 kWh/tonne NH₃) intensive among the processes currently in use.

Table 1.2: Key consumption and GHG emissions for renewable and conventional ammonia production technologies to produce 1 tonne of ammonia.

Technology	Water consumption (kg H ₂ O/ t NH ₃)	(kg of CO ₂ emitted/ t NH ₃)	Energy (electricity and heat consumption (kWh/tonne NH ₃))	Efficiency %	Capital cost per ton/day NH ₃ capacity	References
SMR coupled with Haber-Bosch	ca. 0.656	ca.1.8	ca.9,500	~61-66%	\$500,000	Ganley, Holbrook and McKinley (2007), Soloveichik (2017b), Elgowainy et al. (2015)
Water electrolysis coupled with Haber-Bosch powered by solar /wind	ca.1.588	negligible	ca.12,000	~54%	\$750,000	Pfromm (2017), Ganley, Holbrook and McKinley (2007), Will and Lukas (2018), Soloveichik (2017b)

1.1.1.6 The importance of integrating the ammonia and urea production processes

One approach to manage CO₂ that otherwise would be released into the atmosphere during ammonia production is to produce urea, a key agricultural nutrient. In addition to its importance in the agricultural industry, urea which is readily produced from ammonia and CO₂ is also use extensively in polymers (CICE, 2017). Demand for urea has increased about 3% each year from 2000-2016, keeping pace with ammonia production. Fig.1.10 shows that the increase in global market demand for urea keeps pace with global population growth and this trend is projected to continue. Global population is set to increase by about 7% over the course of 8 years; while between 2016-2019 global urea demand decreased nearly 1.55%, from 2019-2024 it is expected to increase by 0.9% (Fig. 1.10).

Data released by Yara chemical company, indicates that urea makes up most of the nitrogen-based fertilizer market globally (Yara, 2018). Incorporating urea production to consume waste CO₂ utilizes a large share of the end-product ammonia. Significantly, this CO₂ that is used in the urea will be discharged, thus, though the CO₂ in this system is biogenic, it will return to the atmosphere. However, according to the environmental analysis tools it will do so having displaced fossil CO₂ that would increase the atmospheric CO₂ levels. Thus, incorporating a green urea plant may slow, though not abate the GHG crisis, while getting useful services (in this case, offsetting the production of conventional urea, which uses significant fossil resources and leads to significant life cycle GHGs).

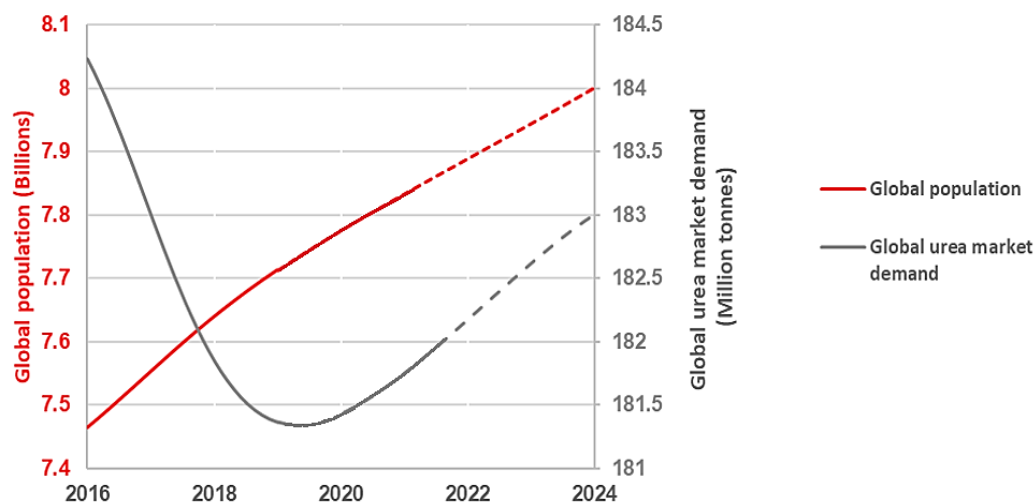


Fig. 1.10: Projected growth of global population and urea demand from 2016-2024 (FAO, 2019).

Urea

Urea is also known as carbamide, a white crystalline organic chemical compound mainly used in the agricultural industry as a fertilizer with a nitrogen content of approximately 46.7% (CICE, 2017). Other than its use in fertilizers, urea is also utilized in the production of melamine, glue, resins, adhesives, pharmaceuticals, coating, and in both Selective Catalytic Reduction (SCR) and Selective Non-Catalytic Reduction (SNCR) for reducing nitrogen oxide (NO_x) emissions (Yara, 2018). Demand for urea in the non-fertilizer sector has the potential to increase mainly in DeNO_x applications in North America, Europe, and East Asia. Selective Catalytic Reduction usage in both United States and Europe has grown from 2009-2016 and is anticipated to increase further (Yara, 2014). This chemical compound is commercially produced via the reaction between synthetic NH₃ and CO₂ gases which are heated to 450 K temperature and 200 atm pressure (Baboo et al., 2016). This reaction forms ammonia carbamate (NH₂COONH₄) which then rapidly decomposes and produces urea after dehydration (Yara, 2018) (see Fig. 1.11), the final product is a prilled/granulated solid. The reaction that takes place for urea production is as follows (see reactions 1.2 and 1.3) (CICE, 2017):

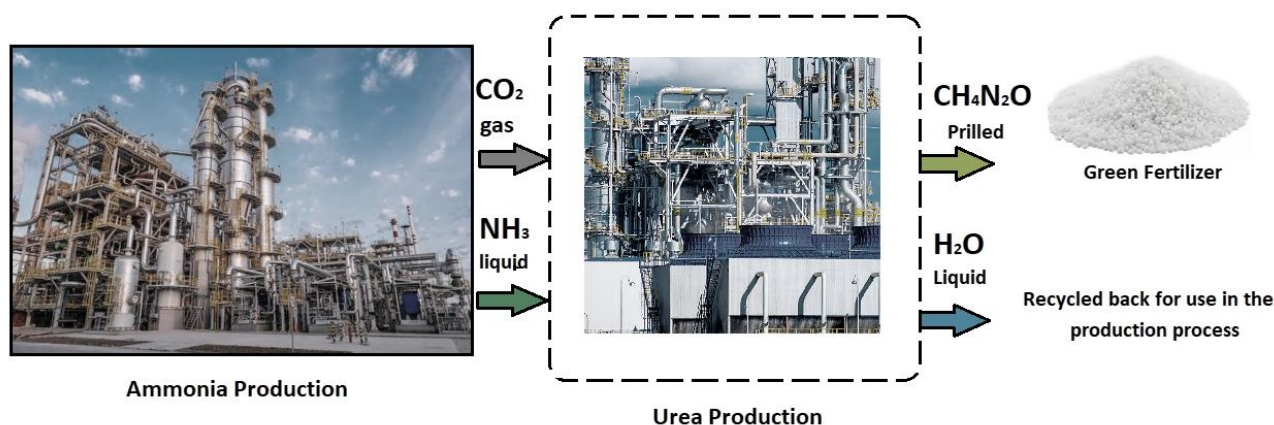


Fig. 1.11: A schematic of urea production process.

During urea manufacturing, an unwanted side reaction known as biuret lowers the production yield due to crop scorching. Urea production processes are classified based on the amount of biuret formation (Li, 2013). The goal of any efficient urea production technology is to lower the formation of biuret as much as possible.

1.1.1.7 Waste as a sustainable source for ammonia production

Bioconversion of wastes such as food and human waste into important chemical compounds such as ammonia and urea ($\text{CH}_4\text{N}_2\text{O}$) offers, to some extent, a new resource recovery alternative for fossil-based chemicals. The overabundance of these waste streams poses significant threats to GHG control. Uncontrolled decomposition of organic waste in landfills, if left untreated, leads to the discharge of methane, a potent GHG trapping approximately 85 times more heat than CO_2 through the first 20 years from when it is discharged (EDF, 2021). Methane accounts for 20% of the global warming that is currently being experienced (Chandler, 2017; IPCC, 2013). In 2015, the U.S. Environmental Protection Agency (USEPA) reported that the GHG emissions resulting from waste landfills was 115.7 Mt of CO_2 eq (Lee et al., 2010). While in the same year, the UK government reported GHG emissions of waste disposed of in landfills was approximately 18 Mt of CO_2 eq (BEIS, 2017).

Both FW and HW are rich in readily biodegradable organic matter, therefore they decompose rapidly, and, in addition to their contributions to global GHG balances, may potentially result in other serious environmental implications if not properly managed. FW and HW are readily biodegradable in the environment which indicates their potential in industrial bioconversion. As a result, designing a sustainable waste management process for ammonia synthesis and reducing the GHG emissions through the utilization of anaerobic digestion bioreactor (ADB) will be an effective pathway to target the replacement of higher impact, fossil-based chemicals. One of the main advantages of a waste-based process such as the green ammonia production technology developed in this study is the potential to prevent the release of methane from uncontained degradation of waste.

Introducing a sustainable waste management approach for ammonia production

Simplified process description

In order to replace the existing high impact ammonia technologies currently in use, a new, waste-based sustainability-driven ammonia production technology is proposed, designed, and modelled here. This process is competitive for carbon emissions, water and power use and has been designed around carbon capture/utilization. The design strategy was devised using life cycle thinking (LCT) and sustainable design principles (SDPs) to guide the design. Crucially, meeting the design targets require the effective management of CO₂.

Through this process, waste (FW and BW) is fed into a two-stage CSTR-bioreactor, resulting in the production of biogas. The produced biogas is upgraded into hydrogen through a series of operating stages (membranes) and reacts with nitrogen derived from the migration of air through a membrane, in order to produce ammonia. The recovered CO₂ along with the ammonia can be used for urea production (a simplified process flow diagram is shown in Fig. 1.12). This process is compared to the case where the CO₂ is not captured/utilized, as well as to cases where the CO₂ is captured, compressed, liquefied, and either injected into the ground Carbon Capture and Storage (CCS) or assumed to enter the commodity liquid CO₂ market (base Carbon Capture and Utilization (CCU)).

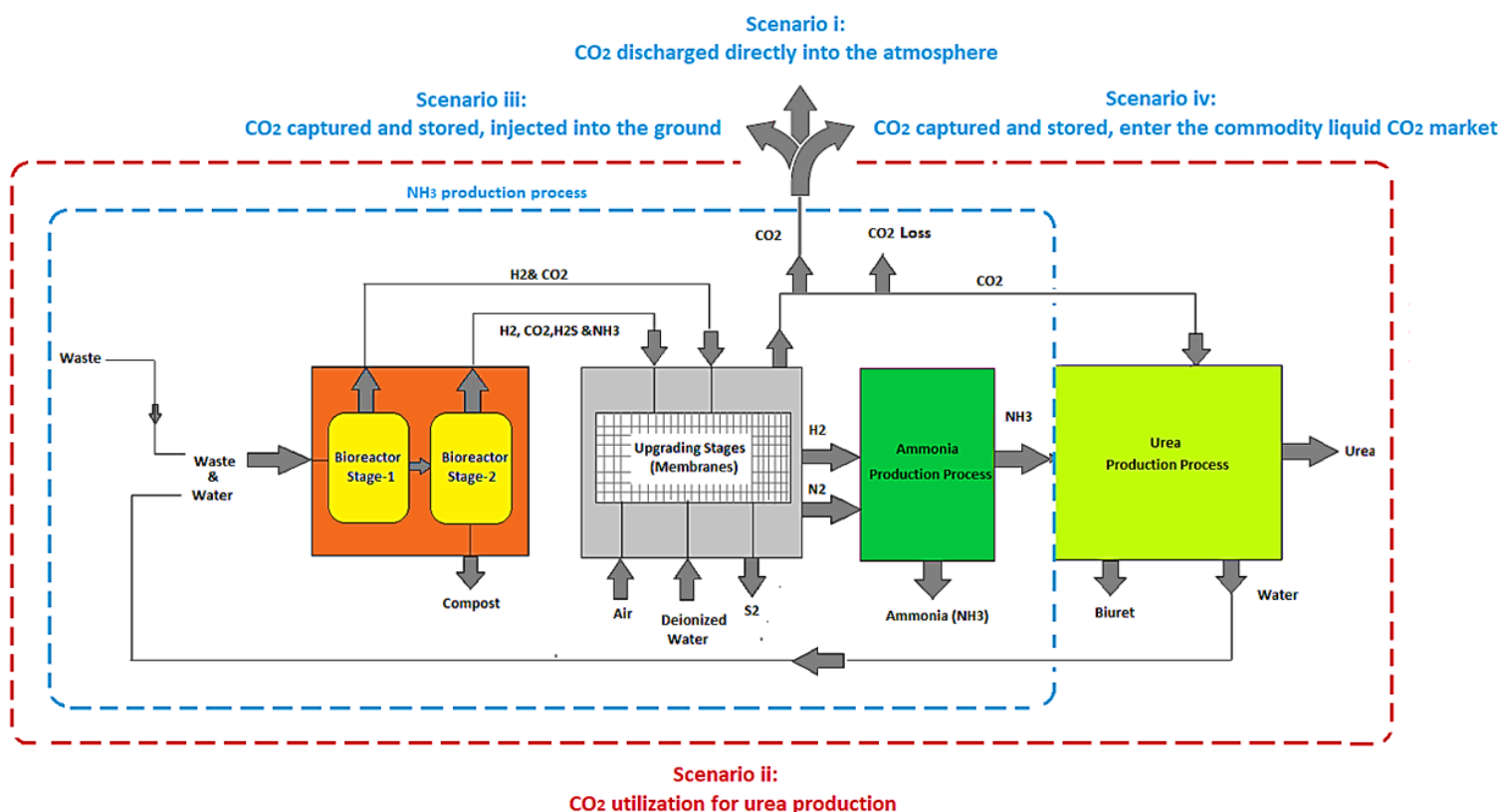


Fig. 1.12: Simplified process flow diagram of the proposed ammonia/ammonia+urea production process from waste.

Significance of the proposed ammonia production process

The primary sustainability design decisions and the rationale for the selection of key components in the process configuration of this study along with its benefits over the conventional ammonia production process are listed in Table 1.3. Feedstock in particular provides a wealth of sustainability benefits mainly in avoiding fossil energy sources as well as utilizing the stream through a valorization strategy which prevents the release of carbon emissions as well as recovering useful chemical compounds and nutrients. In place of conventional processing units, this study focuses on the use of membrane technologies in order to minimize the physical footprint, water, and chemical usage in the designed process. In addition, the byproducts produced through the selected membrane technologies do not need to be upgraded, eliminating associated waste stream or additional process steps for refining (Table 1.3).

Table 1.3: Key sustainability design decisions for this process.

Key elements	Conventional	This study	Benefits over conventional
Feedstock	Natural gas	Food waste and brown water (urban and semi-urban waste streams)	<ul style="list-style-type: none"> -Avoidance of fossil excavation -Decreased processing/treatment demand -Diversion of emissions from improper handling -Valorisation of waste streams -Recovery of key nutrients
Processing units	Reformer, reactor, scrubber, and cryogenic air separation	Bioreactor and membranes	<ul style="list-style-type: none"> -Small physical footprint -Lower cost (lower amount of water and/or chemical usage) -Produces by-products that can be sold commercially without the need to be upgraded
Hydrogen production	SMR coupled with Haber-Bosch	CH ₄ assisted-Solid Oxide Fuel Assisted Electrolysis Cell (SOFEC) (further discussion can be found in <i>Chapter 2</i>)	<ul style="list-style-type: none"> -Higher conversion rate -Smaller physical footprint -Decreased energy draw -Lower cost

Originality of the proposed ammonia production process

Novelty of the technology and Contributions of this research

A previously non-existent waste-based process for sustainable ammonia/ammonia+urea production was developed using LCT and SDPs by designing a flexible modular technology with deliberate utilization of mature and nascent (emerging membranes) technology components, built into a configurable model to allow optimization and evaluation of operating parameters. The technology has been designed for the utilization of mixed waste for the production of ammonia+urea, demonstrating the potential for variable waste stream mixes to support flexibility in deployment. While some of the components of this proposed process technology are well-known/mature, others are at the bench scale/early in the Research and Development (R&D) process. This new technology setup combines the existing and new processes into a configuration/layout that is novel and flexible. Each scenario assessed here presents a new, different, sustainable technology for ammonia production.

This study adds to the body of knowledge in the area of green ammonia production by providing, in addition to this new family of technologies, the first LCA model of a process using these emerging membranes as well as impacts

for these membranes. This provides the first estimates for Global Warming Potential (GWP) and other sustainability impacts that can be used in future research. Based on a thorough review of literature, there has been no research into the engineering of these new membranes in an integrated process or their sustainability. Besides, the additions to the body of research described above, a Visual Basic for Applications (VBA)-based model¹ has been developed for the new technology and family of configurations for public use. This model can be tuned to reflect various operating conditions and ratio of waste types. The model also assesses whether the incorporation of internal energy generation or external renewable energy sources would be more appropriate for a given scenario.

1.2 Research question

The central research question for this thesis is designing and evaluating the potential efficiency and GHG intensity of several configurations of a new, sustainability-driven waste-based ammonia production technology to determine whether a waste-based process designed first around CO₂ capture and utilization can compete with or displace existing ammonia technologies technically and environmentally.

1.3 Aims and objectives

1.3.1 Aims

The aims of this research are, to design and demonstrate the technical viability and sustainability of a family of waste-based green ammonia processes integrating several carbon capture/utilization options. Specifically, the aims are:

- 1- To design a green ammonia technology;
- 2- To apply SDPs in process design;
- 3- To conduct a techno-environmental assessment;
- 4- To design an integrated modelling platform of multiple configurations of core waste-based processes, integrating several carbon capture/utilization options to optimize and assess the technological performance;
- 5- To investigate the use of LCA and LCT early in the green design process;
- 6- To design and conduct an LCA, based on the modelling platform and assess the environmental impacts of a variety of possible configurations

1.3.2 Objectives

The following Table 1.4 shows that the methodology developed has the following objectives, tasks, and requires assessment of certain data.

Table 1.4: Research objectives and methodology for the proposed ammonia/ammonia+urea production process.

No	Objectives	Methodology
I	To design a technology that can produce green ammonia from the waste stream, which targets efficiency, carbon emissions, water, and power use competitiveness.	<p>1.1 By carrying out a thorough literature review on:</p> <ul style="list-style-type: none"> - Various conventional and emerging ammonia production technologies. - Finding sustainable alternatives for each processing unit in the ammonia production plant based on the set sustainability criteria mentioned in <i>Chapter 1</i> and <i>3</i>. <p>1.2 Using SDPs to select component technologies and develop process flow.</p>

¹ [Model available upon request]

2	To develop a numerical model which can be altered in response to variations in types of substrates, air flow rate, and other process conditions through an equation-based approach for the two technologies (DF coupled with AD (DF+AD) and AD-only process).	2.1 By applying the mathematical equations concerning the thermodynamics/ kinetics, chemical equilibria, and 'rules-of-thumb' pertaining to each processing unit of the proposed plant related to mass and energy balance using Visual Basic for Applications (VBA) in Excel software.
3	To estimate the ammonia/ammonia+urea production yield.	3.1 Using the rule of thumb.
4	To develop a DF+AD/ AD-only process models that could calculate the biochemical transformations of FW and BW fermentation/ digestion and the resulting biogas output from the CSTR-bioreactors.	4.1 FW and BW composition analysis (which are the primary feedstock for operating the proposed production process) will be obtained from various literature. The mass balance, electrochemical, and energy balance model calculations will then be conducted based on the data obtained (from waste analysis). Volatile Solid (VS), Total Solid (TS), Total Chemical Oxygen Demand (TCOD), Soluble Chemical Oxygen Demand (SCOD), Total Kjeldahl Nitrogen (TKN), and Biological Oxygen Demand (BOD) from waste analysis will then be fed into the DF+AD/AD model.
5	To model each processing unit (components) of the proposed process, the range of input data entered into these components related to the operational conditions and other membrane/component characteristics were obtained from published literature and were selected based on the design constraints.	5.1 The mass and energy balances pertaining to each processing unit are assessed in various physical and chemical conditions (i.e. temperature, pressure, flow rates, specific heat capacity, thermal conductivity, effectiveness of the heat exchangers, heat loss, drive motor power of the compressor, porosity, tortuosity, flux, and permeability of the membranes, etc.) and sizing of various processing units (i.e. thickness, length, area, number of cells/tubes and modules, etc.). This is done by using the assumptions and mathematical equations (mass transfer, energy transfer, thermodynamics, and kinetics) which are determined for each processing unit. 5.2 Testing the functionality of each component in the proposed plant by using the experimental data from literature related to their input and output parameters.
6	To optimize each model (processing units) in order to increase yields of intermediates and products - To optimize the hydrogen yield which in turn affects the amount of ammonia/ammonia+urea production. Simultaneously, reduce the amount of water and energy consumption. This is done in order to find the optimal process parameters in each processing unit for obtaining the desired output within the design constraints. - To optimize the ammonia/ammonia+urea production process in terms of the amount of hydrogen production (required for ammonia synthesis), water and energy usage based on the aim stated above. In addition, each component in the proposed ammonia/ammonia+urea production process needs to operate in its optimum condition. Optimum condition means that each modelled component will reduce water and energy usage, while increasing production efficiency (e.g., The separated nitrogen required for this process must reach a purity level higher than 99.99% in order to be utilized in the SSAS. Nitrogen with purity levels lower than 99.99% that contain trace amounts of oxygen cause irreversible poisoning of the catalyst in the SSAS.). The goal of an optimization method is to find the values of decision variables which can maximize or minimize the value of a performance criterion (objective function) and to stay within process constraints.	6.1 To optimize each of the components of the proposed process independently in terms of operational conditions (temperature and pressure), membrane characteristics (porosity, tortuosity, pore radius, thickness, etc.), recirculation ratio, waste composition, Hydraulic Retention Time (HRT), H ₂ /CO ₂ and CH ₄ /CO ₂ +H ₂ S+NH ₃ yields etc. and optimize the entire modelled process in terms of water, and energy usage and at the same time operational efficiency using use Multi Objective Optimization (MOO). 6.2 The ToC was carried out in order to consume all the produced CO ₂ for urea production. 6.3 Heat integration method was carried out in order to minimize the need for external energy sources and to maximize heat recovery.
7	To integrate the modelled components in the form of a plant and to conduct a detailed mass and energy balance for the ammonia/ammonia+urea production process resulting from the FW and BW. To provide a modelling platform which is adjustable, having the capability to be applied for other waste compositions and substrate concentrations, etc, and flexible (linkable to other software such as MATLAB, ASPEN PLUS, and DWSIM).	7.1 Using VBA to connect the different components of the proposed plant into a single process resulting in a novel model for the production process of ammonia/ammonia+urea from waste. This requires the modelling of each component separately, then integrating the components as a single process.
8	To conduct a sensitivity analysis in order to define the uncertainty in the output of the proposed model and the identifiability of the parameters involved.	8.1 Defining the degree of variability of different design parameters in the process such as, waste composition, input flow rate, dilution rate, FW-to-BW ratio, air flow rate, etc. to determine which parameter is the most sensitive to change within the selected design constraints.
9	To assess the proposed process through two configurations and four CO ₂ fates, including use for urea production, and several smaller variations, resulting in 72 assessed processes for the LCA model.	9.1 Two hydrogen generating options (two-stage DF+AD and AD-only) are paired with four CO ₂ fates: -Scenario set i (the base case): CO ₂ is discharged directly into the atmosphere -Scenario set ii: (CCU) CO ₂ is used for urea production -Scenario set iii: (CCS) CO ₂ is compressed, liquefied, captured, and injected into the ground -Scenario set iv: (CCU) CO ₂ is compressed, liquefied, captured, and enters the commodity liquid CO ₂ market
10	To determine the environmental impacts of the proposed ammonia production processes, for multiple environmental impact categories including GHG emissions/ GWP as well as potential impacts beyond carbon such as resource use, human health, and ecosystem damage.	10.1 To conduct a cradle-to-gate LCA by means of SimaPro software for the proposed ammonia production process using multiple assessment methods Global Warming Potential (GWP, 20 years and 100 years) (Intergovernmental Panel on Climate Change (IPCC) 2013), ReCiPe 2016 endpoint (H), water scarcity (AWARE), GWP _{biogenic} (Greenhouse Gas Protocol V1.02), CML 2001, and Eco-indicator 99).

		10.2 Geographic location of the proposed ammonia plant is being assessed as a part of the LCA, in order to study the feasibility of adding solar PV or wind power as either an alternative source of power for the proposed plant or to be integrated as a hybrid system and the plant having accessibility to both FW and BW as the main feedstock.
11	To conduct a comparative analysis of different configurations and scenarios.	11.1 In terms of water usage, energy consumption, produced ammonia and urea, and the discharged CO ₂ emissions on a per ton basis for a given amount of ammonia. Comparing the co-product credits, transportation, gas leakage (N ₂ O, CH ₄ , CO ₂ , and NH ₃) from an environmental point of view. In terms of using solar PV or wind power as either an alternative source of power for the proposed plant or to be integrated as a hybrid system.
12	To carry out uncertainty analysis in order to identify the range of possible values of the environmental impact categories evaluated in this study.	12.1 Monte Carlo simulations with 3,000 steps were run for all of the technologies and scenarios, and their substituent parts, to assess distinguishability of technology scenarios and major contributors to uncertainty for the primary impact assessment methods.
13	To carry out sensitivity analysis in order to determine which input variables may substantially change the potential environmental impacts over the technology life cycle.	13.1 As the proposed production processes in this study are comprised of different magnitudes of energy and material inputs, gas leakage, product yields, water use, and distance from waste hub to the facility, it is important to determine which of these variables have the most effect on the proposed processes and whether this could change the relative performance rankings.
14	To compare and evaluate potential environmental impacts, including climate impacts, for the modelled ammonia production processes with available ammonia technologies from library and literature.	14.1 Comparison was carried out using different impact assessment methods (ReCiPe 2016 endpoint (H), IPCC 2013 GWP 100a, CML 2001, and Eco-indicator 99).

1.4 Research scope

The research scope covers a techno-environmental assessment of several configurations of new, sustainability-driven ammonia production technologies in order to determine whether a waste-based process designed first around CO₂ capture and utilization can compete on the basis of key performance indicators for sustainability (carbon emissions, water, and power use) or displace existing ammonia technologies.

Environmental impacts are assessed from cradle-to-gate, including, production of inputs, processing of inputs, and production of primary products at the facility gate. The project concept was based on taking a blended approach to anticipatory/prospective design (this is paired with anticipatory LCA/emerging technologies LCA in the environmental assessment), so mature technologies for base operations are used with more novel components as a means of enabling non-incremental technological advances. Each selected processing unit in the modelled system was chosen based on its potential to decrease environmental impact and increase product yields, while functioning successfully in concert with the other technology components.

Process operations are based on chemical engineering properties and the model utilizes basic thermodynamic, electrochemical, kinetic and stoichiometric equations where relevant. For the bioreactors neither biological aspects of the microbial systems nor fundamental chemistries are within scope of this research. This study elected to focus exclusively on the green design and technical assessment, excluding the economic component (cost estimations or financial assessments), to avoid a tendency to value economic factors over the technical and environmental. As a sustainability-driven design approach, the monetary aspects are intentionally not given primacy.

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Chapter 2

Literature Review

In this chapter, a critical review of different sustainable hydrogen production processes, emerging technologies for sustainable ammonia synthesis, and a comparative LCA of various ammonia production methods was conducted. To change the role of CO₂ in the transition to a circular economy, a review of the two CO₂ fate options (CCS and CCU) for fossil and waste-based ammonia production processes were carried out.

Finally, a CCU option for producing urea as a N-based fertilizer was selected and various urea production technologies were assessed. It has been found that through the review of each of the studied technologies, either large amounts of GHG emissions are produced or high volumes of pretreated water is required or a combination of both these factors occur. As a result, waste-based processes were chosen based on the sustainable design principles.

This chapter was drafted based on the publications submitted to *Frontiers in energy research and International journal of hydrogen energy*:

Ghavam, S., Garcia, G.G. and Styring, P., (2021). A novel approach to ammonia synthesis from hydrogen sulfide. *International Journal of Hydrogen Energy* [online]. 46, 4072–4086. [Viewed 2 May 2021]. Available from: doi: 10.1016/j.ijhydene.2020.10.192.

Ghavam, S., Vahdati, M., Wilson, I.A.G., and Styring, P., (2021). Sustainable Ammonia Production Processes. *Frontiers in Energy Research* [online]. 9, 34. [Viewed 21 October 2018]. Available from: doi:10.3389/fenrg.2021.580808.

2. An introduction to hydrogen, ammonia, and urea production processes

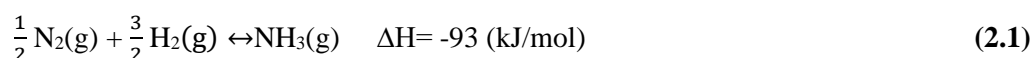
2.1 Literature review methodology

The aim of this section is to review the literature on conventional and new methods for sustainable ammonia production. Based on a thorough review of literature, a number of major apparent deficiencies in sustainable ammonia production technologies are described in *Chapter 1*. More sustainable, lower-carbon pathways for ammonia production described in this section are critical to ensure food security and energy storage in a manner that is compatible with deep decarbonization efforts. In this chapter, a systematic review was performed based on a formulated research question: “How to produce ammonia in a sustainable manner?” The research topics were classified in three main categories: 1) Finding the most sustainable pathways for hydrogen production required for ammonia synthesis 2) Finding sustainable new emerging ammonia production technologies 3) The challenges associated with sustainable hydrogen/ammonia production. The production of green ammonia considered in this chapter focuses on the use of hydrogen obtained from renewable sources. Different technologies for hydrogen production required for ammonia synthesis are evaluated in section 2.2. As hydrogen is the key component for ammonia synthesis, the focus of this study is on sustainable hydrogen production pathways. This section assesses the two most commonly utilized technologies for ammonia production which are SMR and water electrolysis coupled with H-B in terms of GHG emissions, electricity, and water consumption. The other technologies for sustainable hydrogen production, reviewed in this study are produced electrochemically (CH₄ assisted-SOFEC/NGASE) and biologically (DF coupled with other technologies such as photo fermentation and AD). The rationale behind choosing these specific processes is that there is a research gap in available literature in consolidating the evaluation of these technologies for sustainable hydrogen production required for ammonia synthesis. The cost of production for hydrogen through the use of CH₄ assisted-SOFEC is comparable to SMR in addition to being produced in a sustainable manner. The feedstock for this technology can be biogas resulting from the bioconversion of waste. According to the statistics mentioned in the introduction, reported by the EPA, the overabundance of waste streams poses a great threat to GHG control. Therefore, bioconversion of waste through DF, photo fermentation, etc. into important chemical compounds such as ammonia can be a new resource recovery alternative for fossil-based chemicals. Various emerging sustainable ammonia production technologies are presented in section 2.3 and finally, a critical review of different ammonia production technologies using LCA method is described in section 2.4. Based on the aim of this work, the keywords identified and the number of associated articles found were: “green “AND” hydrogen production” (23,825 articles), “green ammonia production” (83,059 articles), “energy carrier” (15,887 articles), “sustainable ammonia production” (37,539 articles), and “ammonia production” AND “Life cycle assessment” (241 articles). The analysis of articles was carried out based on the quality of research and relevancy to the review topic. In determining the papers to assess for this review, focus was exclusively on green and/or sustainable production technologies for hydrogen required for ammonia synthesis and ammonia production technologies. Specifically concentrating on technical and environmental assessment and excluding the economic aspects of these technologies, to avoid a tendency to value economic factors

over the technical and environmental. Moreover, location assessment for determining the site suitability for ammonia production was not included in this review. Although this study's focus is to critically review sustainable hydrogen and ammonia production processes, fossil-based technologies (e.g. conventional production routes using fossil fuels) are also included in the paper for the comparison of the data/results. However, the research strategy was to search for relevant scientific papers published in scientific journals using one of the most recognized academic databases. The databases selected for the purposes of the review were Science Direct, Web of Science, Springer, Wiley, etc. The research was performed considering the period of publication from 1992- May 2020. Following the search of various databases, the results were then filtered and reviewed through three steps: On the basis of the title, keywords, abstract, and after reading the full paper. Articles that were not related to the research questions or which were duplicates have been excluded. In addition, the snowball technique was used to find further relevant papers through checking the references of the collected papers and assessing these as mentioned above. As a result, a total number of 118 relevant publications were identified, of which, 116 papers are in English and two in the Italian language. Regarding the publication type, 43 research items were published as a journal article and the rest were published as dissertations, conference proceedings, government documents, reports, and handbooks. Data was collected from all the relevant papers cited in the references.

2.2 A review of hydrogen production technologies for ammonia synthesis

Ammonia is the result of the exothermic reaction between hydrogen and nitrogen shown by the equilibrium in chemical reaction 2.1. A process in which the equilibrium is pushed further to the right is highly desirable.



The main challenge for ammonia production is finding an economically viable, energy efficient, and more sustainable pathway for the production of hydrogen. As hydrogen is a key factor for all ammonia production processes, it is paramount to have access to a steady supply of this gas. An overview of various production routes for the hydrogen required for ammonia synthesis is depicted in Fig. 2.1.

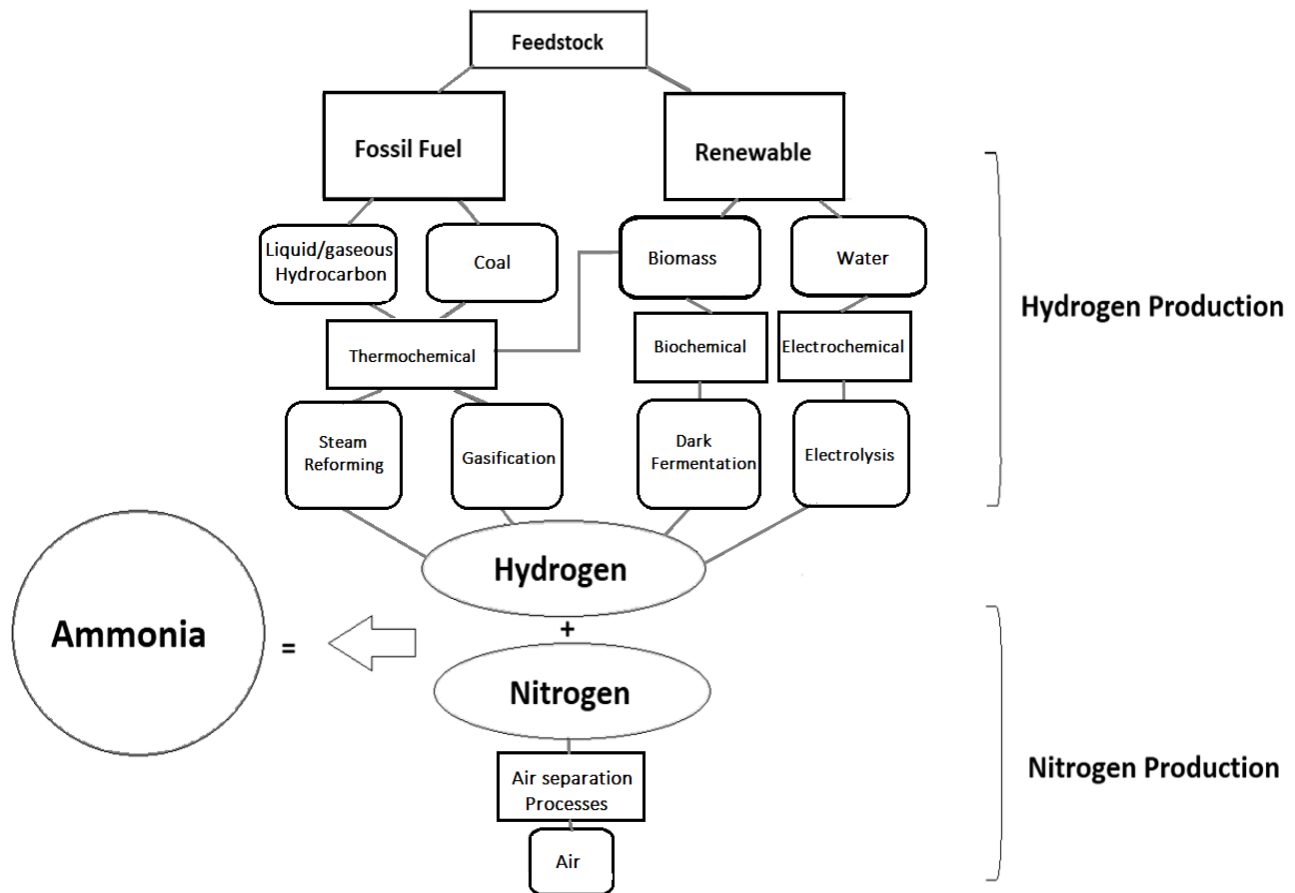


Fig. 2.1: Various hydrogen production routes.

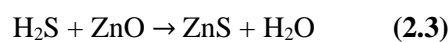
2.2.1 Widely adopted hydrogen production technologies

2.2.1.1 Steam Methane Reforming (SMR)

Globally, 72% of the hydrogen required for ammonia production is produced through SMR process (IEA, 2012). This process is comprised of four stages: Desulfurization, catalytic reforming, carbon monoxide (CO) conversion, and gas separation. Steam reforming process uses nickel (Ni) as the catalyst which is easily poisoned by sulfur (S), as a result, the sulfur compounds present in the feedstock must be removed before the reforming process. This can be accomplished by means of hydro-desulfurization along with a zinc oxide (ZnO) absorbent. The first phase of this process is the reaction between hydrogen and sulfur existing in the feed gas to produce hydrogen sulfide (H₂S). Through the following chemical reaction (2.2) (Morgan, 2013):



The second phase utilizes a bed of ZnO particles for H₂S removal, producing zinc sulfide (ZnS) in the process (2.3) (Morgan, 2013).



The main reforming process utilizes a furnace/heat exchanger comprised of numerous tubes; Ni based catalysts are within these tubes. The heat that is needed for the reaction is transported from the furnace/heat exchanger to the tubes via radiation. The main reformer partially transforms methane to carbon monoxide and hydrogen by means of steam that is provided to the system by burning of surplus natural gas through the following reaction. This process takes place in the pressure range of 2.97- 24.7 atm (Demirbas, 2008). Steam Reforming is an endothermic reaction; it requires heat for the chemical reaction of SMR to take place. This is shown in the following chemical reaction (2.4):



In the secondary reformer, additional energy is provided by internal combustion of natural gas with air (comprised of 21% Oxygen (O₂) and 79% N₂ to enhance the conversion (Morgan, 2013). The process air is compressed and heated up in the temperature range of 500- 600 °C (Morgan, 2013). The reaction is controlled to accomplish a 60% conversion rate based on the methane feed (Morgan, 2013).

The syngas is the product of steam reforming process which is comprised of hydrogen and carbon monoxide. In order to increase the hydrogen and carbon monoxide yield, a Water Gas Shift Reaction (WGSR) is incorporated. A WGSR is a reversible and substantially exothermic chemical reaction. The carbon monoxide shift conversion uses carbon monoxide as the reducing agent for water to produce hydrogen and CO₂. As a result, carbon monoxide which can poison the iron-based catalysts is removed from the gas mixture in favor of CO₂ and hydrogen, based on the following chemical reaction (2.5) (Morgan, 2013):



A schematic of (a) SMR process and (b) SMR coupled with H-B for ammonia production along with a detailed mass and energy balance is shown in Fig. 2.2. The reaction between natural gas, air and water taking place in the SMR process results in the production of CO₂, nitrogen and hydrogen. The nitrogen and hydrogen from SMR then enter the H-B process for ammonia production. The mass balance results adapted from Pfromm (2017) show that for the production of 1000 TPD of ammonia, 414 TPD of methane and 249 MJ/s of input energy is required.

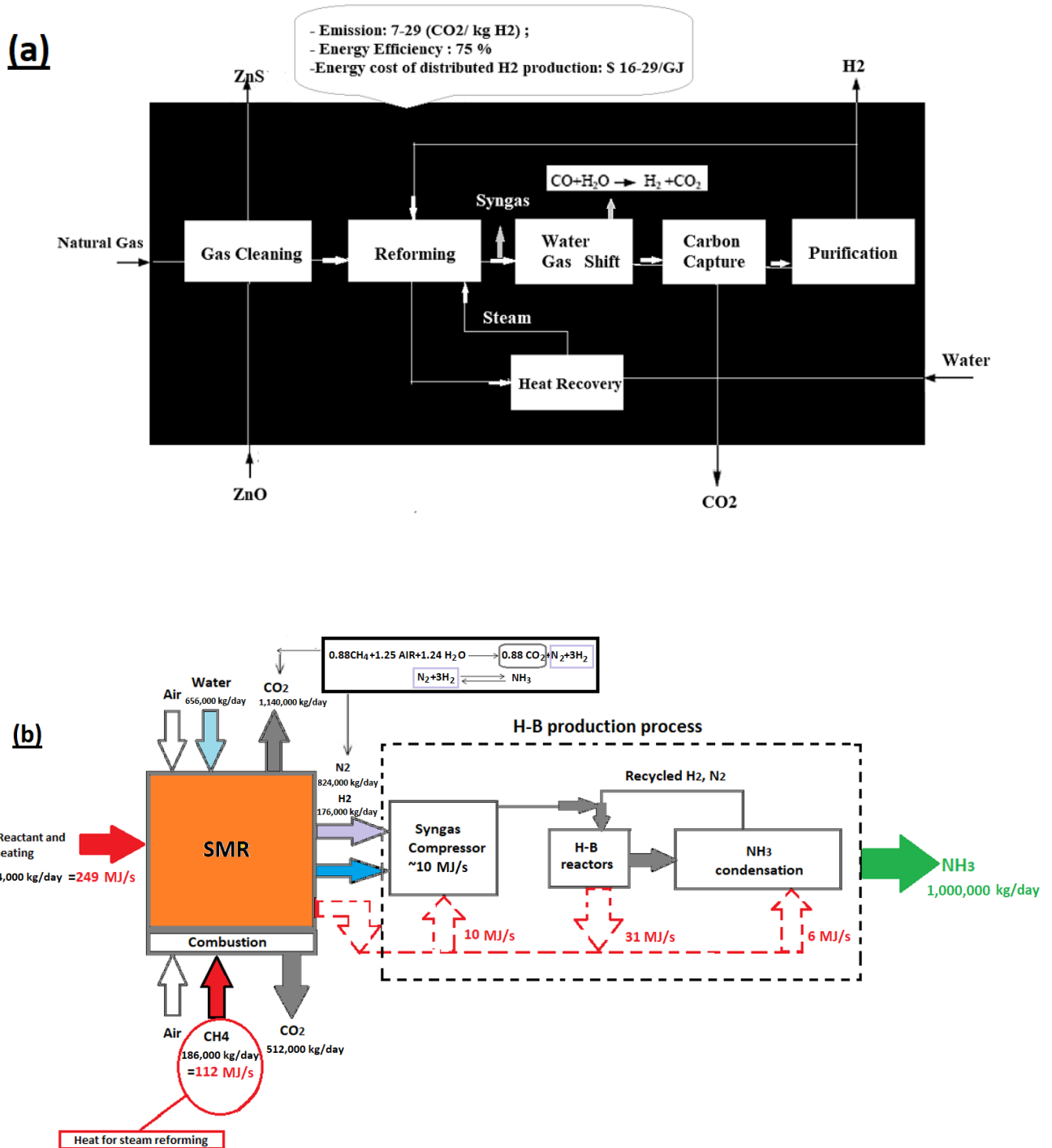


Fig. 2.2: A schematic of (a) Hydrogen production via SMR process (Matzen, Alhajji and Demirel, 2015) and (b) Ammonia production via SMR coupled with H-B process along with a detailed mass and energy balance (adapted from, Pfromm 2017).

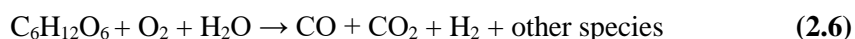
2.2.1.2 Coal gasification

Currently, the second most commonly used process for hydrogen production is coal gasification. Gasification is a thermochemical process through which the gasifier's heat and pressure breaks down coal into its basic chemical constituents. The produced gas is known as synthetic gas or syngas which is mainly comprised of, hydrogen, carbon

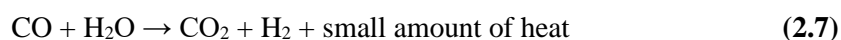
monoxide, and other gaseous compounds. There are primarily two types of coal gasification, one is known as Underground Coal Gasification (UCG) which occurs below the earth's surface, while the other is coal gasification, taking place above the earth's surface. UCG is a process through which coal is consumed by partial combustion with air, oxygen, steam or a combination of these components to produce syngas. The main advantage of using UCG is that the coal seam underground itself becomes the reactor and the coal is not required to be mined for gasification. According to Dincer and Bicer (2015) UCG is a promising option for the future use of unworked coal, generation of electricity, and other products with minimum GHG emissions. Moreover, it avoids the environmental impacts, safety, health risks, and costs associated with mining (Dincer and Bicer, 2015).

2.2.1.3 Biomass gasification

Gasification is a thermochemical process in which organic or fossil-based carbonaceous fuels are converted to a combustible gas (Pradana and Budiman, 2015). This process operates at high temperatures ($>700^{\circ}\text{C}$) with a controlled amount of oxygen/air/steam without combustion (2.6) (Molino, Chianese and Musmarra, 2016).

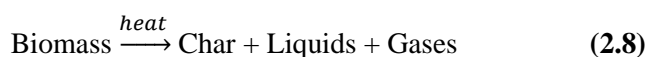


The carbon monoxide produced from 2.6 chemical reaction will then react with water to produce CO_2 and more hydrogen via a Water-Gas Shift (WGS) reaction as follows (2.7):



Generally, all types of biomass can be converted into syngas mostly composed of hydrogen, carbon monoxide, carbon dioxide, and methane via (1) Oxidation (operating in the temperature range of, $700-2000^{\circ}\text{C}$) (2) Drying (operating in the temperature range of, $100-150^{\circ}\text{C}$), (3) Pyrolysis (operating in the temperature range of, $250-700^{\circ}\text{C}$), and (4) Reduction (operating in the temperature range of, $700-1000^{\circ}\text{C}$) (5) Gasification (typical temperature range is between, $800-1100^{\circ}\text{C}$), and (6) Combustion (operating in the temperature range of, $800-1200^{\circ}\text{C}$) (Bridgewater, 1995; Molino, Chianese and Musmarra, 2016). Combustion is required for providing the heat needed for the endothermic gasification reactions to take place. A schematic of main stages for gasification is shown in Fig. 2.3. The produced syngas can be further used for power, heat, and fuel production such as, hydrogen, ammonia, methanol, ethanol, etc.

Biomass gasification has been considered as a promising approach for large scale production of biomass-based fuels and chemicals in terms of, energy security and environmental benefits of efficient utilization of biomass (Demirbas, 2008). However, there are several limitations for commercialization of biomass gasification such as, formation of high amounts of Tar and pyrolysis products, high amounts of ash and dust particles which remain in the gas, and the need for the gas to pass through the oxidation zone in which small ash particles are collected (2.8 and 2.9) (Zhang et al., 2016). Moreover, the fuel must be uniformly sized from 4-10 cm in order avoid blockage of the throat and permit pyrolysis gases to flow downwards (Zhang et al., 2016).



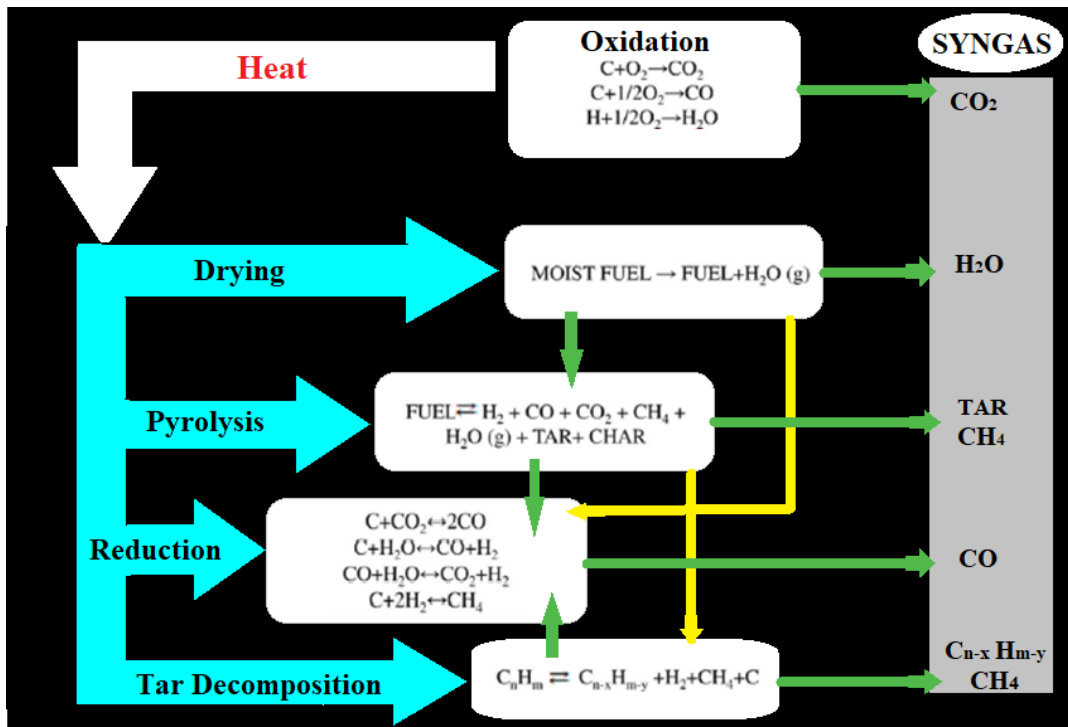
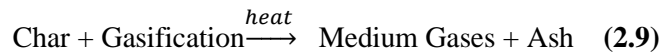


Fig. 2.3: A schematic of main stages for biomass gasification (Molino, Chianese and Musmarra, 2016).

2.2.1.4 Water electrolyzer

Electrolyzers are divided into two categories based on their operational temperatures: Low temperature and high temperature. The overall reaction of both low temperature and high temperature electrolyzers are similar. The current commercial low temperature (<100°C) technologies include Polymer electrolyte membrane (PEM), alkaline electrolysis as well as battolyser². In regards to high temperature technologies, ISPT (2017) refers to SOEC (operating in the temperature range of, 600-1000 °C), several times as an innovation that is able to enhance the economics of renewable ammonia in the future. In water electrolyzers such as alkaline electrolysis, the reaction takes place in a strong ionic solution in order to split the water into oxygen and hydrogen gases. The energy which is required for producing hydrogen gas via electrolysis is 118.7 kJ/mol as cited by the United States Department of Energy (USDOD) (Reaume, 2009). Oxygen and hydrogen are separated by applying voltage to the two electrodes in water. According to, Wijers (2011) this method is very inefficient because of the high decomposition voltage of water. Research was conducted in order to increase the yield of this process by applying SOFC as an electrolysis device. This device is known as Solid Oxide Electrolysis Cell (SOEC), it was found that the efficiency of this system is close to the efficiency of large scale SMR (Fig. 2.4). One of the benefits of

² Battolyser is a dual function device which is able to function as a normal battery during charging and discharging, this device is able to initiate the electrolysis of water.

operating at high temperatures is that the required electrical energy input is reduced. As cited by, ISPT (2017) the electrical input energy at 800°C is 25% lower than of 100°C. However, at the same time, this type of electrolyzer requires surplus input heat.

A comparison of various hydrogen production processes (thermochemical, biochemical, and electrochemical) along with a brief description of their feedstock and their source of energy is shown in Table 2.1. Various

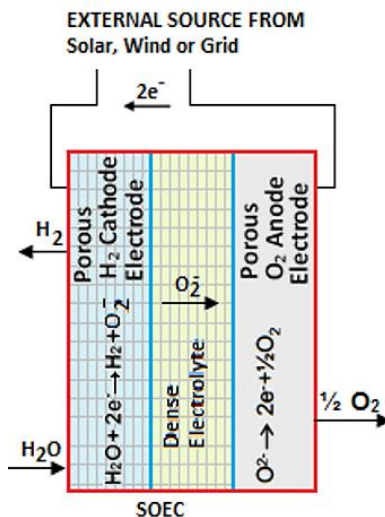


Fig. 2.4: A schematic of SOEC electrolyzer.

technologies for hydrogen production with their energy inputs and state of commercialization are described in Table 2.1. These technologies produce hydrogen directly without the need to be upgraded into pure hydrogen.

Table 2.1: A brief description of various hydrogen production processes (Acar and Dincer, 2018; Wijers, 2011).

Main energy inputs	Technologies	Brief description	State of commercialization
Electrical	Water electrolysis	Direct current is applied in order to split water into hydrogen and oxygen.	Large
	CH ₄ assisted-Solid Oxide Fuel Electrolysis Cell (SOFEC)/ Natural Gas Assisted Steam Electrolysis (NGASE)*	The entire process of an CH ₄ assisted -SOFEC is based on substituting high value electricity with cheaper methane. In the CH ₄ assisted-SOFEC, methane is added to the anode side of the electrolyzer, the decomposition potential (voltage) of water is decreased, and this results in a lower energy usage and higher conversion ratio of electricity for hydrogen production.	Medium/small
	Plasma arc decomposition	Purified natural gas (without H ₂ S, CO ₂ , H ₂ O, etc.) is passed throughout the plasma arc in order to produce hydrogen and carbon soot.	Large
Electrical & thermal	High Temperature Electrolysis (HTE)	Both electrical and thermal energy are utilized in order to initiate, water splitting for hydrogen production.	Large
	Hybrid thermochemical cycles	Both electrical and thermal energy are utilized in cyclical reactions.	Medium
Thermochemical	Coal Gasification (CG)	Conversion of coal through thermochemical process into syngas.	Large
	Fossil fuel reforming	Fossil fuels are converted into hydrogen and CO ₂ .	Large
	Thermolysis	Thermal decomposition of steam at temperatures higher than 2,226.85 °C.	Large
	Thermochemical processes	-Cyclic reactions (net reaction: water splitting into hydrogen) -Thermo-catalytic conversion -Biomass conversion into hydrogen	Large
Photonic	Photo-electrochemical cells (PEC)*	A hybrid cell which generates voltage and current through absorption of light simultaneously.	Small
	Artificial photosynthesis	Mimicking photosynthesis process for hydrogen production.	Small
	Photo-catalysis	Direct water splitting via photo-catalyst.	Small
Photonic & Biochemical	Bio-photolysis*	Biological processes (microbes/bacteria, etc.) through which water dissociates into hydrogen and oxygen in the presence of light.	Small
Biochemical	Dark fermentation (DF)*	Biological processes are utilized for hydrogen production in the absence of light.	Small
	Photo-fermentation (PF)*	Fermentation process initiates through exposure to light.	Small

2.2.2 CH₄ assisted-Solid Oxide Fuel Electrolysis Cell (SOFEC)

SOFEC technology is a type of electrolysis which aims to produce hydrogen at lower costs compared to other available electrolysis technologies. In the CH₄ assisted-SOFEC, methane is added to the anode side of the electrolyzer, the decomposition potential (voltage) of water is decreased, and this results in lower energy usage and a higher conversion ratio of electricity for hydrogen production. The system efficiency is up to 70% with respect to primary energy. Wijers (2011) also mentions a laboratory test based on SOFEC which showed an 85% decrease in the demand of electrical energy in comparison to the best alternative electrolysis available. University of California (2000) was the first study to propose adding fuel (methane) to the anode, thus lowering the voltage needed for the electrolysis process. The final cost of hydrogen through CH₄ assisted-SOFEC is competitive compared to hydrogen prices via SMR method (Luo et al., 2014). However, its high operational temperatures and long-term instability limit its practical application. Fig. 2.5 shows a schematic of CH₄ assisted-SOFEC with the chemical reactions involved.

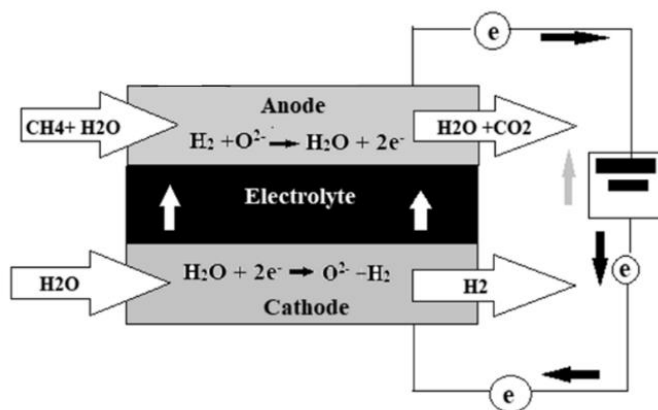


Fig. 2.5: A schematic of a CH₄ assisted-SOFEC (Wijers, 2011).

2.2.3 Natural Gas Assisted Steam Electrolyzer (NGASE)

Martinez-Frias, Pham and Aceves (2003), created a lab-scale model known as NGASE in which the operating voltage of this electrolyzer could be decreased by as much as 1 volt (from approximately 1.2 volts to 0.2 volts). This decrease in voltage is the result of applying natural gas to the anode side of the electrolyzer. In this technology, natural gas replaces air in the anode side while the cathode side is filled with water. Thus, this approach functions similarly to a fuel cell, generating electricity using an electrochemical reaction (Gross, 2008). NGASE is a specific type of CH₄ assisted-SOFEC in which methane has been added to the anode side of the electrolyzer for hydrogen production. Initially, NGASE was based on the theory that adding methane to the anode would decrease the electrolysis voltage.

2.2.4 Photoelectrochemical hydrogen production

Both studies conducted by Wang et al. (2018) and Bicer (2017) are focused on the H₂/NH₃ production process using solar energy-based systems. Wang et al. (2018) states that if ammonia could be produced directly from nitrogen and water, powered by sunlight, in an efficient and cost-effective manner, and through a technologically advanced process, this so-called green ammonia process could change the world. Bicer (2017) concludes that the use of

photoelectrochemical and catalytic hydrogen production processes are developing but a feasibility study for these methods needs to be conducted to investigate their viability. In photoelectrochemical approaches, a photosensitive material such as a semiconductor is required in which an electrodeposition system is mainly used. There are various types of deposition routes which operate at different temperatures (some higher than 100 °C). Wang et al. (2018) has presented various processes for ammonia production such as the study conducted by Ali et al. (2016) using solar energy. The obtained results show that the yields of solar ammonia along with the light powered nitrogen reduction processes are presently in the $\text{nmol g}_{\text{cat}}^{-1} \text{h}^{-1}$ to $\mu\text{mol g}_{\text{cat}}^{-1} \text{h}^{-1}$ range and are not enough for implementation on an industrial scale.

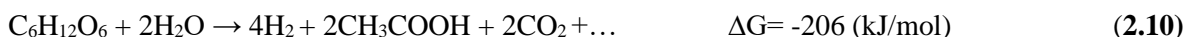
2.2.5 Biological hydrogen production processes

One of the main challenges of ammonia production from biomass using a biological hydrogen production process according to Arora et al. (2016) is that ammonia production from biomass is only feasible in large volumes (global level ammonia production). Due to economies of scale, smaller plants are at a disadvantage when compared to large scale plants. Arora et al. (2016) also mentioned that transporting biomass at longer distances (> 100 km) is not economically viable since the cost of transportation will exceed the value of energy in the biomass. This is due to the fact that biomass has a lower energy density when compared to fossil fuels. When assessing the hydrogen production processes for ammonia production this issue needs to be taken into account.

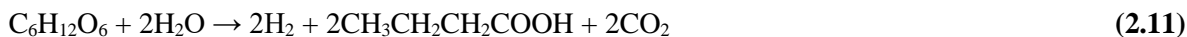
2.2.5.1 Dark Fermentation (DF)

Dark fermentation is a fermentative conversion and versatile bioprocess for production of molecular biohydrogen from various biodegradable renewable feedstocks by means of a wide range of different types of bacteria (Kothari et al., 2017; Yaswanth, 2018). This process takes place in anoxic and anaerobic conditions (in the absence of oxygen) in which, during this process, a large spectrum of anaerobic fermentative bacteria such as clostridium, facultative anaerobes such as *Enterobacter*, and aerobes such as *Bacillus* are involved in the fermentation process (Ghimire et al., 2015). The main mechanism for this process to take place is by the decomposition of carbohydrate rich substrates through microorganisms such as, *Clostridia Sp.*, *Enterobacter Sp.* to hydrogen and carbon dioxide gases and other intermediate products such as Volatile Fatty Acids (VFAs) and alcohols. The main by-product of DF process are volatile fatty acids, lactic acids, alcohols, and hydrolyzed residues. These by-products can be utilized in other biological processes for valorization through energy recovery or can be utilized as a feedstock for chemical production. Reddy (2016) states that temperature is one of the factors that affect the fermentation process which shifts the metabolic pathway to hydrogen production. These temperature ranges are: Mesophilic (operate at temperatures in the range of 25–40°C), thermophilic (operate at temperatures in the range of 40-70°C), extreme thermophilic (operate at temperatures in the range of 65-80°C), and hyperthermophilic (operate at temperatures higher than 80°C). Anaerobic bacteria which are more active in mesophilic and thermophilic temperatures are utilized for converting a wide spectrum of waste such as, sucrose, cellulose, glucose, and starches with pure strains and genetically improved cultures as seen in the reaction 2.10 (Arslan et al., 2015). Enhancing the hydrogen yield from 4 mol H₂/mol glucose to 12 mol H₂/mol glucose can increase the hydrogen production yields as shown in reaction 2.10 (Sen, Shakhdiwepe and Banerjee, 2008). Improving the hydrogen yield is related to the fermentation path and final products (Ghimire et

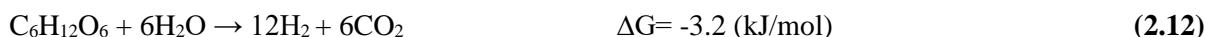
al., 2015). If the acetic acid (CH₃COOH) is the byproduct of the reaction 2.10, a theoretical maximum of 4 mol H₂/mol glucose will be achieved as (Ghimire et al., 2015; Sen, Shakdwipee and Banerjee, 2008):



Furthermore, when butyrate is the sole product in the process, according to reaction 2.11, a theoretical maximum of 2mol H₂/mol glucose is obtained:



For the complete oxidation of glucose to hydrogen and carbon dioxide as shown in reaction (2.12), a theoretical maximum of 12 mol H₂/mol glucose is acquired as (Sen, Shakdwipee and Banerjee, 2008):



The reaction in 2.10 is for complete oxidation and is based on theory and not yet applied experimentally. The actual hydrogen yield will always be lower than the theoretical yield. The main challenge with DF as cited by Sen et al. (2008) is the low hydrogen concentration which is in the range of 40-60%. Increasing hydrogen yield to over 4 mol H₂/mol glucose makes the hydrogen economically viable. Another pathway to enhance the hydrogen yield of DF is to couple it with other processes, such as photo-fermentation, methanogenesis, Microbial Electrolysis Cell (MEC) and Microbial Fuel Cell (MFC) (Reddy, 2016; De Gioannis et al., 2013). A schematic of biochemical stages of organic waste decomposition for biogas production is shown in Fig. 2.6. These stages are comprised of, hydrolysis, acidogenesis, and acetogenesis.

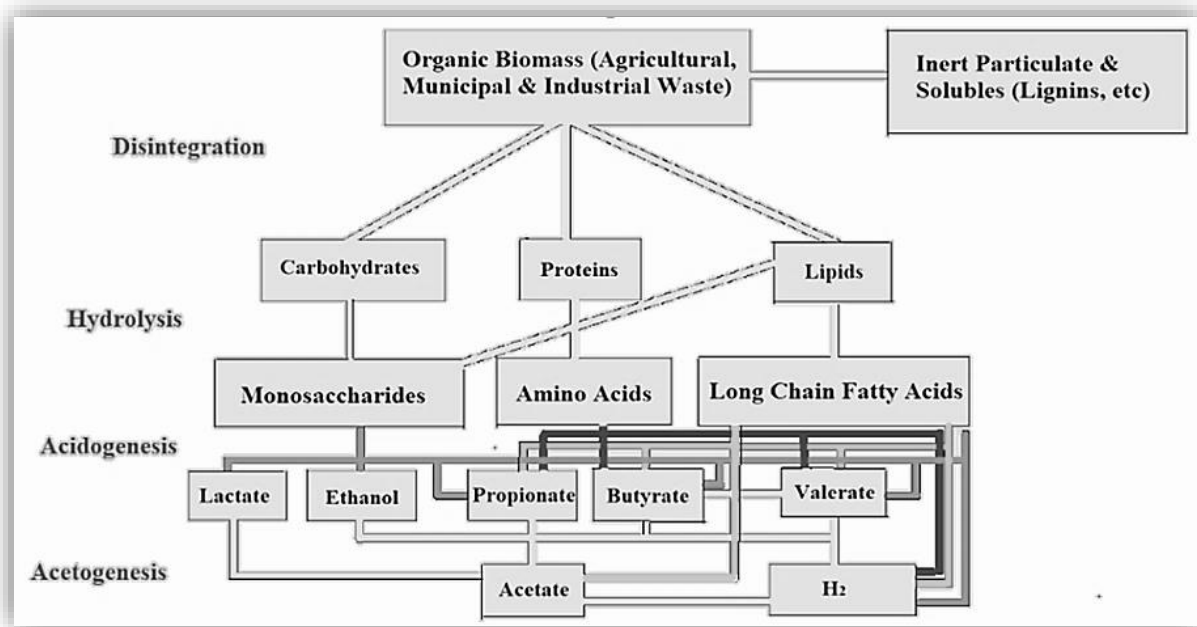


Fig. 2.6: The biochemical process of waste decomposition for biogas production (Ghimire et al., 2015).

DF coupled with AD

According to Liu (2008) a two-stage process which combines biohydrogen and biomethane production is one possible solution for enhancing the efficiency of the DF process. Producing hydrogen solely from DF is not economically viable because of low hydrogen yields and difficult operating conditions with many variables, such as maintaining the pH, temperature, Organic Loading Rate (OLR) and specific OLR at a set point. For example, experiments have been conducted on FW for a two-stage AD process under different operating conditions (pH, temperature, OLR, and HRT) as shown in Table 2.2 (Cavinato and Pavan, 2011; Bolzonella et al., 2018). This shows that the highest Specific Hydrogen Production (SHP) rate and Specific Gas Production (SGP) rates were attained at a pH of 5.5 and HRT of 1.3, which is the lowest when compared to the two other mentioned studies. However, the recirculation rate is the highest when compared to other studies. The inhibition of the methanogenic activity can be accomplished by monitoring the operating parameters such as pH, temperature (heat treatment of inoculum can inactivate hydrogenotrophic methanogens, enhance hydrogen producing bacteria, and select anaerobes that form spores.), OLR or using additives (De Gioannis et al., 2013).

Table 2.2: The effect of changing the recirculation rate on two-stage DF+AD.

References	Substrate	Recirculation rate	First phase				Second phase				
			T	pH	HRT	OLR	SHP	T	HRT	OLR	SGP
		Qr/Qin	(°C)		(day)	(kg TVS/m ³ d)	(lH ₂ /kg TVS)	(°C)	(day)	(kg TVS /m ³ d)	(m ³ biogas/kg VS fed)
Kataoka et al., (2005)	Food waste	0.25-0.5	55	5-6	2.5-6	8.45	20-30	55	18-30	1.18	0.49
Chu et al., (2008)	Food waste	2	55	5.5	1.3	38.4	205	35	5	6.6	0.61
Lee et al., (2010)	Food waste	1	55	5.5-5.57	1.9	39	83	55	7.7	8.4	0.21(CH ₄)

Anaerobic digestion is a continuous biochemical process in which complex substrates are decomposed and digested via microbial actions and converted into biogas (Pengyu et al., 2017). The AD process takes place in the absence of oxygen, and occurs through four main steps: Hydrolysis, acidogenesis, acetogenesis, and methanogenesis. Biogas production from an AD process is a complex mechanism where several chemical and biochemical phenomena take place. Through these steps, large organic materials that make up biomass are broken down into smaller molecules by using microorganisms in the absence of oxygen. The output from the reactions of one group of microorganisms are the substrates for the next set of reactions. As a result of the AD process, biomass is converted to biogas composed of: Methane, carbon dioxide, sulfur compounds such as hydrogen sulfide (H₂S), and trace amounts of other gases such as ammonia, nitrogen, methane, steam, etc.

In a two-stage biohydrogen and biomethane process with household solid waste as substrate operating at 37°C, a hydrogen yield of 43 mL/gVS added was accomplished (Liu 2008). Furthermore, the methane production in a double-stage process was 21% higher than in conventional one-stage methanogenesis process since it enhanced the hydrolysis of the household waste, which proved to be the main impediment to AD of household solid waste. Micolucci et al., (2018) conducted an experiment on a single-stage AD process on FW on a laboratory scale and

reported a methane yield of $0.45 \text{ m}^3 \text{ CH}_4/\text{kgVS}$, with a VS removal rate of 83% achieved. Anaerobic digestion was also performed in a two-phase process and showed a substantial reduction in the yield of volatile solids from 1,751 kg/day to 1,233 kg/day compared to a single stage process. The resulting energy and mass balance demonstrate that the single-phase processes were 33% superior in terms of biogas production and energy yields (Micolucci et al., 2018). However, by comparing energy and mass balance with a two-stage reactor, the final results show that the average methane concentration for the two-phase process was 68% with a Soluble Microbial Products (SMPs) of 351 $\text{LCH}_4/\text{kg VS}$. For the single stage, methane concentration was 55% with 404 $\text{LCH}_4/\text{kg VS}$. Eventually, the author points out that the two-stage AD process can increase energy recovery from biomass compared to a single-stage process. Micolucci et al., (2018) also carried out an experiment in order to determine how the AD of an organic feedstock with a Chemical Oxygen Demand (COD) composition of almost 1 g/L of FW or Organic Fraction of Municipal Solid Waste (OFMSW) could be consumed in both single-stage and two-stage processes. By comparing both AD processes, it was found that the two-stage process has a removal efficiency which is 17% higher than of a single-stage process. In addition, by applying a digestate dewatering treatment after the process, the two-stage system showed 33% less disposable sludge. The SGP in the second-stage was higher and about $0.88 \text{ m}^3_{\text{biogas}}/\text{kg VS}$ compared to the single-phase reactor which was $0.75 \text{ m}^3_{\text{biogas}}/\text{kg VS}$. The overall two-stage system efficiency for removal was 16% higher when compared to a single-phase AD process. This indicates resilience and high biogas production yields, using a two-stage rather than a single-phase configuration process that will significantly affect the methanogenesis process. Fermentation plays the role of pretreatment for the FW as it enhances the conversion efficiency of the volatile fraction to biogas production (Micolucci et al., 2018).

2.2.5.2 A comparison of various biological hydrogen production processes

The main barriers for implementing large-scale DF for hydrogen production are: (a) low hydrogen yields, and (b) high production costs because of the high costs of feedstock. By choosing a low-cost feedstock such as biomass, including agricultural residues, and organic waste resulting from industries and municipalities, this challenge can be solved (Ramirez-Morales et al. 2015). According to Zilouei and Taherdanak (2015), Chong et al. (2009) and Kapdan and Kargi (2006), this will give DF a competitive economic advantage compared to other methods currently being utilized for hydrogen production such as water electrolysis and biomass gasification. A comparison of different types of biohydrogen production methods are shown in Table 2.3.

Dark fermentation is superior to other biological hydrogen production processes mentioned in this study, since it does not require light to operate. As a result, it can be implemented even in locations without accessibility to an intensive light source and the high costs associated with halogen lamps. The hydrogen production rate rises when the light intensity increases and reaches a saturation point, depending on the feedstock and microorganisms. Lack of infrared light between 750-950 nm wavelengths will lower hydrogen production by 39%. According to Argun and Kargi (2010), both the source and the intensity of light affect the yield and rate of hydrogen gas production in photo-fermentation. Liu et al. (2009) carried out a study to assess the effects of light intensity and light/dark cycle on biohydrogen production with a combination of *Clostridium butyricum* and *R. faecalis* RLD-53. Throughout the combination process, the highest yield was stated to be $5.374 \text{ mol-H}_2/\text{mol-glucose}$.

Argun and Kargi (2010) also conducted a study on the same cycle (DF/photo-fermentation) for biohydrogen production by *R. sphaeroides*-RV. Halogen lamps were found to be the most appropriate light source with a light intensity of 5 klux. There was minimal production of hydrogen when accessibility to light was below 5 klux while at light intensities higher than 5 klux no production took place. Thus, the optimum hydrogen production is achieved at precisely 5 klux. Total hydrogen yield for the dark/light cycle was stated to be 4.55 molH₂/mol-glucose. Both dark and photo-fermentation can accept a wide spectrum of organic substrates as their feedstock to operate. Other biohydrogen methods such as direct and indirect bio-photolysis require water for hydrogen and oxygen production. The hydrogen production rate for DF is higher compared to the technologies stated in Table 2.3. The products resulting from DF according to 2.10 and 2.11 chemical reactions are hydrogen, carbon dioxide and volatile fatty acids which can be used as the substrate for AD to produce biomethane. A mixture of hydrogen produced from DF along with the methane resulting from AD process can produce bio-hythane, a mixture of hydrogen and methane (Bolzonella et al., 2018). According to Table 2.3, as cited by Tenca (2011), Valdez-Vazquez and Poggi-Varaldo (2009), Hawkes et al. (2007), and Akroum-Amrouche et al. (2013), it can be concluded that among the biohydrogen production methods, DF is the most efficient biological technology when coupled with methods mentioned for hydrogen production required for ammonia synthesis.

Table 2.3: A Comparison of different types of biological hydrogen production methods.

Technology	Organisms	Reactions	Products	Hydrogen yield (mmol H ₂ /Lh)	Advantages	Disadvantages	References
Dark-Fermentation	Anaerobic bacteria	$C_6H_{12}O_6 + 2H_2O \rightarrow 2CH_3COOH + 4H_2 + 2CO_2$ (2.13)	H ₂ , CO ₂ , VFA	77	<ul style="list-style-type: none"> -The configuration of the reactor is simple. - High yield of H₂ production. - Low cost -It can produce H₂ continuously without light. -This system is an anaerobic process so there is no O₂ limitations. - Utilizes waste streams. - Mixed culture friendly 	<ul style="list-style-type: none"> - O₂ is a resilient inhibitor of Hydrogenase. - Comparatively lower yields accomplished through this process. - As yields increase H₂ fermentation appear to become thermodynamically unfavorable according to Le Chatelier's principle. -The product gas stream contains CO₂ that needs to be separated from the H₂ stream. 	Valdez-Vazquez and Poggi-Varaldo (2009), Hawkes et al. (2007), Tenca (2011), Akroum-Amrouche et al. (2013), Singh et al. (2015)
Photo-Fermentation	Purple non-sulfur bacteria	$2CH_3COOH + 4H_2O \rightarrow 8H_2 + 4CO_2$ (2.14)	H ₂ , CO ₂	145-160	<ul style="list-style-type: none"> -An extensive range of spectral light energy by means of bacteria. - H₂ production from different carbohydrates and organic wastes -High hydrogen yield 	<ul style="list-style-type: none"> - Scaling-up the system. -O₂ has an inhibitory effect on hydrogenase. -Low conversion efficiency approximately, 1 to 5%. 	Tenca (2011), Akroum-Amrouche et al. (2013), Singh et al. (2015), Ciranna (2014)
Direct bio-photolysis	Hydrogenase (microalgae, cyanobacteria)	$2H_2O + (\text{light energy}) \rightarrow 2H_2 + O_2$ (2.15)	H ₂ , O ₂	0.07	<ul style="list-style-type: none"> - Can produce H₂ directly from water or sunlight. - A complete carbon free process - The solar conversion energy had a growth of ten times in comparison to trees and crops 	<ul style="list-style-type: none"> - Needs high intensity light. -O₂ can be detrimental to this system. - Lower photochemical efficiency. - Challenges for designing bioreactor in order to maximize light. 	Tenca (2011), Singh et al. (2015)
Indirect bio-photolysis	Nitrogenase (cyanobacteria)	$12H_2O + 6CO_2 (\text{light energy}) \rightarrow C_6H_{12}O_6 + 6O_2$ (2.16) $C_6H_{12}O_6 + 6H_2O (\text{light energy}) \rightarrow 12H_2 + 6CO_2$ (2.17)	H ₂ , O ₂	0.36	<ul style="list-style-type: none"> -Does not require organic electron donors (aside from CO₂) 	<ul style="list-style-type: none"> -Challenges for designing bioreactor in order to maximize light. -O₂ has an inhibitory effect on Nitrogenase. 	Tenca (2011), Ciranna (2014)

2.3 A review of sustainable technologies for ammonia production

Due to the important role of ammonia as a fertilizer in the agricultural industry and its promising prospects as an energy carrier, many studies have recently attempted to find the most environmentally benign, energy efficient, and economically viable production process for ammonia synthesis. There are a number of sustainable technologies for ammonia production, such as electrochemical ammonia production, Non-Thermal Plasma (NTP) synthesis for ammonia production, and nitrogenase-motivated peptide-functionalized catalyst for electrochemical ammonia production. These technologies will be assessed in sections 2.3.1, 2.3.2, and 2.3.3 respectively.

2.3.1 Electrochemical ammonia production

Electrochemical ammonia production technologies are divided into three categories based on the operational temperature range of the electrochemical cell: Low temperatures, under 100 °C, intermediate temperature in the range of 100-400°C and high temperatures in the range of 400-750 °C (Amar et al., 2011). According to Soloveichik (2017), the advantages of electrochemical technology compared to thermochemical (H-B) are in four major areas:

1. Higher efficiency, which permits energy saving.
2. Higher selectivity, meaning that less purification is required.
3. Lower temperatures and pressures, resulting in reduced Capital Expenditure (CapEx) costs through lower balance of plant.
4. Modularity, which makes these plants suitable for small to medium scale utilization.

2.3.1.1 Electrochemical synthesis of ammonia through low temperatures (<100°C)

For temperatures lower than 100 °C, a cell with a potassium hydroxide (KOH) solution as electrolyte and Nafion as the separation membrane, a platinum (Pt) anode and a ruthenium (Ru)/C cathode are utilized in order to synthesize ammonia (Kordali, Kyriacou and Lambrou, 2000). The maximum production rate for this is stated as *ca.* $2 \times 10^{-11} \text{ mol s}^{-1} \text{ cm}^{-2}$, operating at the temperature of 90 °C, resulting from steam and nitrogen with a 0.2-1 % Faradaic Efficiency (FE), which is defined as the proportion of protons that are converted to ammonia by migrating throughout the electrolyte. The electrolytes which are utilized for low temperature electrochemical ammonia synthesis in place of polymeric electrolyte membrane are, Sulfonated-Poly-Sulfone (SPSF) membranes, Nafion membranes or NH_4^+ in substitute to Nafion membranes (Lan, Irvine and Tao, 2013). Xu et al. (2009) investigated a maximum ammonia production rate of $1.13 \times 10^{-8} \text{ mol s}^{-1} \text{ cm}^{-2}$ operating at a low temperature of 80 °C with an applied voltage of 2 volt by means of a Nafion membrane (as the electrolyte), a Ni-doped SDC (Ni-SDC), $\text{NiO} \cdot \text{Ce}_{0.8}\text{Sm}_{0.2}\text{O}_{2-\delta}$ anode and a $\text{SmFe}_{0.7}\text{Cu}_{0.3-x}\text{Ni}_x\text{O}_3$ ($x=0-0.3$) (SFCN) cathode. Hydrogen and nitrogen were used as the reactants in the process, operating at atmospheric pressure. High FE, above 90% (90.4%) was accomplished. This figure is higher than was reported by other studies, when testing low temperature ammonia synthesis processes. As stated by Lan, Irvine and Tao (2013), ammonia is a weak base which can react with acidic membranes such as Nafion resulting in a reduction in proton conductivity. As a result, it has been stated that Nafion membrane utilization converted from H^+ form to the NH_4^+ form via exposing the cell to a flow comprised of ammonia solution with a FE

lower than 1%. Lan, Irvine and Tao (2013) carried out an experiment for ammonia production from air and water at ambient temperatures. The low FE of this experiment is due to the type of catalyst used (Pt) which is not the most appropriate choice for nitrogen reduction. Lapina (2013) states that air can be used in place of pure nitrogen, although some authors claim that oxygen poisons the catalyst used for the ammonia synthesis process (Marrony, 2015). Lapina (2013) specifies that the effect of using pure nitrogen or air (as the nitrogen source) on FE has not been reported in any study. Lapina (2013) also state that at low temperatures, ammonia production from nitrogen and hydrogen is spontaneous and, as a result, the minimum voltage needed is negative, meaning that there is no need to apply a voltage. Although in reality, applying voltage is required to overcome the electrode over-potential and ohmic losses in the electrolyte, while a limited current pass throughout the cell. If water is utilized in place of hydrogen, an applied voltage is needed to drive the reaction (Lapina 2013).

2.3.1.2 Electrochemical synthesis of ammonia through high temperatures (> 400 °C)

For high temperatures, in the range of 400 -750 °C, a solid-state proton conductor or oxide ion conductor is utilized as the electrolyte for electrochemical ammonia synthesis. Several studies have been conducted on the utilization of both proton ion conductors and oxide ion conductors such as, Marnellos, Zisekas and Stoukides (2000) and Skodra and Stoukides (2009). Skodra and Stoukides produced ammonia via steam and nitrogen at temperatures in the range of 450-700 °C using ruthenium as the catalyst supported on silver (Ag) or palladium (Pd) as the cathode. In their study, $\text{SrCe}_{0.95}\text{Yb}_{0.05}\text{O}_{3-\delta}$ as the proton conductor or $\text{ZrY}_{0.92}\text{Y}_{0.08}\text{O}_{2-\delta}$ as oxide-ion conductor were used as the electrolytes. For both, the production rates are respectively: 10^{-12} and 10^{-11} mol s^{-1} cm^{-2} with FE of 0.01 %. The FE stated by Marnellos and Stoukides (1998) and Marnellos, Zisekas and Stoukides (2000) was 90%, which was accomplished by using hydrogen and nitrogen in a cell with $\text{SrCe}_{0.95}\text{Yb}_{0.05}\text{O}_{3-\delta}$ electrolyte and palladium electrodes (Lapina 2013). In all the mentioned studies, the ionic currents, meaning the rates of ion migration throughout the electrolyte, were at the same scale. The ammonia production rates were approximately 3 orders of magnitude lower in the experiment conducted by Skodra and Stoukides (2009). One of the major downsides of high temperature ammonia synthesis is that it can decompose thermally after production. Liu et al. (2006) have reported ammonia production rates in the range of $7.2\text{-}8.2 \times 10^{-9}$ mol s^{-1} cm^{-2} operating in the temperature range 400- 800 °C by means of $\text{Ce}_{0.8}\text{M}_{0.2}\text{O}_{2-\delta}$ (M = La, Y, Gd, Sm) as electrolyte and Ag-Pd as electrodes. These authors claimed that a FE of 100% was achieved. There are other studies such as Wang et al. (2011) using the same type of electrode (Ag-Pd) doped with barium operating in the temperature range 400 – 600 °C with the ammonia production rate reported to be in the range of $1\text{-}5 \times 10^{-9}$ mol s^{-1} cm^{-2} and with FE of 40-50%. Amar et al. (2011) have also utilized carbonate-oxide composite electrolytes operating in the temperature range 400-450 °C, with the highest ammonia production rate reported to be 5.39×10^{-9} mol s^{-1} cm^{-2} , operating at the temperature of 450°C with a $\text{La}_{0.6}\text{Sr}_{0.4}\text{Fe}_{0.8}\text{Cu}_{0.2}\text{O}_{3-\delta}$ - $\text{Ce}_{0.8}\text{Sm}_{0.2}\text{O}_{2-\delta}$ composite cathode, $\text{NiO-Ce}_{0.8}\text{Sm}_{0.2}\text{O}_{2-\delta}$ anode, and composite $\text{Ce}_{0.8}\text{Sm}_{0.2}\text{O}_{2-\delta}$ Li_2CO_3 - Na_2CO_3 - K_2CO_3 as the electrolyte.

2.3.1.3 Different types of polyelectrolytes utilized for electrochemical ammonia synthesis

There are four main classifications of electrolytes utilized for electrochemical ammonia synthesis which are: (i) liquid electrolyte operating near room temperature; (ii) molten salts operating at intermediate temperatures of 180-500°C;

(iii) composite membranes comprised of a conventional solid electrolyte mixed with a low melting salt, operating in the temperature range of 300-700°C; (iv) solid-state electrolytes with an extensive operating temperature range from approximately ambient temperature to 700-800°C which depends on the type of electrolyte membrane utilized (Dicer and Bicer, 2018 ; Hughes et al., 2015). These electrolytic ammonia production routes are presented in Fig. 2.7 with brief descriptions.

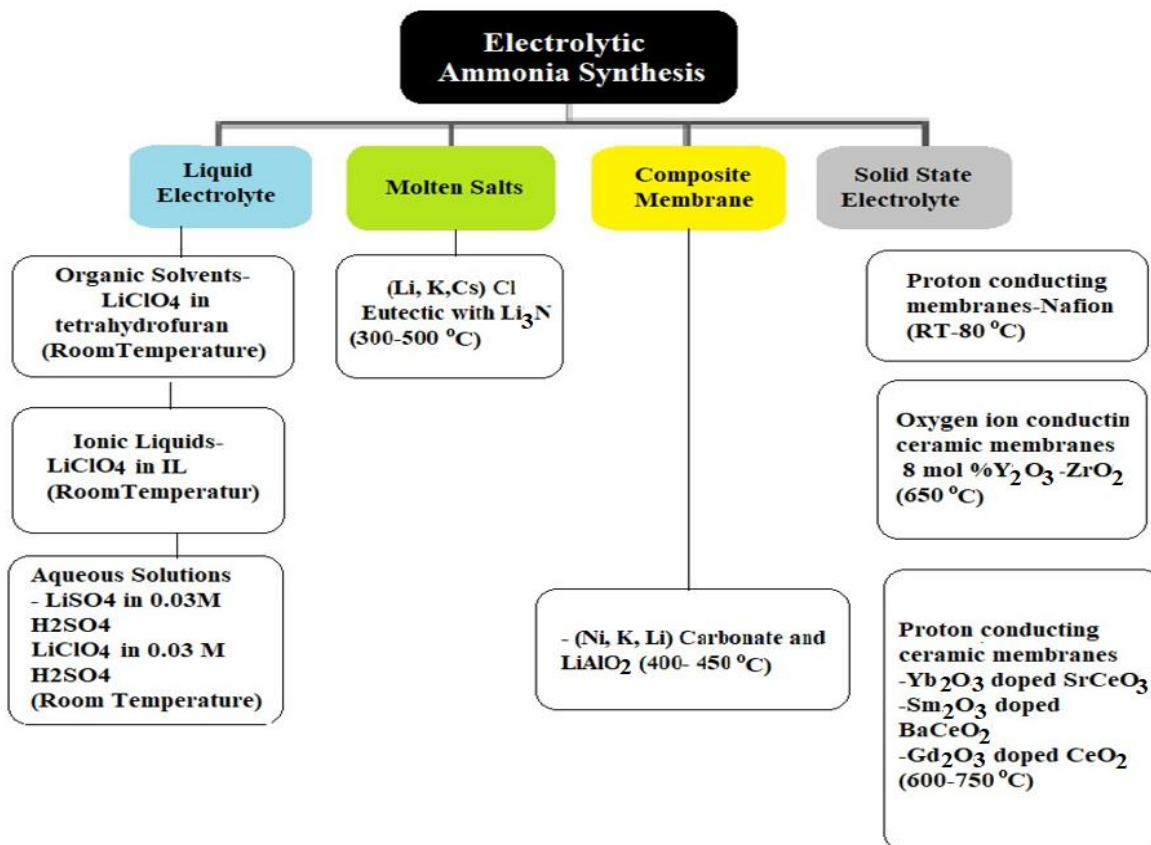


Fig. 2.7: Different electrolytic routes for ammonia production (Giddey, Badwal, and Kulkarni, 2013).

There are several issues associated with the catalytic process for ammonia synthesis such as, low conversion, severe environmental pollution, and high energy usage. These problems are addressed by utilizing electrolytic ammonia synthesis technologies (Amar et al., 2011). There are a number of problems associated with electrolytic ammonia synthesis such as low production rates (usually in the range of 10^{-13} - 10^{-8} mol s^{-1} cm^{-2}) except for polymer electrolyte membranes which have a 10^{-8} mol s^{-1} cm^{-2} production rate and instability issues of the acidic electrolyte membrane.

Current studies suggest that electrolytic reduction of nitrogen using heterogeneous catalysts has been shown to be a green and sustainable pathway for ammonia production. In this process, ammonia is synthesized from water and nitrogen powered by renewable energy sources such as solar/wind under ambient conditions. The most important elements for producing ammonia through electrochemical Nitrogen Reduction Reaction (NRR) system powered by renewable energy sources are electrocatalysts. Electrocatalysts need to be designed for optimizing the mass transport, physisorption, chemisorption, and transfer of electrons and protons to reach high selectivity and catalytic performance. Although producing ammonia through NRR is a promising sustainable technology, many of the

electrocatalysts for this system have a low FE and ammonia yield rate compared to the conventional H-B process (Guo et al., 2019).

2.3.2 Non-Thermal Plasma (NTP) synthesis for ammonia production

The volatility of fossil fuel prices, which are the main feedstock for the H-B process, the need for large volumes of fossil fuels to power the process, and the high operational costs associated with its high operating pressure (150-300 bar) and temperature (400-500°C) make this technology energy intensive (Peng et al., 2018). According to Peng et al. (2018), all the stated factors make the current process for ammonia production not appropriate for implementation on a small and decentralized scale. They conducted research on plasma-assisted ammonia synthesis, using a NTP, which operates at low temperatures (approximately 50 °C) and pressure conditions of approximately 1 atm. This technology is able to address some of the problems associated with the H-B process, such as, the high capital costs, fossil fuel usage, etc. The two most critical challenges of this technology as stated by Peng et al. (2018) are: (a) nitrogen gas fixation and (b) back reactions. In addition, they state that the conversion and efficiency rates need to be improved as this technology is still in the research and development stage (available on a small scale). However, the advantages of this system according to Peng et al. (2018) are that the NTP process does not require fossil fuels to operate, has low capital costs (related to low operational conditions, transportation, and storage) and has a small physical footprint. This process is more compatible for distributed ammonia production in local farms and can be located where the end users are. The West Virginia University Research Corporation (WVURC) is also developing a technology known as Microwave-Plasma Ammonia Synthesis. This technology converts renewable electricity, water, and air into ammonia by means of plasma excitation (WVURC, 2016). In this process, the aim is to lower the operational pressures and temperatures which will lead to the production of ammonia at five times the conversion rate of the H-B process. According to WVURC (2016), this method differs from both electrochemical conversion processes such as Solid-State Ammonia Synthesis (SSAS) and catalytic processes such as the H-B process. In this form of physical activation, the microwave plasma process is able to activate both nitrogen and hydrogen, and produce ions and free radicals that react over the catalyst surface in order to produce ammonia. One of the benefits of this process is that under the appropriate conditions, microwave heating is able to heat the catalyst selectively to reach the required temperature without the need for reactions to take place and without heating the bulk environment. This arrangement of a catalyst with a high temperature within a cool environment result in lower overall reaction temperatures and enhances the energy efficiency. In addition, as stated by WVURC (2016), the simplified design of this process is due to its low operational pressure. The low operational pressure of this process enables it to be a better fit with renewable energy sources, since the system is reportedly able to be turned on and off easily.

2.3.3 Nitrogenase motivated peptide-functionalized catalyst for electrochemical ammonia production

Ammonia is produced in nature through nitrogenase enzymes, with an efficiency of approximately 75%. As the efficiency of ammonia production in nature is very high, electrochemists have attempted to utilize these enzymes for industrial applications of ammonia synthesis such as in the study conducted by Loney et al. (2017). According to this study, electrochemical ammonia synthesis is a promising technology but its low operating temperature and pressure conditions have shown efficiencies of less than 1%, which would require a catalyst for enhancing the efficiency of

ammonia production. Furthermore, peptide functionalized catalysts were developed and tested in an Anion Exchange Membrane (AEM)-based system. The material used in this catalyst shows promising results compared to conventional catalyst approaches. Szymanski and Gellett (2017) also state that the electrochemical processes are modular and are able to be coupled with renewable energy sources such as solar and wind and also have the capability to function at relatively lower temperatures and pressures compared to the larger scale conventional ammonia production processes. For this reaction to occur, a catalyst is required that is selective to ammonia production. In order to address this issue, Szymanski and Gellett (2017) conducted a feasibility study in order to enhance ammonia selectivity by tailoring a nanoparticle catalyst morphology and utilizing peptides resulting from nitrogenase (a naturally occurring nitrogen splitting enzyme) in order to direct the desired reaction. Greenlee et al. (2017) addressed the selectivity issues for electrochemical nitrogen reduction by designing nano-particle catalysts, such as non-precious metal-based catalysts comprised of iron and nickel, that are bimetallic materials and are theoretically predicted to lead to optimum surfaces for nitrogen reduction. Greenlee et al. (2017) also reported that they are able to control the local surface environment of the catalyst by means of specifically structured short chain peptide series that had been inspired by the structure of the nitrogenase enzyme.

2.3.4 Hydrogen sulfide byproduct as the feedstock for ammonia production

Hydrogen/ammonia can be produced from chemicals such as hydrogen sulfide. Hydrogen sulfide is toxic, hazardous, and highly flammable under normal conditions and becomes explosive when it is mixed with air. When a fuel is reformed, gasified or digested, sulfur appears in the form of hydrogen sulfide (Winnick and Liu, 2003). Significant work has been carried out to reduce hydrogen sulfide to ppm levels before it can be used in applications such as for the production of sulfuric acid and in fuel cells (Zhang, Peng and Yu, 2015; Mbah, 2008). Hydrogen sulfide has a number of industrial uses, with the main application being the production of sulfuric acid and elemental sulfur (ATSDR, 2016). This chemical compound can be commercially obtained through two different methods: (1) Capture from gas mixtures and chemical means, and (2) Capture from natural gas and gases that are related to crude oil production, which are comprised of different levels of hydrogen sulfide, from trace to high amounts (70–80%) (ATSDR, 2016). There are also a number of companies that purify hydrogen sulfide at different levels and transport it in high volumes (>1500 gal/day) with specific handling conditions to ensure safety. Annually, over 12 Mt of hydrogen sulfide is produced in the US as a byproduct of industrial activities (Mbah, 2008). This amount of hydrogen sulfide is not sufficient to solely meet the ammonia production demand. There are many routes for separating hydrogen sulfide from carbon-based gases, of which many are inefficient or produce other pollutants as their byproducts. Moreover, some of these methods are multistage processes that require large capital investments (Li et al., 2016). However, up to the time of publication of “A novel approach to ammonia synthesis from hydrogen sulfide” no studies assessed using hydrogen sulfide as the feedstock for ammonia production. Ghavam, Garcia Garcia and Styring (2021) has proposed a novel model for ammonia production from hydrogen sulfide through a series of compact processes (membranes). This novel production process is a clear example of considering the circular economy by using waste hydrogen sulfide to obtain an important, value-added product such as ammonia, specifically, highlighting the relevance of utilizing hydrogen sulfide for ammonia production. In this method, compressed air

enters an Ion Transport Membrane (ITM) for oxygen separation. The resulting oxygen is routed to a Solid Oxide Fuel Cell (SOFC). The remaining nitrogen after oxygen separation is divided into two streams: One stream is directed to an Electrochemical Membrane Separation (EMS) process as sweep gas and the other stream goes to SSAS as a feedstock for ammonia production. The hydrogen needed for ammonia synthesis is separated from hydrogen sulfide by EMS. Hydrogen sulfide is converted into hydrogen and sulfur in the presence of a sweep gas (nitrogen) which is the byproduct from the ITM. The hydrogen along with the nitrogen from the ITM enter the SSAS proton (H^+) conducting membrane for ammonia production. 25% of the hydrogen from EMS is fed into a SOFC for generating heat, power, and steam for the entire process. However, higher gas separation through the use of a single membrane in real world operation is not realistic. Therefore, hybrid processes such as, membrane separation technology integrated with a unit operation such as: Pressurized water scrubber, amine swing absorption, PSA along with EMS is necessary. Including a unit operation along with EMS would significantly increase the overall energy consumption. The aforementioned membranes along with their functionality and composition materials will be described in *Chapter 3*. Through the above-mentioned process, 10 TPD of hydrogen sulfide is required to produce 3 TPD of ammonia, this amount of produced ammonia is not sufficient for industrial applications. The amount of hydrogen sulfide required for industrial ammonia production would need to be approximately 300 times higher than the current amount to be commercially viable.

2.4 Environmental impacts of various ammonia production processes

LCA is a primary technique used to support decision making for sustainable development in production. A number of studies have been conducted on the comparative LCA of sustainable ammonia production pathways. These studies include Bicer et al. (2016) on a comparative LCA of different ammonia production methods and Frattini et al. (2016) on a system approach in energy evaluation of different renewable energy sources integrated into ammonia production plants. The same approach (producing an LCA) was carried out by Tallaksen and Reese (2013) and Arora et al. (2018), both selecting the Functional Unit (FU) of 1 kg of ammonia for its production using fossil fuels and renewable sources. Tallaksen and Reese (2013) compared both approaches in terms of the usage of energy and carbon emissions. However, Arora et al. (2018) identified the carbon emissions and costs related to ammonia production. The system boundary by Tallaksen and Reese in their study for ammonia production powered by wind was comprised of wind power, water electrolyzer, hydrogen compression, nitrogen separation/compression, ammonia production, and ammonia storage (Matzen, Alhajji and Demirel, 2015). However, the system boundary selected by Arora et al. (2018) was more detailed in comparison. Arora et al. (2018) estimated the emissions resulting from coal mining, biomass harvesting, transportation, electricity production, and utilities in their study, and also conducted an LCA on ammonia production. They concluded that the GWP of coal gasification with 4.22 kg CO_2 eq /kg NH_3 is the highest when compared to biomass gasification with 1.2 kg CO_2 eq /kg NH_3 , while SMR of natural gas falls in between with GWP of 2.81 kg CO_2 eq /kg NH_3 . However, in this study, coal gasification to ammonia production was priced lower than the other processes discussed due to lower energy consumption, feedstock cost, and not consuming significant amounts of energy related to CO_2 stream compression. Makhlof, Serradj and Cheniti (2015) also conducted an LCA and presented the results for production of 1 tonne of ammonia by SMR of natural gas in Algeria. The results indicated

that the GWP is high, which is due to the amount of GHG emissions of 1.44 t CO₂ eq/ t of NH₃. Although this figure (1.44t CO₂ eq/ t of NH₃) is lower when compared to the results reported by Arora et al., (2018) for the production of ammonia from natural gas, which is said to be 2.81 t CO₂ eq/ t of NH₃) of GHG emissions. The system boundary for the LCA differs in the two studies. In Makhlouf, Serradj and Cheniti (2015), the system boundary consists of an upgrading stage along with a SMR process for ammonia synthesis. In addition, Makhlouf, Serradj and Cheniti (2015) stated that when calculating the GHG balance, only the amount of natural gas utilized as fuel was considered and the amount of process gas was not taken into account. The outcome of the study shows that the energy requirement for ammonia production by the SMR of natural gas in Algeria was 25.16% higher than of other locations globally. This figure was said to be 51.9×10^3 MJ/t of ammonia while the global energy requirement for ammonia production is reported to be 41.5×10^3 MJ/tonne (IEA, 2007). Arora, et al. (2017) conducted their LCA in order to compare the GWP of biomass to ammonia production processes through three different configurations, SMR, Auto-thermal Reforming (ATR) and carbon dioxide reforming. All three configurations were modelled and compared for utilization of three different types of biomass feedstock: Straw, bagasse, and wood, in order to understand the effects of their composition on supply chain, economics, and environmental factors for ammonia production. Their study emphasized that GWP will be lowered if biomass is used as the feedstock for ammonia synthesis. Among the three types of biomass used for ammonia synthesis in the study, bagasse has the lowest GWP followed by wood and straw pellets. However, Arora et al. (2017) concluded that the GWP of straw used as biomass for ammonia production is similar to the GWP of natural gas for ammonia synthesis when there is no electricity cogeneration. Among the three different types of biomass, wood has the highest ammonia production rate. Arora et al. (2017) conducted a Multi-Objective Optimization (MOO) showing that one route for reducing the GWP of biomass to ammonia process can be through the utilization of a proportion of the produced syngas resulting from biomass gasification which can also be used for electricity production. With this solution, the discharge of GHG emissions from the use of electricity will be lowered. However, this strategy will decrease the amount of ammonia produced, resulting in an increased output product price. Arora et al. compared the trade-off between ammonia production and electricity generation for three different types of feedstock and different results were obtained. All variables such as the specific type of biomass, economics, and the environmental profile correlate to a specific location. As reported for the production of a specific amount of ammonia using the same production process, the amount of water depletion when using bagasse is higher compared to using wood as the feedstock. For example, when using the SMR process for ammonia production, the amount of water depletion by means of bagasse is said to be 2.95×10^{-2} m³ while wood was reported to be 3.3×10^{-3} m³.

Tallaksen and Reese (2013) conclude that hydrogen production through water electrolysis powered by wind requires approximately 60 GJ of electricity/tonne NH₃. This total energy is considerably higher compared to conventional fossil fuel-based ammonia production, which is 36.6 GJ energy for production of 1 tonne of ammonia. According to Tallaksen and Reese (2013) the process requires less fossil energy since the system operates with wind power, resulting in lower GHG emissions when compared to running the system from the grid which was reported as 58.7 GJ/tonne. Whereas, Frattini et al. (2016) concludes that producing ammonia from renewable energy sources increases

the security of supply. Both studies agree that ammonia production from renewable energy sources results in lower CO₂ emissions.

Bicer et al. (2016) conducted this study on four different ammonia production methods by the H-B process using a feedstock of electrolytic hydrogen. They concluded: (1) ammonia production from a water electrolyzer powered by biomass and municipal waste offers a reliable alternative for distributed ammonia production facilities and can increase fertilizer production; (2) municipal waste-based ammonia production can be considered as one of the most environmentally benign methods among the proposed processes, since it has the lowest abiotic depletion, global warming, and human toxicity values (3) the renewable sources with their improved efficiency are able to lower the overall environmental footprint and can replace the current fossil fuel-based centralized ammonia production facilities. Frattini et al. (2016) on the other hand compared the efficiency of the energy flows and GHG emissions for the H-B ammonia production process by means of different hydrogen production pathways. Through this study they assessed three scenarios for renewable hydrogen production: (i) biomass gasification, (ii) electrolysis of water and (iii) biogas reforming. They compared these technologies with the conventional SMR of natural gas. Concluded that ammonia has the capability to be produced through an efficient manner using renewable energy sources, leading to an alternative method of a distributed, efficient, and sustainable ammonia production process. This results in a decrease in CO₂ emissions and costs, and an increase in production output. Moreover, this process allows for storing of renewable energy as a seasonal energy vector which has a high energy density with low emissions.

Frattini et al. (2016) made a clear case for the advantages of electrolytic hydrogen production compared to biomass gasification /biogas reformation in regards to the energy flux of each system. In regards to energy flows, they concluded that all proposed processes, including the conventional methods of SMR, have the same primary power usage within the range of 14-15 kWh/kg NH₃. New configurations have no effect on the amount of primary energy utilized for ammonia synthesis. This demonstrates that applying renewable energy does not limit the efficiency of the process. They made an explicit case for the advantages of electrolytic hydrogen production in comparison to biomass gasification or biogas reformation. Both studies aim to quantify the costs and advantages of integrating the H-B process with a renewable hydrogen feedstock resulting from biomass gasification, electrolysis of water operating by solar, wind, hydropower, nuclear power, and biomass. In summary, both projects investigated the carbon intensity of ammonia production. However, Bicer et al. (2016) expands its area of research to a full LCA, including GWP, Human Toxicity, and abiotic depletion, while the study conducted by Frattini et al. (2016) emphasized primarily on energy efficiency. The LCA study by Tallaksen and Reese (2013) on the other hand was more focused on environmental issues rather than raw material depletion. Another study conducted by Bicer and Dincer (2018) highlights the advantages of ammonia utilization in transportation (passenger cars) and power plants by evaluating different environmental impacts including: GWP, acidification, abiotic depletion, and ozone layer depletion. In this study ammonia is produced using water electrolysis in an electrochemical reactor using molten salt electrolyte powered by wind energy. According to Bicer and Dincer (2018) the GHG emissions for vehicles utilizing the aforementioned ammonia is approximately 37% lower compared to gasoline powered vehicles. This also applies to the production of about 0.27 kWh electricity in ammonia fired power plants compared to power plants operating on

natural gas, resulting in approximately 64% less kg CO₂ eq. Both Frattini et al. (2016) and Bicer and Dincer (2018) conclude that electrolytic hydrogen production for ammonia synthesis is advantageous from the environmental point of view due to the potential absence of GHG emissions. Bicer and Dincer (2018) also makes an explicit case for replacing conventional fuels with carbon free ammonia, thereby reducing significantly the GHG emissions associated with the transportation and power generation sectors.

2.5 Production capacity and distance from waste hub to the plant

One of the main challenges of ammonia production from biomass using a biological hydrogen production process according to, Arora et al. (2016) is that it is feasible only in large volumes (global level ammonia production). Due to economies of scale, smaller plants are at a disadvantage when compared to large scale plants. Arora et al. (2016) also mentions that transporting biomass at longer distances (> 100 km) is not economically viable since the cost of transportation will exceed the value of energy in the biomass. This is due to the fact that biomass has a lower energy density when compared to fossil fuels. When assessing the hydrogen production processes for ammonia production this issue needs to be considered.

2.6 Carbon dioxide fates resulting from fossil-based and biogenic sources

The resulting CO₂ from different sources (fossil-based and biogenic) produced alongside hydrogen can be captured, compressed, liquefied, and either injected into the ground (CCS) or assumed to enter the commodity liquid CO₂ market (CCU). The difference between CCS and CCU is the final use of the captured CO₂. CCS extracts the CO₂ from a gas stream resulting from major sources and transport it to a geographical site for long-term storage, including depleted oil and gas reservoirs. While CCU converts the captured CO₂ into value added products, materials, fuels, chemicals, etc. (Aldaco et al., 2019). According to Aldaco et al. (2019) when comparing CCS and CCU technologies in terms of reduction in CO₂ emissions it shows that CCS is a better option. However, CCU technology is economically viable and consumes lower fossil fuels when using renewables (Aldaco et al., 2019). Incorporating a urea production process is one approach to consume waste CO₂ which utilizes a large share of the end-product ammonia.

2.6.1 Carbon capture and utilization

2.6.1.1 Incorporating the urea production process

Incorporating urea production to consume waste CO₂, utilizes a large share of the end-product ammonia. Significantly, this CO₂ that is used in the urea will be discharged, thus, though the CO₂ in this system is biogenic, it will return to the atmosphere. However, according to the environmental analysis tools (e.g. SimaPro, GaBi) it will do so having displaced fossil CO₂ that would increase the atmospheric CO₂ levels. Thus, incorporating a green urea plant may slow, though not abate the GHG crisis, while getting useful services (in this study, offsetting the production of conventional urea, which uses significant fossil resources and leads to significant life cycle GHGs). Further discussion can be found in the LCA section. There are different methods for urea production such as Montedison urea process, solution recycle process, UTI HEAT- Recycle process, etc. (Mavrovic et al., 2000). However, the main processes that are currently being used for urea production are: Once through process, partial recycle, and total

recycle. A comparison of these processes is shown in Table 2.4. Among the processes assessed in Table 2.4, total recycle is the most efficient technology for urea production which has the highest product yield. The three main technologies of total recycle are, Snamprogetti process, Stamicarbon, and Advanced Cost and Energy Saving (ACES) by TEC (UN Industrial Development Organization and Int'l Fertilizer Development Center, eds. 1998). Snamprogetti is the most efficient process due to its high production yield (Li, 2013) (Table 2.5).

Table 2.4: A comparison of different urea production processes (UN Industrial Development Organization and Int'l Fertilizer Development Center, eds. 1998).

Technology	Description
The once through process	Is the simplest and most cost effective amongst all the aforementioned processes, although the production yield is low.
Partial recycle	Only a portion of the off gas is recycled back to the reactor. The production yield is higher than the once through process and its cost is lower than the total recycle process.
Total recycle	The unconverted NH ₃ and CO ₂ are recycled back to the reactor with a conversion of 99.8%. Moreover, its flexibility is higher in comparison to partial recycle and once through process, it's operational and investment cost is higher.

Table 2.5: A comparison of different urea production technologies (Baboo et al., 2016; UN Industrial Development Organization and Int'l Fertilizer Development Center, eds. 1998).

Characteristics	Snamprogetti Thermal stripping	Stamicarbon CO ₂ stripping	TEC ACES process
Description	Is based on an inner recycling system in which the solution of carbamate is recycled and recovered by a stripping process. This technology functions at temperatures in the range of 180 -190 °C and a pressure of 130 atm. In this system, the unreacted NH ₃ and CO ₂ are recycled back to the system and recovered.	In this process, heated, high-pressurized gaseous CO ₂ is used as a stripping agent for the carbamate solution. The stripper functions at 3 atm and a temperature of 120 °C. This technology for the recovery of its off gases uses a high pressurized pump system where the gases are compressed and condensed at a temperature of 65 °C and a pressure of 3 atm. In this system, 15% of the carbamate from the stripper is uncovered. The temperature of the discharge from the reactor is 185 °C and is recycled back to the stripper at a pressure of 140 atm.	The purpose of this system is to diminish the input energy for the urea plant; this is accomplished by combining the solution with the recycling and stripping steps. An efficient separation of unconverted materials is achieved along with a high CO ₂ conversion. This results in a CO ₂ conversion that is higher than all other urea processes. The consumption of steam in this technology is significantly lower than other total recycle systems.
Reactor pressure, atm	156	140	175
Reactor temperature, °C	188	183	90
Molar NH ₃ /CO ₂	3.3-3.6	2.95	4.0
Molar H ₂ O/CO ₂	0.5-0.6	0.39	0.6
CO ₂ conversion in reactor %	64	60	6.8
NH ₃ conversion in reactor %	41	36	34
CO ₂ conversion in synthesis %	84	79	N.A
NH ₃ conversion in synthesis %	47	79	N.A
NO. of high-pressure vessels-synthesis	5	4	5
Recirculation-stages	2	1	2
NH ₃ consumption	0.566	0.566	0.568
N.A= Not Available			

A schematic of urea production process through Snamprogetti process is shown in Fig. 2.8. This figure shows the urea production process based on a total inner recycling system, where unconverted NH_3 and CO_2 are recycled back to the reactor and recovered. The solution of carbamate is also recycled and recovered by a stripping process. In order to prevent high biuret formation, a vacuum evaporation system is utilized followed by a cooling system.

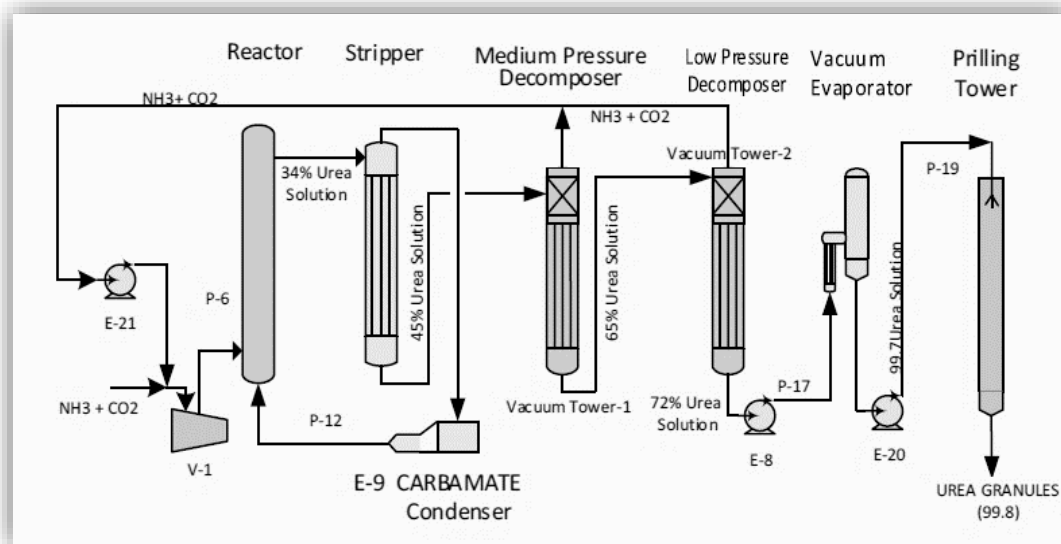


Fig. 2.8: A schematic of urea production through Snamprogetti process.

Due to its high operational temperature and pressure, the Snamprogetti process is rather inefficient. Recent studies have attempted to increase efficiency by lowering the operational conditions of these technologies. A study conducted by, Yahya suggests a green method for urea synthesis through lowering the operational temperatures and pressures (when compared to the above-mentioned urea production processes) by means of an electromagnetic induction and Nano-catalyst (Hematite and nickel oxide (NiO)) through a low energy consumption methodology (UN Industrial Development Organization and Int'l Fertilizer Development Center, eds. 1998; Yahya, 2018). However, this is operational on a small scale and requires more research and development in order to be commercially utilized on an industrial scale.

Sustainable urea production by employing the theory of change

The main obstacles to producing urea through conventional methods are the use of significant fossil resources leading to significant life cycle GHGs and the high energy intensity needed for operating such plants. Offsetting the production of conventional urea will be an important step toward sustainability. In order to synthesize low impact urea, based on the ToC, sustainability in the production of H_2 required for NH_3 and NH_3 needed for urea synthesis must take place. Unsustainability throughout each stage of the integrated H_2 - NH_3 -urea production process is the main problem associated with current urea production methods. Therefore, sustainable design principles need to be adopted in each of the urea production process steps (H_2 and NH_3). For this to occur, this study aims to review sustainable H_2 production processes and emerging technologies for sustainable NH_3 synthesis in order to address the stated issue by replacing current high impact production processes.

Conclusion

Ammonia can play the role of a fuel for energy storage as well as its primary use as the main ingredient for fertilizers, transport fuels, and many other applications, therefore, sustainable routes for its production are needed. As hydrogen is the main feedstock for ammonia synthesis, a review of various sustainable hydrogen and ammonia production processes has been carried out. In addition, an assessment of different studies on the environmental performance of ammonia production through LCA has been conducted. Two pathways (CCS and CCU) in which the CO₂ byproduct from fossil and waste-based hydrogen/ammonia production processes were studied. Finally, a CCU method through which urea is produced was assessed and different urea production processes were reviewed.

The review of ammonia production technologies shows that current processes are either multistage, energy or carbon intensive, or require significant amounts of water resources to operate. Identifying greener pathways (low carbon, low water, and low energy usage) for ammonia production is important to ensure food security and its application in energy storage. After reviewing several studies, there seems to be a lack of focus on processes that aim to reduce the amount of water required for sustainable ammonia production. However, there are a number of studies that have assessed the effect of water usage in different ammonia production processes (SMR and water electrolysis) by focusing on food security, environmental sustainability, and economics through conducting LCA. Two mature technologies, SMR and water electrolysis, both coupled with H-B and powered by renewable technologies are compared in this study. The former consumes less water while having higher GHG emissions and the latter emits less GHGs with higher water consumption. Of course, each hydrogen production technology has its pros and cons, the selection of these requires various criteria that would be specific to a particular project and context. These criteria include environmental impact, efficiency, cost effectiveness, resources and their use, commercial availability and viability, and system integration options (e.g., DF+AD) which need to be considered.

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Chapter 3

Methods and Tools

for

The modelling and Simulation

This chapter focuses on the scope and specifically, the action plan for modelling the proposed waste to green ammonia production. This is followed by a method section which is comprised of assumptions, research boundaries, and a selection of processing unit models along with the factors taken into consideration in selecting these models and equations pertaining to each component in the proposed process.

Through this study, waste is fed into a two-stage DF+AD/AD-only process, producing biogas. The resulting gas stream is then upgraded to hydrogen by passing through a sequence of process steps comprised of different types of membranes described further in Tables 3.2 and 3.3. The upgraded hydrogen will then react with nitrogen which is the product of the migration of air throughout the membrane, in order to produce ammonia. The separated CO₂ from the bioreactors along with ammonia can be discharged directly in the atmosphere or captured and enters the commodity liquid market, or can be utilized for urea production.

This chapter was drafted based on the publications submitted to the International journal of hydrogen energy and Frontiers in energy research:

Ghavam, S., Garcia, G.G. and Styring, P., (2021). A novel approach to ammonia synthesis from hydrogen sulfide. *International Journal of Hydrogen Energy* [online]. 46, 4072–4086. [Viewed 2 May 2021]. Available from: doi: 10.1016/j.ijhydene.2020.10.192.

Ghavam, S., Taylor, C.M. and Styring, P., (2021). Modelling and Simulation of a Novel Sustainable Ammonia Production Process from Food Waste and Brown Water. *Frontiers in Energy Research* [online]. 9, 42. [Viewed 22 July 2021]. Available from: <https://doi.org/10.3389/fenrg.2021.600071>.

3. Process description overview

In this modelled system, two configurations with four possible CO₂ fates are assessed for this green design-based process (Fig. 3.1): Technology-1: Ammonia production through a two-stage DF+AD and Technology-2: Ammonia production through AD-only.

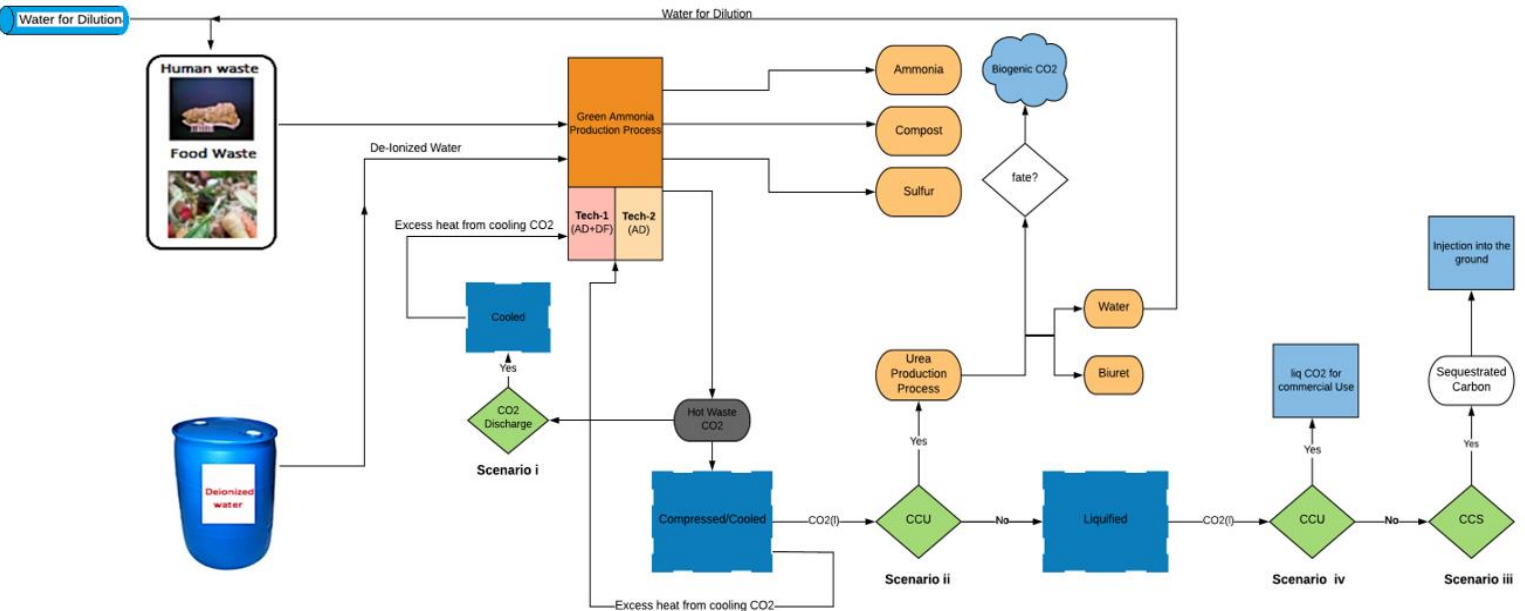


Fig. 3.1: Proposing a new sustainably driven waste-based ammonia production route along with four possible CO₂ fates for each process configuration.

- Scenario set-i (the base case): CO₂ is discharged directly into the atmosphere
- Scenario set-ii: (CCU) CO₂ is used for urea production
- Scenario set-iii: (CCS) CO₂ is compressed, liquefied, captured, and injected into the ground
- Scenario set-iv: (CCU) CO₂ is compressed, liquefied, captured, and enters the commodity liquid CO₂ market and likely will return to the atmosphere based on its usage

3.1 Technology pathways

The rationale behind choosing the co-digestion of FW and BW in the modelled system is that digestion efficiencies in co-digestion of FW and HW are generally higher when urine has been removed (Rajagopal, Ahamed and Wang, 2014). This separation is done in order to increase the hydrolytic and acidogenic potential of co-digestion of FW and BW (Colón, Forbis-Stokes and Deshusses, 2015). Moreover, co-digestion of excreta along with other organic compounds enhances the process efficiencies that are prevented by excreta characteristics. General technology structures are shown in Fig. 3.2 (two-stage DF+AD and AD-only process).

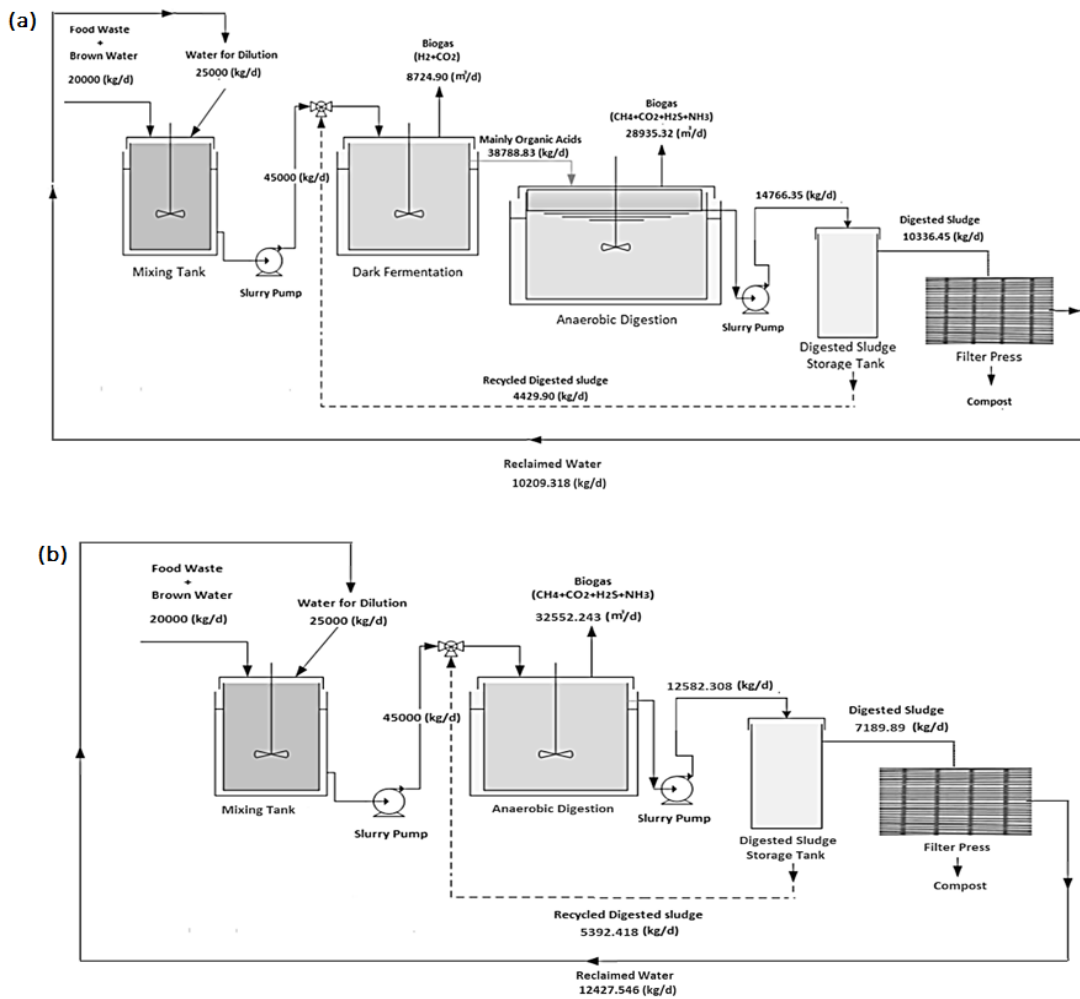


Fig. 3.2: A schematic of waste processing portions of the ammonia production processes through (a) two-stage DF+AD and (b) AD-only.

3.1.1 Selecting the appropriate reactor for hydrogen and methane production

CSTR, that is utilized for biogas production has been selected over other types of reactors due to its following advantages: This reactor is the most utilized bioreactor for biohydrogen production running continuously, due to its ease of operation, simpler configuration, uniform stirring mechanism, and effective control of temperature and pH. In this type of bioreactor microbial population is completely circulated and is suspended with the mixed liquor in the bioreactor, in this condition the best mass transfer and inoculum substrate interface is accomplished. As a result, due to its rapid mixing functionality mechanism, CSTR is capable of maintaining higher amounts of fermenting microbes

(Saratale et al., 2019). Since CSTR generally operates at low TS concentrations, the input waste needs to be pre-treated and diluted to meet the desired TS for CSTRs (Igoni et al., 2008). Comparison with previous studies on hydrogen and methane production for two-stage DF+AD using different types of substrates, bioreactors, and different operational temperatures is shown in Table 3.1. The table shows that the type of bioreactor and operational temperature has an effect on both hydrogen and methane production yields and OLR. However, there are other factors that influence these variables which will be discussed in *Bioreactor calculations* section. The results obtained in this study closely resemble the results attained by Chu et al. (2008).

A type of reactor which is filled once with the raw feed (waste) for a given amount of time and sealed until the process is completed, is known as a batch reactor. Throughout the degradation process there will be no output from this reactor. Batch reactors are not appropriate for continuous production and are more suited to high value products, however, they can generally operate at high TS concentrations of waste.

Table 3.1: A comparison of previous studies on hydrogen and methane production for two-stage DF+AD with various substrates and operating at different temperatures.

Dark Fermentation					
Substrate	Maximum production yield (ml H ₂ /g VS)	Operational temperature	OLR (g VS/L.d)	Reactor type	References
OFMSW	205	55	38.4	Continuous two-stage	Chu et al. (2008)
Household solid waste	43	37	37.5	Continuous two-stage	Liu et al. (2006)
Dairy manure	35.1	36	70	Batch	Xing et al. (2010)
FW	65	40	22.65	Semi- continuous two-staged	Wang and Zhao, (2009)
BW	2.52	N. A	4.5	Semi- continuous	Seong, Yoonand and Seo (2014)
FW +BW	99.8	37	106	Continuous two-stage	Paudel et al. (2017)
FW + BW	113.878	55	36.309	Continuous two-stage	This study
Anaerobic digestion					
Substrate	Maximum production yield (ml CH ₄ /g VS)	Operational temperature	OLR (g VS/L.d)	Reactor type	References
OFMSW	464	35	6.6	Continuous two-stage	Chu et al. (2008)
Household solid waste	0.5	37	5	Continuous two-stage	Liu et al. (2006)
OFMSW+cow manure	0.71	55	4	Batch CSTR	Hartmann and Ahring (2005)
FW +cattle manure	0.6	36	1.2	CSTR	Maranon et al. (2012)
Agro-industrial waste	0.25	37	2.01	Continuous two-stage	Dareiotti, Vavouraki and Kornaros, (2014)
FW + BW	0.72/0.67	37	1.24/1.76	Continuous two-stage	Paudel et al. (2017)
FW + BW	524.045	35	1.19	Continuous two-stage	This study

N.A: Not Applicable

3.2 Significance of membrane incorporation in the proposed process

A waste-based, CO₂ aware, ammonia production technology leveraging emerging membrane technologies in concert with local infrastructure can provide a viable route to green ammonia and to green fertilizers, providing an effective strategy to address multiple sustainability/sustainable development needs simultaneously.

The proposed process is designed around membranes to address the challenges in necessary gas upgrading and purification, reduce the need for external sources of both chemicals and water, while minimizing the physical footprint of the processing units. To obtain the necessary purity level from biogas resulting from waste (FW and BW), the methane stream needs to be upgraded to separate impurities such as CO₂, H₂S and traces of other compounds. The cost of the available technologies for upgrading biogas such as water scrubbing, Pressure Swing Adsorption (PSA), chemical absorption, cryogenic distillation, amine scrubber, etc. are comparatively high due to

energy, water, chemical usage, and large physical footprint, and/or the combination of these factors (Fouladvand, 2016).

In place of processing units, such as an amine scrubber, with a large physical footprint, a Micro Filtration Index (MFI) membrane is used for the separation of hydrogen and CO₂ from DF. For example, a single MFI module has the same throughput/output as a large, expensive and energy-intensive amine scrubber (Korelskiy et al., 2015).

This proposed process is also designed in order to increase the production of hydrogen required for ammonia synthesis through an environmentally benign, energy efficient, and cost-effective manner. The design objectives have been achieved by utilizing CO₂ for urea synthesis, converting hydrogen sulfide into elemental sulfur (S₂) and hydrogen via a membrane, converting the byproduct of the AD process into compost, utilizing renewable energy sources, and processing units with a low physical footprint for its operation. These processing units include certain types of membranes which reduce the production costs, such as ITM that is used for air separation (Sun, Larpudomlert and Thepwatee, 2011).

3.2.1 Membranes

Membrane technology is a promising method compared to conventional energy-intensive gas separation processes such as amine scrubber (Chowdhury et al., 2005). Cost-effective operations and other attractive features such as, modular design, ease of operation, low maintenance, etc. enables membrane technology to be utilized in different industrial applications from gas separation to water purification, etc. (Chowdhury et al., 2005). Membranes are selective obstacles that can regulate the transport rate of various types of chemical compounds as they pass through the said membrane. They can be permeable, semi-permeable, and impermeable to different types of materials (Fouladvand, 2016). To assist transport via the membrane, a driving force, needs to be applied, such as: The chemical potential, the electrical potential, and the hydrostatic pressure, which are the typical driving forces for transport throughout the membranes. For gas separation via membrane, the driving force is typically shown as partial pressure differences, migrating from the high-pressure feed side to the lower pressure permeate side (Fouladvand, 2016). For gas separation process via membranes, one component preferably permeates throughout the membrane and the other components will permeate at lower rates or will not permeate at all. Permeate is the fragments of the feed passing

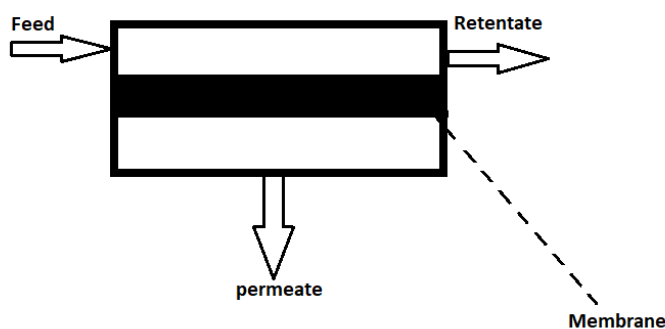


Fig. 3.3: A schematic of membrane technology.

throughout the membrane, whereas the retentate is the stream which is refused via the membrane. Fig. 3.3 shows a schematic of membrane technology.

3.3 Process components

3.3.1 Technology Readiness Level (TRL) and potential technical viability

In designing this waste-to-ammonia/ammonia+urea technology, mature technologies for base operations are used with more novel components as a means of enabling non-incremental technological advances. It is a deliberately novel, untried (when working in concert) technology, but it is helpful to have a sense of its operational possibility. It is a function of both the future viability of the proposed technology and its distance from the developmental stage. This is to provide a broad idea of the potential future viability of the process developed and modelled in this work that is based on mixed maturation components, categorized by Technology Readiness Level (TRL) (Sauser et al., 2006). The TRL scale is a tool for evaluating the maturity of technologies during complex system development (Fig. 3.4) and can be used to provide a sense of the components and, as a result, their intersection³. TRL has been applied to a variety of CCU technologies such as the study conducted by, Armstrong (2015a).

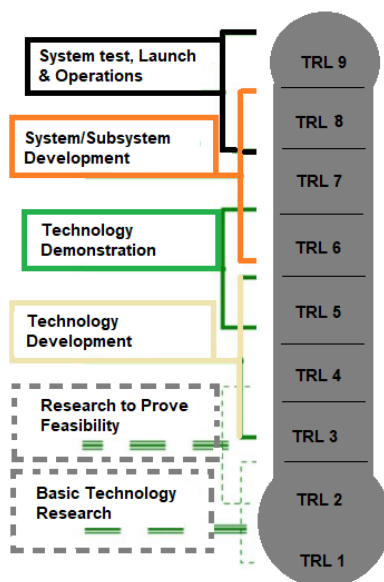


Fig. 3.4: National Aeronautics and Space Administration (NASA) TRL scale (NASA, 2012).

The system is built up of individual components (DF, AD, MFI, EMS, ITM, CH₄ assisted-SOFEC, SSAS, SOFC) at various TRLs (a logical flow diagram is used to describe the modelling method for each component, separately shown in section 3.5.2.2). The description of the plant components along with the TRL and material composition of each of the membranes, are shown in Table 3.2 and Table 3.3 respectively.

³ A complete view of the system readiness would be based on a more comprehensive evaluation based on detailed System Readiness Level (SRL) and Integration Readiness Level (IRL) evaluations (see, Sauser et al. (2006)).

The AD, DF, and urea production processes are ready to be commercialized with a high TRL of 7-8. The bulk of membranes incorporated into the studied technology are also ready to be commercialized. A few of the membranes, such as EMS and SSAS, require further physical and material development prior to commercialization. An equation-based modular approach model was devised to allow one to tune the input parameters/variables for different production volumes/scale, to accommodate the varying TRLs for the membranes incorporated into the proposed process and allow exploration of scale and other factors.

As a general 'rule-of-thumb', the integrated technology with hybrid TRLs can have a TRL no greater than the lowest TRL (Sauser et al., 2006). Another key element to the viability of the technology will be interoperability at scale. Because the technology's viability relies on ability to operate at large scale, it is important to have a sense of whether the most nascent technologies used here have the potential to function at the desired (ultimately industrial) scale.

The TRL for most of the membrane technologies are around 7, active, or probably at scale. The developers of MFI membranes evaluated the long-term potential application of their membranes for gas separation on an industrial scale (for the separation of approximately 300 TPD of CO₂) with comparable technologies (amine scrubber and polymeric membrane) performing the same task (Fouladvand, 2016). ITM has gone through five developmental stages and has been tested for tonnage oxygen production on a commercial scale (Armstrong, 2015b). SOFC is a technology that is approaching commercialization, while the CH₄ assisted-SOFEC electrolyzer with potential applications in hydrogen production has a similar structure except that the oxidant on the cathode side of the cell is steam in place of air. Due to the structural and material similarity of this electrolyzer to SOFC, the prospects for commercialization of it are promising, however, the potential of this technology is limited by the accessibility to biogas/natural gas (Nielen, 2016). The LCA results show that high uncertainty is due to the speculativeness of these membranes and the technology being novel (*Chapter 6*). Although some of these membranes have low TRL, the long-term outlook for the commercialization of these membranes is positive.

With TRLs of 3-4, SSAS and EMS membranes have the lowest readiness/maturation of the technologies used. SSAS membranes are operating at bench scale level and are yet to be commercialized for ammonia synthesis (Bartels, 2008). Further development of this membrane requires advances in materials and appropriate operational conditions. However, it shows potential in terms of price, CO₂ emissions, and ease of integration with renewable sources of energy with comparable technologies such as SMR and water electrolysis coupled with H-B at scale (Ganley, Holbrook and McKinley, 2007). The EMS membrane is proposed and designed on a bench scale and is yet to be determined for commercialization, further development of this membrane requires advances in appropriate cathode material sourcing (Winnick and Liu, 2003). However, one intent for its use is in Integrated Gasification Combined Cycle (IGCC) at industrial scale, though the time to reach that level needs more evaluation. Thus, while not yet demonstrated, the concepts behind both of these technologies are for large scale applications, consistent with the other technology components and the intent of the proposed technology.

Table 3.2: Description of the plant components incorporated in the modelled waste-to-ammonia and ammonia+urea production process (Ghavam, Taylor and Styring, 2021; Brémond et al., 2018; Li, 2013; Philbin,2020).

Processing unit	Description	Reactions	TRL readiness
CSTR- Dark Fermentation Bioreactor (DFB)	DF is the decomposition of carbohydrate rich substrates in the absence of light and O ₂ to produce H ₂ and CO ₂ (detailed information is provided in <i>Chapter 2</i> , section 2.2.5).	$C_6H_{12}O_6 + 2H_2O \rightarrow 2CH_3COOH + 4H_2 + 2CO_2$ (3.1)	7
CSTR- Anaerobic Digestion Bioreactor (ADB)	AD is a continuous biochemical process in which complex substrates are decomposed and digested via microbial actions and converted into biogas in the absence of O ₂ (Pengyu et al., 2017). This transformation takes place through four main steps: Hydrolysis, acidogenesis, acetogenesis, and methanogenesis. (detailed information is provided in <i>Chapter 2</i> , section 2.2.5).	$C_6H_{12}O_6 \rightarrow 3CH_4 + 3CO_2$ (3.2)	7-8
Snamprogetti-Urea Production process	Urea is the result of the dehydration of carbamate. Carbamate is the intermediate product resulting from the reaction between NH ₃ and CO ₂ .	(1) $NH_3(g) + CO_2(g) \leftrightarrow NH_2COONH$ (3.3) (2) $NH_2COONH_4(s) \leftrightarrow NH_2CONH_2(s) + H_2O(l)$ (3.4) (1) + (2): $NH_3(g) + CO_2(g) \leftrightarrow NH_2CONH_2(s) + H_2O(l)$ (3.5)	9

Table 3.3: Descriptions, material compositions, and chemical reactions used for membranes, electrolyzer, and fuel cell incorporated into the modelled waste-to-ammonia and ammonia+urea production process.

NO	Membrane	Description	Composition	Reactions	TRL readiness	References
1	Electrochemical Membrane Separation (EMS)	Electrochemical Membrane Separation converts H ₂ S into H ₂ and S ₂ in the presence of N ₂ used as the sweep gas.	Cathode: Gd _{1-x} Ti _{2-x} Mo _x O ₇ (x = 0.0-2.0), Electrolyte: La _{0.7} St _{0.3} VO ₃ Anode: NiO	Cathode: $H_2S + 2e^- \rightarrow H_2 + S^{2-}$ (3.6) Anode: $S^{2-} \rightarrow \frac{1}{2} S_2 + 2e^-$ (3.7) The overall reaction: $H_2S \rightarrow \frac{1}{2} S_2 + H_2$ (3.8)	3-4	Winnick and Liu (2003)
2	Ion Transport Membrane (ITM)	This membrane is a solid inorganic oxide ceramic material that transports O ₂ ions at high pressures (10-30 bar) and temperatures (800-900 °C).	SrCo _{0.9} Sc _{0.1} O _{3-δ}	Non permeate side: $\frac{1}{2} O_2 + 2e^- \rightarrow O^{2-}$ (3.9) Permeate side: $O^{2-} \rightarrow \frac{1}{2} O_2 + 2e^-$ (3.10)	7-8	Armstrong (2015b) Sun, Larpudomlert and Thepwater (2011) Da Costa et al. (2013)
3	Membrane Filtration Index (MFI)	An electrochemical zeolite-based membrane known as Membrane Filtration Index has been incorporated into the system for the separation of H ₂ from the H ₂ and CO ₂ gas mixture.	Ceramic MFI zeolite membranes	$H_2 + CO_2 \rightarrow CO_2$ (Permeate side) (3.11) H_2 (Non permeate side (retentate)) (3.12)	7-8	Fouladvand (2016) Cousins et al. (2019)
4	Solid Oxide Fuel Cell (SOFC)	SOFC is an electrochemical conversion device that generates electricity via electrochemical conversion of fuel gas mainly H ₂ at high temperatures of 700-1000 °C.	Cathode: La _{1-x} Sr _x MnO ₃ (LSM) Electrolyte: YSZ Anode: Ni-YSZ composite	Cathode: $\frac{1}{2} O_2 + 2e^- \rightarrow O^{2-}$ (3.13) Anode: $H_2 + O^{2-} \rightarrow H_2O + 2e^-$ (3.14) Overall reaction: $\frac{1}{2} O_2 + H_2 \rightarrow H_2O$ (3.15)	7-9	Jimenez (2013) Küngas (2020)
5	CH ₄ -Solid Oxide Fuel Assisted Electrolysis Cell (CH ₄ - assisted SOFEC)	In the SOFEC, CH ₄ is added to the anode side of the electrolyzer, the decomposition potential (voltage) of H ₂ O is decreased, and this results in lower energy usage and a higher conversion ratio of electricity for H ₂ production.	Cathode: LSM- ScSZ Electrolyte: ScSZ Anode support layer: Ni-YSZ composite Anode active layer: Ni-ScSZ composite	Cathode: $H_2O + 2e^- \rightarrow H_2 + O^{2-}$ (3.16) Anode: $\frac{1}{4} CH_4 + O^{2-} \rightarrow \frac{1}{2} H_2O + \frac{1}{4} CO_2 + 2e^-$ (3.17) Overall reaction: $\frac{1}{2} H_2O + \frac{1}{4} CH_4 \rightarrow H_2 + \frac{1}{4} CO_2$ (3.18)	5-6	Xu et al. (2016) Hrbek (2018)
6	Solid State Ammonia Synthesis (SSAS)	Solid State Ammonia Synthesis produces ammonia through an electrochemical conversion process in a proton-conducting solid electrolyte cell from gaseous H ₂ and N ₂ .	Cathode: SmFe _{0.7} Cu _{0.3-x} Ni _x O ₃ (x=0-0.3) (SFCN) Electrolyte: Nafion (membrane) Anode: Ni-doped SDC (Ni-SDC) NiO-Ce _{0.8} Sm _{0.2} O _{2-δ}	Cathode: $N_2 + 6H^+ + 6e^- \leftrightarrow 2NH_3$ (3.19) Anode: $3H_2 \leftrightarrow 6H^+ + 6e^-$ (3.20) Overall reaction: $N_2 + 3H_2 \leftrightarrow 2NH_3$ (3.21)	3-4	Xu et al. (2009) Ganley, Holbrook and McKinley (2007)

3.3.2 Electrochemical Membrane Separation (EMS) for hydrogen sulfide separation (1)

The upgrading stage used in the proposed process for removing hydrogen sulfide is an EMS system. Via this method, hydrogen sulfide is removed in one continuous phase at temperatures of 600-700 °C, which leads to the production of hydrogen and elemental sulfur (Winnick and Liu, 2003). However, the optimum performance of EMS is at 650 °C, temperatures higher than this result in gas crossover, this crossover results in either electrolyte evaporation/solidification. A schematic of EMS is shown in Fig. 3.5.

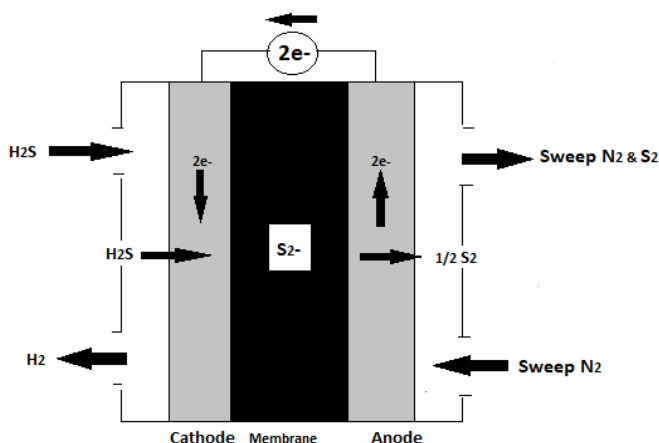


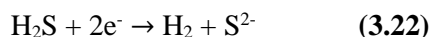
Fig 3.5: A schematic of an EMS.

In the EMS, hydrogen sulfide is removed from the fuel gas stream and is converted to pure hydrogen, which is the main feedstock for ammonia production. The sulfur by-product can be sold commercially to industries involved in the production of sulfuric acid, agricultural industries for fertilizer production, etc. The basic separation principle relies on applying an electrochemical potential gradient which provides the driving force for the charged species across the membrane. According to Burke et al. (2004), in comparison to pressure-driven membrane separations, this membrane produces selectivity significantly higher due to the applied electric field which only affects the charged species.

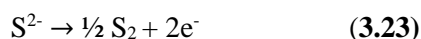
There are seven steps required for electrochemical removal of hydrogen sulfide: (1) gaseous diffusion of hydrogen sulfide to the electrode, (2) hydrogen sulfide diffusion through the electrode pores to the electrolyte-electrode interface, (3) adsorption and reduction of hydrogen sulfide at the cathode surface, (4) production of a sulfide ion, (5) migration and diffusion of sulfide ions through the electrolytic membrane, (6) oxidation of sulfide ions to elemental sulfur at the anode, and (7) diffusion of sulfur away into the bulk purge stream (Winnick and Liu, 2003). This process works continuously and takes place in one step, making the technology economical due to lower costs associated with manpower and operation (Burke et al., 2004). An efficient design of the cell stack ensures that the physical footprint of the plant is kept to a minimum (Burke et al., 2004).

The electrolytic cell has the following basic components: (1) cell housing, (2) an inert ceramic membrane, (3) an electrolyte, (4) an anode, and (5) a cathode. The chemical reactions that occur in an EMS are as:

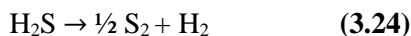
Hydrogen sulfide is passed through the cathode, as shown in chemical equation 3.22:



Chemical equation 3.23 shows the transport of sulfide ions throughout the membrane to the anode side:



The overall reaction resulting from both reactions taking place in the anode and cathode at the temperature of 650 °C is (3.24):



3.3.3 ITM for air separation (2)

This process consists of an ITM for oxygen separation from air. This membrane generally operates at temperatures of 800-900 °C and pressures of 10-30 bar (Han et al., 2018). Pressure gradient is the driving force mechanism in this type of ITM. This pressure driven ITM generally consists of mixed ion and electron-conducting ceramic materials with high oxygen separation selectivity. Various types of ceramic materials will lead to different separation efficiency/gas permeation. There is no need to apply a voltage to this system as membrane materials have the capability to conduct the electrons and oxygen ions from high to low pressure, resulting in low-cost operation (Sun, Larpudomlert and Thepwater, 2011). Increasing the pressure gradient provides the necessary driving force for mass transfer of O₂ component across the ITM. The three factors which affect the oxygen productivity/separation efficiency of this membrane are, pressure, temperature and flow pattern. This membrane is an innovative technology for air separation which has a simple configuration with a lower energy penalty when compared to mature technologies currently in use such as cryogenic distillation. A schematic of ITM can be seen in Fig. 3.6, which shows that oxygen molecules pass the membrane, while the nitrogen molecules do not pass and accumulate behind the membrane.

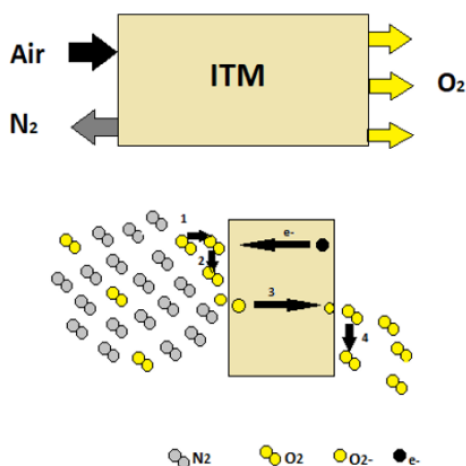


Fig. 3.6: A schematic of the ITM separation process.

A comparison of different types of air-separation technologies (cryogenic and non-cryogenic) is shown in Table 3.4. The purity level of oxygen resulting from ITM is higher than polymeric membranes, PSA, and Vacuum Swing Adsorption (VSA) with 99-100% purity level. However, the purity level of the resulting oxygen from ITM is almost the same as cryogenic air separation. Since the physical footprint of this processing unit (ITM) is small compared to

cryogenic air separation, it is a suitable option for the proposed process. The separated nitrogen required for this proposed ammonia production process must reach a purity level higher than 99.99% in order to be utilized in the SSAS. Nitrogen with purity levels lower than 99.99% that contain trace amounts of oxygen cause irreversible poisoning of the catalyst in the SSAS (Marrony, 2015).

Table 3.4: A comparison of different types of air separation technologies (cryogenic and non-cryogenic) (Chemsystems, 2010; Da Costa et al., 2013).

	ITM	Polymeric membranes	Cryogenic air separation	Pressure Swing adsorption (PSA) and vacuum Swing adsorption (VSA)
Production capacity	≥100 t/day	< 20 t/day	>3000 t/day	Plant size is up to about 56.7 t/day
Purity level	99-100%	~40%	99+	95%
Current status	Semi-Mature	Mature	Mature	Mature
Description	This membrane is a solid inorganic oxide ceramic material that transports oxygen ions at high pressures (10-30 bar) and temperatures (800-900 °C).	The membrane system is based on the variance between particle diffusion rates throughout the membrane. The main drawback is its low chemical resistance.	The technology is based on the fact that each of the components that make up air have different boiling points. This process operates at a temperature of approximately 185°C.	Under pressure, gases tend to be adsorbed to solid surfaces. As the pressure increases, the adsorption rate increases and as the pressure decreases the gas is desorbed and released.
Advantages	Simple in design, low energy penalty, low cost, high tonnage, and low environmental impact.	Flexibility in scale (due to modularity), and a mature and well-developed technology.	The most mature and well-developed technology, cost effective, and efficient.	Mature and well-developed technology, continuous oxygen production, capable of maintaining a high purity level of 99%, low capital costs, flexible design for different adsorbents.

3.3.4 Micro Filtration Index (MFI) for gas (H₂ and CO₂) separation (3)

CO₂-selective membranes currently in use are low flux polymeric membranes with limited chemical and thermal stability. Fouladvand (2016) assesses the effect of resilient and high flux ceramic MFI zeolite membranes for separation of CO₂ from H₂, this process is an important method for treating syngas taking place at a temperature in the range of -38_37°C and at pressure of 8.882 atm. The results obtained from the performance of ceramic MFI zeolite membranes show that they are superior to other sophisticated zeolite and polymeric membranes stated for CO₂ selective in terms of both flux and selectivity. Fouladvand (2016) also concluded that the ceramic zeolite membranes are more compact than a process based on polymeric membrane. This study also states that ceramic zeolite membranes are economically viable, and have promising results for selective, and sustainable removal of CO₂ from syngas. Currently, CO₂ is removed via absorption processes such as the energy intensive and expensive amine scrubbing technology. Moreover, absorbent utilization is corrosive, not environmentally friendly, and the absorption units are relatively large and complex. Membrane separation has also gained attention recently due to its high efficiency, sustainability, and low energy usage. The volume of energy needed for 90% recovery of CO₂ by means of an efficient membrane has been projected to be ca. 16% of the power produced via power plants, while the energy needed by an amine absorption and desorption process is ca. 50% of that power (Merkel et al., 2010). From a commercial point of view, polymeric membranes show promising results, for example, the Membrane Technology and Research (MTR), Inc. Polaris membranes are known as the first commercial polymeric membrane capable of

CO₂ separation from syngas. Currently, the most effective polymeric membrane can accomplish CO₂/H₂ selectivity of 10-12 with a CO₂ permeance of ca. 2-10 mol s⁻¹ m⁻² Pa⁻¹ at room temperature (Baker and Low, 2014). This low permeance, integrated with a relatively low selectivity requires the usage of a comparatively large membrane area for a separation process. Moreover, one of the problems with polymeric membranes is plasticization resulting from CO₂ that substantially lowers the membrane selectivity and stability over a period. Because of the porous configuration, zeolite membranes exhibit higher fluxes than polymeric membranes. For example, a much smaller area is required for a separation process. In addition, zeolite membranes display other benefits towards polymeric membranes in terms of high chemical and thermal stability (Fouladvand, 2016). A schematic of an MFI membrane is shown in Fig. 3.7.

There are three categories in which zeolite membranes can be classified: Molecular sieving, selective adsorption, and diffusion. A combination of these mechanisms direct the separation process in zeolite membranes, for e.g., if the

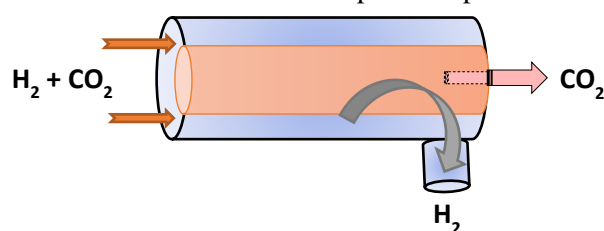


Fig. 3.7: A schematic of an MFI membrane.

separation is directed by adsorption, one/a number of components are transported throughout the membrane, whereas, the non-adsorbing components do not pass through. For the diffusion-controlled separation, components which have higher diffusivity in the membrane pores diffuse faster and permeate. In molecular-sieving, the molecules smaller than the pores can permeate through the membrane, while molecules larger than the pore size will not permeate. Hydrogen and CO₂ have a smaller kinetic diameter than the pores of zeolite MFI, thus, both adsorption and diffusion play vital roles in the transport throughout the membrane in this study (Fouladvand, 2016). In order to avoid CO₂ condensation in the pores, based on the study conducted by Fouladvand (2016) a nondestructive method known as permoporometry was adopted to allow detailed characterization of micropore and mesopore defects in ultra-thin high-flux MFI membrane. Through this method, the permeance of non-adsorbing gas, in this case, helium (He) is measured as a function of the relative pressure of an adsorbing gas, for instance n-hexane in the feed stream. When the concentration of added adsorbate to the feed stream is increased, capillary condensation will result in more pores and defects to be blocked.

3.3.5 Solid Oxide Fuel Cell (SOFC) for heat and power production (4)

In the modelled process, fuel cell is used for steam and electricity generation. Fuel cells are competitive sources of power since they have a number of advantages, such as high efficiency, flexibility in their usage, and lack of noise (Abdalla et al., 2018). They can also be used in an extensive range of operating temperatures; this means that they are capable of being used in multiple applications. SOFC operates at 700-1000 °C, these temperatures are higher than for other types of fuel cells and are the reason for its use in power generation and hybrid power applications (Ramadhani et al., 2017). This fuel cell was selected mainly due to its ability to generate up to 3 MW power when compared to other types of fuel cells (Uttamote, 2011). A schematic of an SOFC is shown in Fig. 3.8.

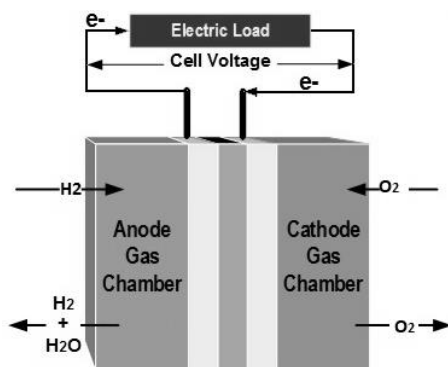
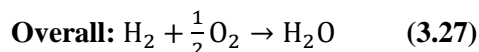
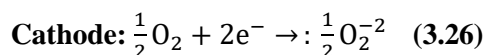
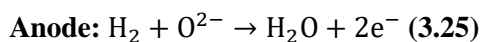


Fig. 3.8: A schematic of SOFC.

The SOFC reactions in anode, cathode and overall are as shown in chemical equations 3.25, 3.26, and 3.27.



3.3.6 CH₄ assisted- SOFEC for upgrading methane into pure hydrogen (5)

Detailed information on CH₄ assisted-SOFEC is provided in the literature review section (*Chapter 2*). A schematic of CH₄-assisted SOFEC is shown in Fig 3.9.

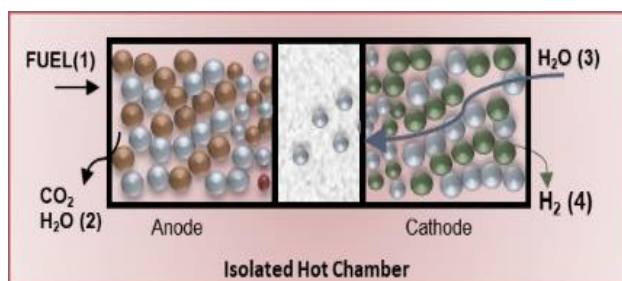
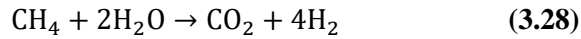
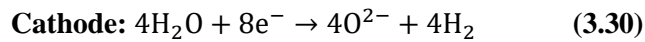
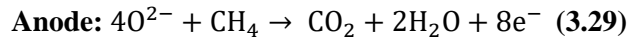


Fig. 3.9: A schematic of CH₄-assisted SOFEC.

Oxygen ions are separated from water leaving a flow of hydrogen and unused steam 3.28.



Anode and cathode half reactions are given as 3.29 and 3.30.



3.3.7 Solid State Ammonia Synthesis (SSAS) for ammonia production (6)

There are several issues associated with the catalytic process for ammonia synthesis (Haber Bosch) such as low conversion efficiency, severe environmental pollution, and high energy usage. These problems are addressed here by utilizing a SSAS (Amar et al., 2011). The overall chemical reaction that takes place in the cell for ammonia production is divided into two electrode reactions. Each of the reactions takes place at one of the electrodes. The exact form of the electrode reactions is related to the type of electrolyte: Either a H^+ ion conductor or an O_2 ion conductor. Moreover, the source of H^+ can be hydrogen or water. The reaction rates obtained from O^{2-} conducting solid electrolyte cells were lower than those achieved from H^+ cells. However, O^{2-} conductors are advantageous in terms of producing pure oxygen as the byproduct.

The use of water in place of hydrogen, results in a new method for ammonia synthesis, this approach is based on the use of oxygen ion conductors. A schematic of ammonia synthesis in O^{2-} cell along with the chemical reactions taking place in this cell are shown in the following Fig. 3.10 (Garagounis, et al., 2013).

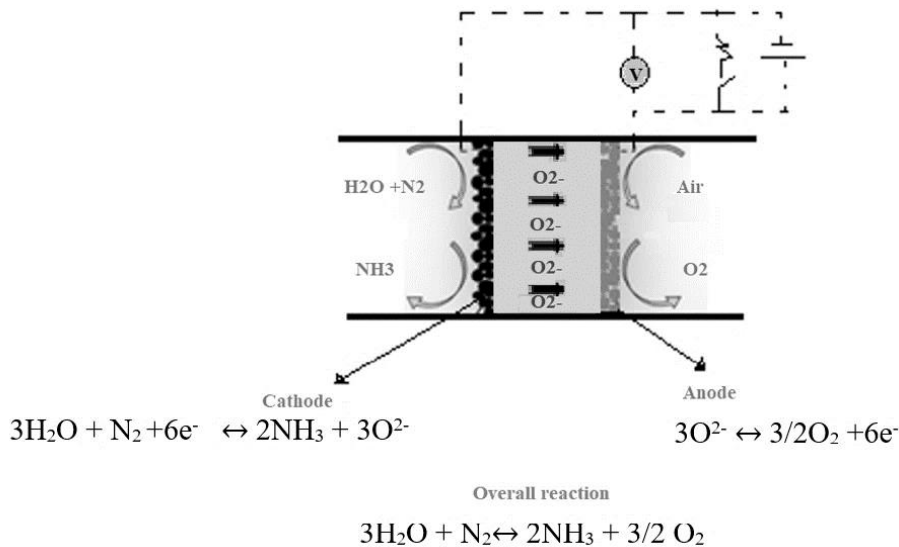
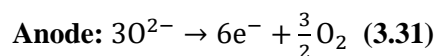
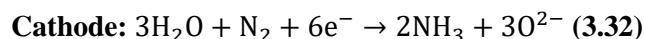


Fig. 3.10: A schematic of a solid-state ammonia synthesis device; via an O^{2-} conducting electrolyte.

At the anode, oxygen ion is converted to oxygen molecules as (3.31):



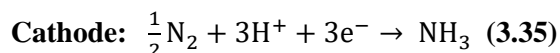
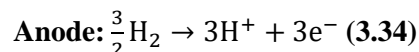
Water and nitrogen enter at the cathode side where the reactions taking place are as follows (3.32):



The overall reaction is (3.33):



For a cell with a H^+ conducting electrolyte, the reactions that take place in the electrodes, are as follows (3.34 and 3.35).



A schematic of a proton-conducting membrane along with the chemical reactions taking place inside the cells are shown in Fig. 3.11. The cell is comprised of a solid-state H^+ conductor and two porous metal films located on the two sides of the solid electrolyte and function as electrodes. Hydrogen migrates throughout the electrolyte in the form of H^+ to the cathode where the half-cell reaction occurs (Marrony, 2015).

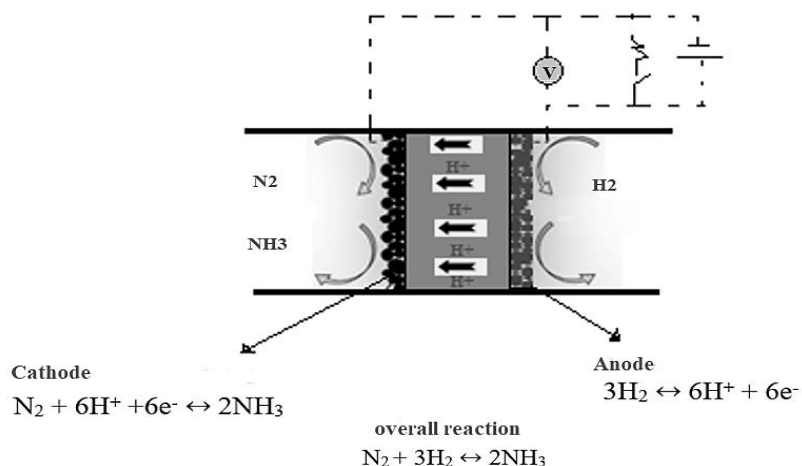


Fig. 3.11: A schematic of a solid-state ammonia synthesis device; via a proton conducting electrolyte.

All studies on electrochemical ammonia production are divided into two categories based on the operational temperature range of the electrochemical cell: temperatures lower than 100°C are considered low temperature while temperatures in the range of $400\text{--}750^\circ\text{C}$ are considered high temperatures. According to Soloveichk, et al. (2017) the advantages of the electrochemical technology compared to thermochemical (Haber Bosch) are:

- Higher efficiency allowing greater energy saving

- Reduced amount of purification needed due to higher selectivity
- Reduced Capital Expenditure (CapEx) costs thanks to lower temperatures and pressures
- Suitability for small to medium scale utilization thanks to the linear scalability of these plants

One of the major disadvantages of high-temperature electrochemical ammonia synthesis is that it can decompose thermally after being produced. This issue is addressed in the proposed study by incorporating a low-temperature SSAS into the proposed production process by using the same material and operational conditions (temperature and pressure) as in the study by Xu et al. (2009). The study examined a maximum ammonia production rate of $1.13 \times 10^{-8} \text{ mol.s}^{-1}.\text{cm}^{-2}$ operating at a low temperature of 80 °C with an applied voltage of 2 V by using a Nafion membrane (as the electrolyte), a Ni-samaria-doped ceria (Ni-SDC) $\text{NiO}\cdot\text{Ce}_{0.8}\text{Sm}_{0.2}\text{O}_{2-\delta}$ anode and a $\text{SmFe}_{0.7}\text{Cu}_{0.3-x}\text{Ni}_x\text{O}_3$ ($x=0-0.3$) (SFCN) cathode, and by using hydrogen and nitrogen as the reactants, operating at atmospheric pressure. In this study a high Faradic efficiency of 90.4% was attained. This figure is higher when compared to other studies, when testing low-temperature ammonia synthesis processes.

3.4 Methodology

Fig. 3.12 shows all the process configurations, scenarios, and CO₂ fates designed and evaluated here.

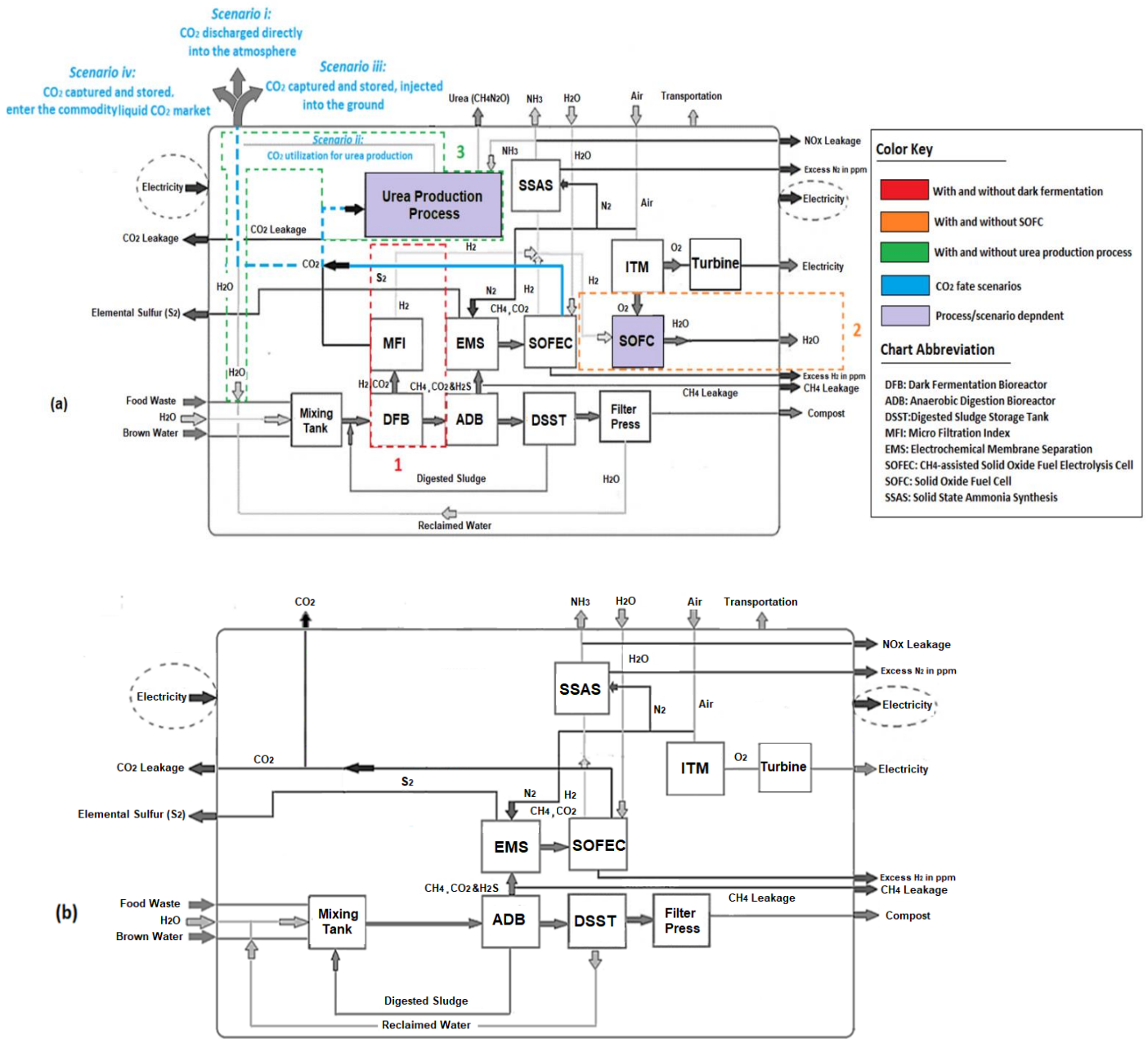


Fig. 3.12: A schematic of (a) a two-stage DF+AD with SOFC (b) AD-only without urea production process and without SOFC.

In these processes, waste (FW and BW) is fed into a two-stage DF+AD, panel (a) or one-stage AD-only, panel (b), producing biogas. Hydrogen is separated from the gas mixture through a series of operating stages (membranes) and reacts with nitrogen derived from the migration of air via ITM (Table 3.3), for the production of ammonia. The CO₂ recovered together with the ammonia can be utilized for urea production (scenario set-ii). This process is compared to the scenario where the CO₂ is not captured/utilized, as well as to scenarios where the CO₂ is captured, compressed,

liquefied, and either injected into the ground (CCS) or assumed to enter the commodity liquid CO₂ market (base CCU) (scenario sets i-iv). Each process configuration is shown as a dotted line in three different colours in Fig 3.12(a): (1 red dashed box)- with and without DF, (2 orange dashed box)-with and without SOFC, and (3 green dashed box)-with and without urea production process. Fig 3.12(b) shows the production process (AD-only without urea production process and without SOFC) with the three components (DF, SOFC, and urea production process) removed from Fig 3.12(a).

3.4.1 Modelling approach

As described in section 3.1, this proposed process is assessed through two configurations: Technology-1: Ammonia production through a two-stage DF+AD and Technology-2: Ammonia production through AD-only. Each configuration has four possible CO₂ fates, Scenario i: CO₂ is discharged directly into the atmosphere, Scenario ii: (CCU) CO₂ is utilized for urea production, Scenario iii: (CCS) CO₂ is compressed, liquefied, captured, and injected into the ground, and Scenario iv: (CCU) CO₂ is compressed, liquefied, captured, and enter the commodity liquid CO₂ market. All four scenarios are evaluated for two situations, one where SOFC is used, and one where it is not.

The process configuration and computational model behavior change depending on scenario configuration. For scenarios i, ii, and iv all the produced CO₂ is compressed, cooled, and liquefied, then either discharged directly, captured and injected into the ground, or sold commercially. The methane and hydrogen resulting from AD/DF are upgraded into pure hydrogen for ammonia synthesis via multiple membrane types (MFI and SOFEC). If the process does not utilize SOFC, the calculation ends at this point. When SOFC is incorporated into the process, the SSAS/SOFC hydrogen ratio is set, the SOFC calculations are conducted and the ITM, nitrogen throughput is attenuated.

For scenario iii the entirety of the CO₂ produced is utilized for urea production and the upgraded hydrogen is used for the production of the required ammonia for urea synthesis. As with the other scenarios, the inclusion of SOFC determines the algorithm from here. If SOFC is incorporated into the process, the SOFC calculations are conducted and the SSAS/SOFC hydrogen ratio is set at this point. In the absence of the SOFC module, the nitrogen from ITM is used without attenuation along with the excess hydrogen for ammonia synthesis rather than entering the SOFC module (Fig.3.13).

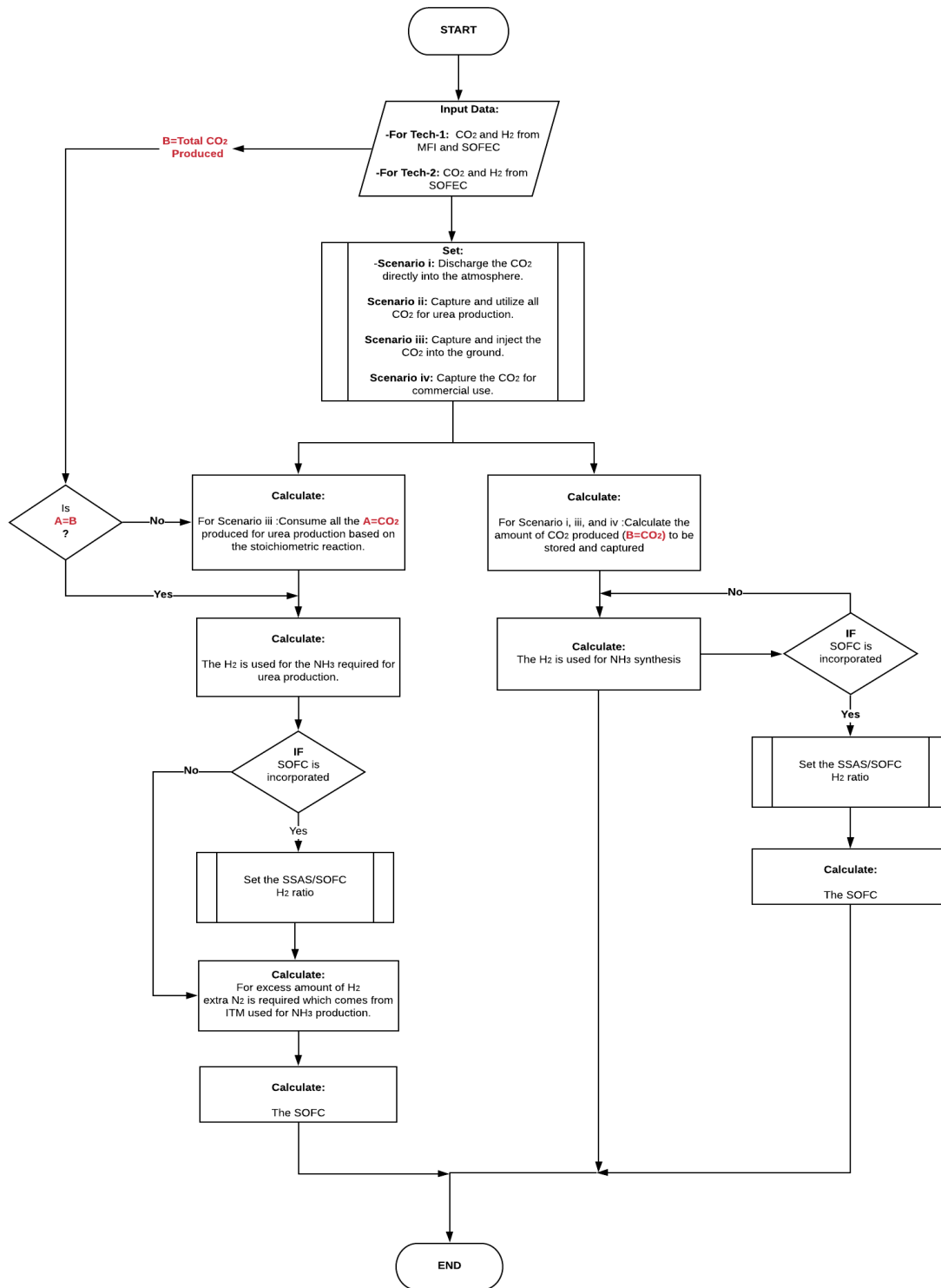


Fig. 3.13: Modelling approach flow diagram for the proposed process.

3.4.1.1 Technology-1: Process description of ammonia production through a two-stage DF coupled with AD

Hydrogen is separated from the hydrogen and CO₂ gas mixture resulting from DFB by using an MFI. The separated hydrogen provides the process with the required hydrogen for ammonia synthesis. The hydrogen along with the needed nitrogen resulting from the ITM, enters into the SSAS for ammonia production. The organic acids which are the byproducts of DF are used as the substrate for AD in order to produce biogas which is comprised of methane, CO₂, and hydrogen sulfide. Hydrogen sulfide must be removed from the biogas stream, which is accomplished here using an EMS system. This hydrogen sulfide is converted into traces of hydrogen and sulfur in the presence of a sweep gas (nitrogen) which is separated via ITM. The CO₂ along with methane is introduced into a CH₄ assisted-SOFEC for hydrogen production. Throughout this conversion, CO₂ is also separated from the hydrogen stream in this electrolyzer. The hydrogen then enters the SSAS, producing ammonia which is required in the event where urea is produced (only for scenario ii). A portion of the hydrogen resulting from the CH₄ assisted- SOFEC is fed into a SOFC for generating heat, power, and steam for a part of the process. The ammonia produced along with the CO₂ resulting from both MFI and SOFEC enter the urea production process or the CO₂ is released directly into the atmosphere (scenario i), captured and injected into the ground (scenario iii) or assumed to enter the commodity liquid CO₂ market (scenario iv).

3.4.1.2 Technology-2: Process description of ammonia production through AD-only

Biogas resulting from AD, needs to be upgraded in order to provide the hydrogen required for ammonia synthesis. The hydrogen along with the needed nitrogen resulting from the ITM, enters into the SSAS for ammonia production. Hydrogen sulfide must be removed from the biogas stream, accomplished here using an EMS system. Hydrogen sulfide is converted into traces of hydrogen and elemental sulfur in the presence of a sweep gas (nitrogen) which is separated via ITM. The CO₂ along with methane are introduced into a CH₄ assisted- SOFEC for hydrogen production. Throughout this conversion, CO₂ is also separated from the hydrogen stream in the electrolyzer.

The hydrogen along with the nitrogen resulting from the separation of air in an ITM then enters the SSAS for producing ammonia which in turn is required for urea production. A portion of the hydrogen resulting from the SOFEC is fed into a SOFC for generating heat, power, and steam for part of the process. The ammonia produced along with the CO₂ resulting from CH₄ assisted- SOFEC enter the urea production process (only for scenario ii). The CO₂ resulting from the CH₄ assisted- SOFEC can be released directly into the atmosphere (scenario i), captured and injected into the ground (scenario iii) or assumed to enter the commodity liquid CO₂ market (scenario iv).

3.4.1.3 Energy flows of the proposed ammonia production through a two-stage DF coupled with AD process

The need for external energy sources is minimized and heat recovery is maximized when the heat integration method is adopted. The energy balance across each processing unit follows the logic: “Heat input + ΔH_R - heat output = Rate of accumulation”. A heat balance model is presented in Fig. 3.14 (a) and (b) for the proposed ammonia production process. It illustrates the energy flow diagram utilizing heat integration and is divided into three parts **I**, **II**, **III**, and **IV** described below:

I: The process streams are cooled with the input air flow at 25 °C before entering the ITM and heated with recirculated steam at about 974.8 °C resulting from an external source of water at 920 °C which enters a compressor before being used for heating up the process at a steady state condition. The input air enters a compressor in order to reach the desired pressure in the range of 10-30 atm before entering the ITM. This air stream is heated from ambient temperature to 850 °C. The separated oxygen is divided into two streams. The first stream enters the SOFC as one of the main feedstocks for its operation. The remaining oxygen passes through the SOFC hot box in order to enter the gas turbine system for power generation. The remaining nitrogen is also divided into two streams. The first stream enters the relief valve to reach the pressure of 1 atm and is cooled down with air before entering the SSAS at 80 °C. The second stream is also cooled down with air and lowered to 650 °C before entering the EMS used as the sweep gas.

II: FW and BW enter the process at 2 °C and are heated to 90 °C in a mixing tank along with the water for dilution. The mixture is then cooled with air to 55 °C in the DFB. The temperature is monitored through the entire process to increase the hydrogen produced. The hydrogen and CO₂ resulting from DF is compressed and passes through a refrigerator in order to reach a pressure of 20 atm and temperature of -39°C before entering the MFI. The sludge is then pumped into the ADB and is cooled to 35 °C.

III: The biogas resulting from the ADB enters a heat exchanger to reach 650 °C before entering the EMS. The resulting nitrogen + sulfur from the EMS enter a condenser in order to separate nitrogen from sulfur. The separated nitrogen will then be recirculated back into the EMS as the sweep gas. The remaining biogas stream from the EMS is then heated to 850 °C and the steam is cooled to the same temperature (850 °C) in order to enter CH₄ assisted-SOFEC for CO₂ separation and hydrogen production. The resulting sludge from the ADB passes through a filter press to remove its moisture for producing compost. The reclaimed water is then recycled back into the mixing tank used as the diluted water.

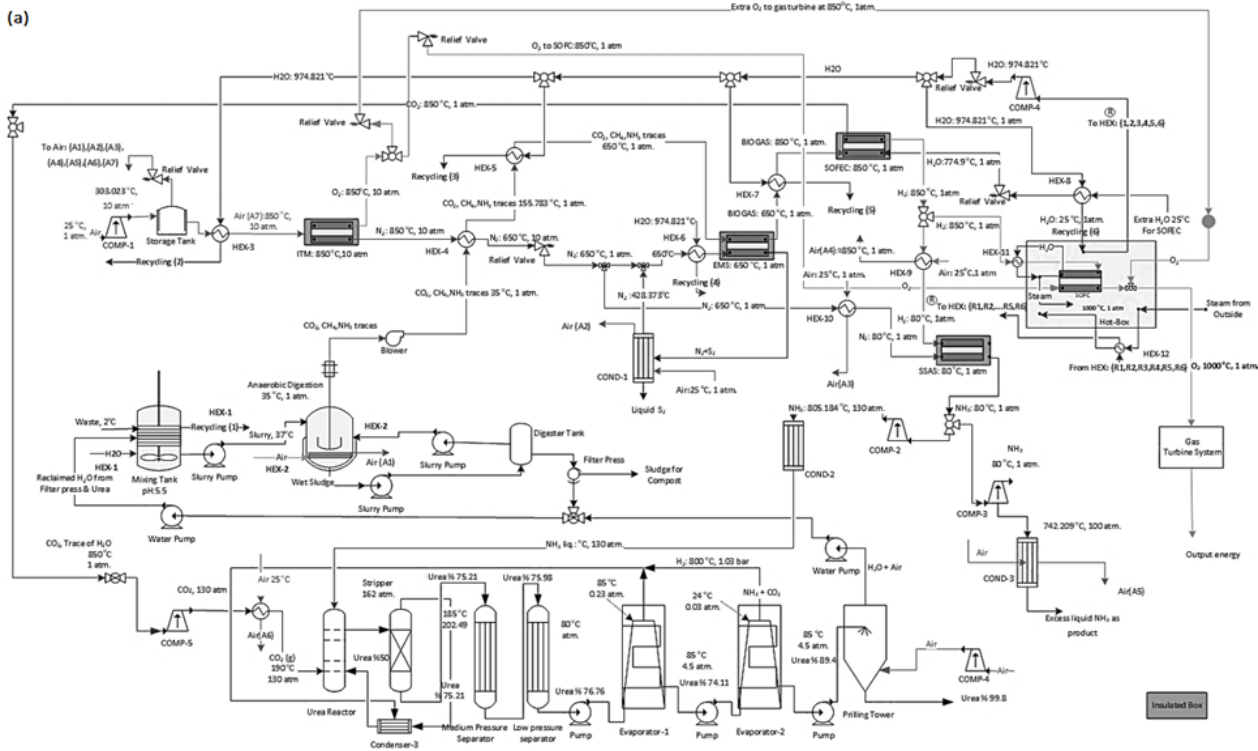
IV: The separated CO₂ from both the MFI and CH₄ assisted- SOFEC are mixed, compressed, and cooled before entering the urea production process at 130 atm and 190 °C (Fig. 3.14 (a)). While for the process without urea production the separated CO₂ is compressed and cooled to 100 atm and 25.1 °C before being captured and injected into the ground or sold commercially (Fig. 3.14 (b)). Simultaneously, the separated hydrogen from both the MFI and CH₄ assisted- SOFEC is also mixed before entering the SSAS at 80 °C and 1 atm. The ammonia produced from the SSAS is divided into two streams, the first stream enters the urea production process (Fig. 3.14 (a)). The second stream is compressed to 100 atm, cooled, and finally liquified (Fig. 3.14 (b)). The remaining hydrogen is heated to 1000 °C before entering the SOFC along with the oxygen from the ITM.

3.4.1.4 Energy flows of the proposed ammonia production through AD-only process

A heat balance model for the proposed ammonia production process demonstrating the energy flow diagram with heat integration is presented in Fig. 3.15 (a) and (b). Part **I** and **III** have the same energy flows as described above. While part **II** and **IV** have different configurations that are described below.

II: The waste stream enters the AD process at 37 °C and is cooled to 35 °C.

IV: The separated CO₂ from the CH₄ assisted- SOFEC is mixed, compressed, and cooled before entering the urea production process at 130 atm and 190 °C (Fig. 3.15 (a)). While for the process without urea production, the separated CO₂ is compressed and cooled to 100 atm and 25.1 °C before being captured and injected into the ground or sold commercially (Fig. 3.15 (b)). Simultaneously the separated hydrogen from the SOFEC reaches 80 °C before entering the SSAS. The ammonia produced from the SSAS is divided into two streams, the first stream enters the urea production process (Fig. 3.15 (a)). The second stream is compressed to 100 atm, cooled, and finally liquified (Fig. 3.15 (b)). The remaining hydrogen is heated to 1000 °C before entering the SOFC along with the oxygen from the ITM.



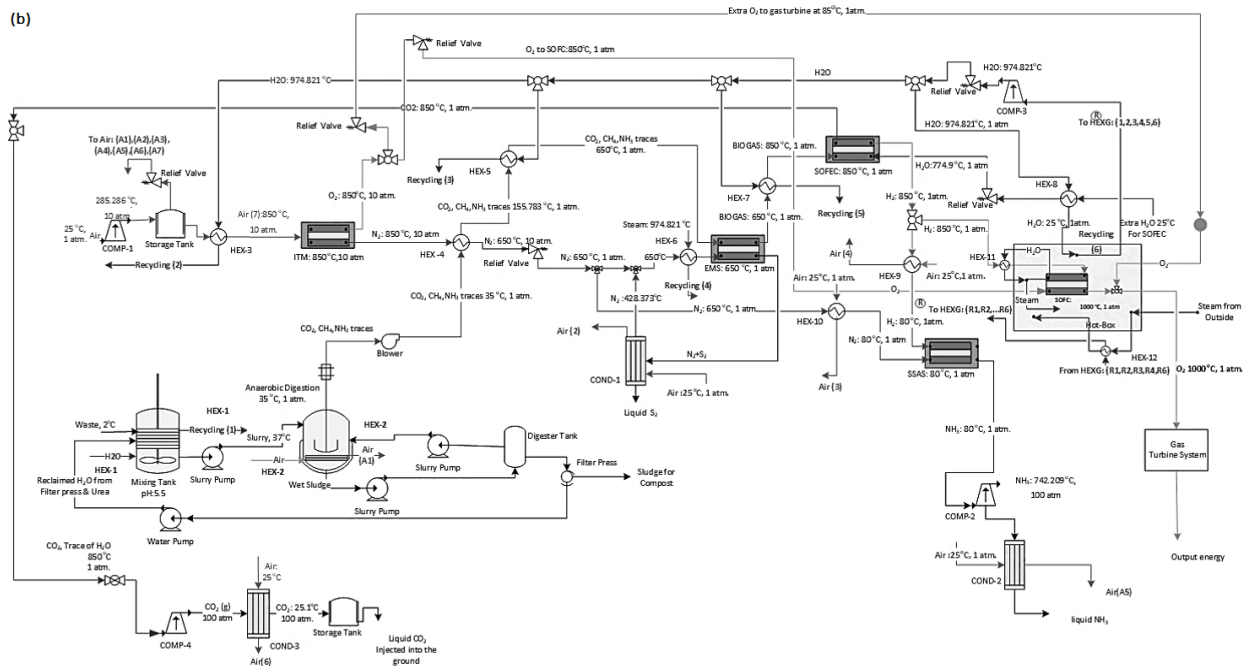


Fig. 3.15: A schematic of the process flow diagram of the proposed ammonia production process through, (a) AD with urea production and by incorporating SOFC and (b) AD without urea production with CCS and by incorporating SOFC.

3.5 Evaluation of the modelling software for the proposed process

In this modelled system, a number of different types of novel membranes (MFI, EMS, ITM, and SSAS) are utilized. Therefore, the selection of the appropriate software for modelling the proposed process was based on having the thermodynamics and kinetic details on these membranes in its database. There are different thermodynamic simulators such as, UniSim®, HYSYS, CHEMCAD, aspenONE, ProMax®, Aspen HYSYS, etc. which have the capability to model and optimize different processes. However, none of the mentioned simulators offer membranes among their standard process functions (Hoorfar, Alcheikhhamdon and Chen, 2018). Nguyen (2014) stated that when modelling for a complex process, a single piece of software may not be enough and other components may need to be coupled to build a robust interoperable tool. While there are several modelling tools which are available for flowsheeting, only a few are appropriate for the optimization and simulation of this modelled system.

Commercial tools such as AspenPlus® do not have the option to model the membrane operation, and so it is necessary to program the membrane in Matlab, FORTRAN, VBA, or other programs. According to, Darkwah, Knutson and Seay (2018) traditional Process Systems Engineering (PSE) tools such as AspenPlus® do not have built-in models that can easily simulate integrated fermentation and in situ product recovery processes. Darkwah, Knutson and Seay (2018) also emphasized that PSE tools do not have the features required to simulate fermentation processes. Without detailed models' optimization is not possible. In addition, one of the major challenges in developing the DF, AD simulation model by AspenPlus® is that it requires a specific analysis for the feed in order to simulate it properly. The digestion/fermentation taking place in the bioreactors involve microorganisms, as a result, their activity cannot be simulated in Aspen and only the kinetics would be specified (Al-Rubaye et al., 2017). Aspen is

categorized as a sequential modular simulator with a loop analyzer for handling the recycle flows (Nguyen, 2014). A library comprised of different industrial operations is included in Aspen, known as build in modules. One can create the process flowsheet by connecting the modules through the mass and heat streams. The modules in Aspen provide a platform for the communication of FORTRAN and Excel for customization and carrying out mathematical calculations. The spreadsheet in Aspen is more robust when compared to other commercial tools such as UniSim as it can connect to user models in order to deal with more complex spreadsheet models (Nguyen, 2014). AspenPlus® has a vast database including data for conventional chemicals, solids, and polymers which are updated frequently by the US National Institute of Standards and Technology (NIST). It contains a wide range of build in models such as pumps, compressors, heat exchangers, reactors, mixers, separators, etc. This process simulator has the capability to be linked with other programming languages such as Excel, FORTRAN, Visual Basic, and MATLAB. According to, Darkwah et al. (2018) nondatabank components are simulated in a communication platform such as VBA in excel or component object model interface in MATLAB and finally connected to a powerful optimization platform. One of the main advantages of using commercial software such as AspenPlus® and Aspen HYSYS is that sensitivity analysis using these tools can be conducted in a relatively short amount of time (Al-Rubaye et al., 2017). Noncommercial tools can also be linked to the databases of a number of commercial tools for obtaining more accurate results. In addition, the system can be tailored and manipulated based on the system component design and desired production output. The physical setup of the components mentioned above in a laboratory would cost significantly higher than simulating a process using software.

3.5.1 Visual Basic for Applications (VBA)

VBA is a programming language built into most of the Microsoft office applications, meaning that users can run the code within a host application without the need for specialized numerical programming packages (Norton and Tiwari, 2010). This software offers a route to activate a variety of built-in as well as writing add in procedures. It also has the flexibilities of other programming languages and has the capability to program any standard numerical algorithm for solving systems of equations, linear systems, nonlinear systems, Ordinary Differential Equations (ODEs), and Partial Differential Equations (PDEs).

This is done by developing a mathematical model with mass and energy balance equations to simulate the performance of the ammonia production process with VBA (embedded in Microsoft Excel) (Computer codes can be found in Appendix A).

3.5.2 Modelling approach

The CO₂ emissions, water, and energy usage of this novel process for the production of ammonia and urea from waste are computationally analyzed. A mathematical model to simulate the performance of the ammonia production process from co-digestion of FW and BW is developed with mass, heat, and energy balance equations. This is implemented in the VBA platform embedded in the Microsoft excel program. The coupled mass and energy balance of this simulated model is assessed under various physical and chemical conditions (temperature, pressure, flow rates, specific heat capacity, porosity, tortuosity, flux, and permeability) and sizing of various processing units (thickness,

area, and number of modules). Assumptions and mathematical equations (mass transfer, energy transfer, thermodynamics, and kinetics) are determined for each processing unit. Since the entire process operates sequentially, the output and the performance of each component affects the input of the other components except for the bioreactors and ITM which are the initial processing units of this proposed process. The modelling framework is comprised of equation-oriented and sequential modular approaches shown in Fig. 3.16. Through this approach, the components (processing units) are modelled using an equation-based approach in sequence, starting with the feed stream and the

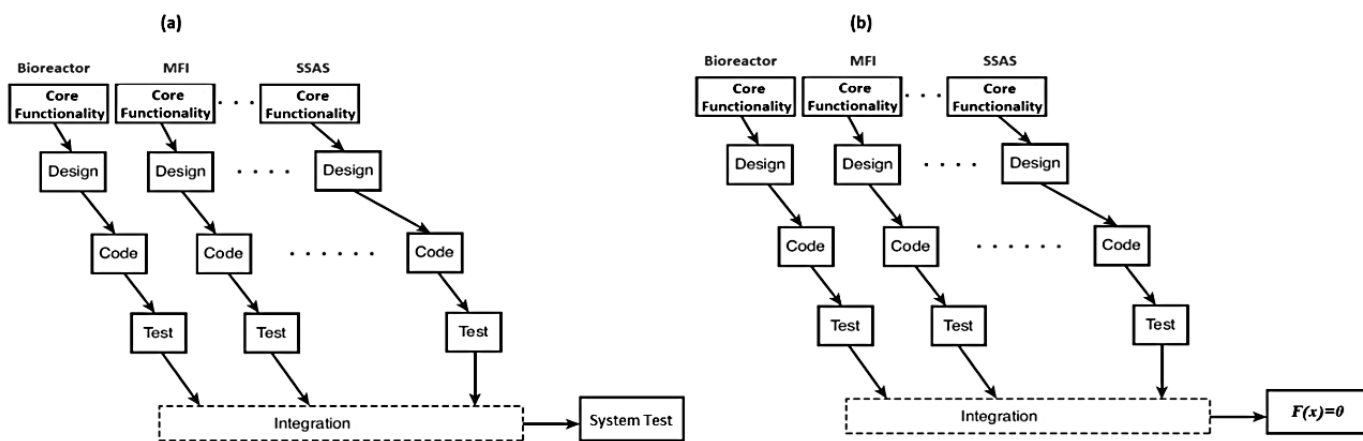


Fig. 3.16: A simplified schematic of the process framework, (a) sequential modular approach and (b) equation-oriented approach.

entire process flow is treated as a set of mathematical equations which need to be solved simultaneously.

Although there are a variety of different thermodynamic simulators capable of modelling and optimizing different processes, none offer membranes among their standard process functions (Hoorfar et al., 2018). Commercial tools such as AspenPlus® do not have the option to model the membrane operation, and so it is necessary to program the membranes in Matlab, FORTRAN, VBA, or other programs. VBA enables us to expose direct optimization of membrane parameters.

3.5.2.1 Assumptions

The results presented in *Chapter 4* are based on the calculations for 20 tons per day (TPD) of input waste (FW and BW). Although other scaling can be evaluated with the implemented model, this figure is calculated to roughly show the size of a mid-size city such as Bakersfield, California. The main assumptions used in this study are listed in Table 3.5.

Table 3.5: List of assumptions used in this study.

Assumptions	
1. Process conditions	2. Operational conditions
<p>- The process operates at a steady state condition</p> <p>-The flow in the membrane, fuel cell, and electrolyzer channels are considered as laminar (Reynolds number<2300)</p> <p>-The composition of gases produced from the DFB is kept fixed at 58.7% H₂ and 41.3% CO₂</p> <p>-The composition of biogas produced from the ADB is kept fixed at 81.5% CH₄, 18.47% CO₂, 0.010 %H₂S, and traces of other gases</p> <p>-The calculations are based on 10 t of FW and 10 t of BW and 25 t of water for dilution.</p>	<p>-The input gas flow enters this process at ambient temperature (25 °C) and pressure (1 atm)</p> <p>-The operating pressures and temperatures are applicable to production processes of any size. As a result, once the size of the plant is selected, the flow rates through the plant can be estimated and the processing units can be properly sized, based on the waste composition, substrate concentration, and dilution rate</p> <p>-Solar radiation and effective temperature are neglected</p> <p>-Physical properties of digester, membrane, fuel cell, and electrolyzer material and the hot box material are uniform over the temperature range considered</p> <p>-The temperature of the substrate inside the bioreactor is constant</p> <p>-The sorted and pretreated FW and BW will be fed to the process at temperatures lower than 4 °C</p> <p>-The temperature within the membranes, fuel cell, and electrolyzer is distributed uniformly</p> <p>- Two-stage CSTR process was selected for continuous hydrogen and methane production using FW and BW. The CSTR was simulated over different ranges of %TS concentration.</p>
<p>1.1 Gas behaviors</p> <p>-Air properties are constant</p> <p>-All gases involved in this production process (H₂, CO₂, CH₄, H₂S, NH₃, O₂, N₂, H₂O, CH₄N₂O, and NH₄CO₂NH₂) are considered as ideal gases ($PV = nRT$)</p> <p>-The gas mixtures are assumed well mixed at the molecular level with all components having the similar velocity, pressure, and temperature</p>	<p>3. Mass and heat transfer</p> <p>-The internal mass transfer resistance between the gas and the membrane surface is negligible</p> <p>-Radiation heat transfer in this process is neglected</p> <p>-The internal heat generation in the two-stage DF and AD is negligible</p> <p>-Heat transfer is linear under steady state condition</p> <p>-The heat transfer coefficient is constant</p> <p>-Heat and mass flows are two-dimensional</p> <p>-The ~99.9% recovery considered in MFI for H₂ and CO₂, ITM for O₂ and N₂, and EMS for H₂S separation were models carried out as a screening analysis with coarse grain data to establish the model and the suitable boundaries</p> <p>- Any product stream that has not been separated completely alongside the permeate gas with a separation efficiency of <0.01% is considered negligible and does not need an additional step for its separation, unless it causes irreversible poisoning of the catalyst used in the processing units.</p>
<p>1.2 Electrolytic assumptions</p> <p>-Anode and cathode gases are not allowed to crossover</p> <p>-The electronic and ionic conductors are spread evenly and continuously throughout the electrodes</p> <p>-Total reactions take place in the SOFEC and SOFC</p> <p>-99.9% of hydrogen produced in this process is diverted into SSAS for ammonia synthesis and the remainder goes to SOFC</p>	<p>4. Material loss</p> <p>-There will be no leakage (material loss) from the process except for CH₄ from the AD, and CO₂ for urea production (NH₃ and N₂O losses are included only in LCA chapters 5 and 6.</p>

Bioreactor calculations

Bioreactor Dimensions

V is the bioreactor useful volume (m^3) and is calculated using Eq. 3.1.

$$V = \frac{m \cdot t}{\rho} \quad (\text{Eq. 3.1})$$

Where, m is the mass flow rate (kg/d), t the HRT, (d), and ρ the density of the feed stream (kg/ m^3).

Assuming, $L = 1.5D$ by substituting it in Eq. 3.2 one can obtain the dimensions of the bioreactor (L, D) (L is the bioreactor height (m) and D is the bioreactor diameter (m)).

$$V = \pi \times \left(\frac{D^2}{4}\right) \times L \quad (\text{Eq. 3.2})$$

V_{total} is the total bioreactor volume (m^3) and derived as Eq. 3.3.

$$V_{total} = V + (0.15 \times V) \quad (\text{Eq. 3.3})$$

Mechanical Design

Agitator Dimensions

Agitator dimensions are calculated based on the equations shown in Table 3.6.

Table 3.6: The equations for calculating the agitator dimensions.

Agitator Dimensions	Equations
Impeller diameter ($D_{impeller}$), (m)	$D_{impeller} = (D/3) \quad (\text{Eq. 3.4})$
Impeller height, ($H_{impeller}$), (m)	$H_{impeller} = D_{impeller} \quad (\text{Eq. 3.5})$
Length of impeller blade, ($L_{impeller}$), (m)	$L_{impeller} = (D_{impeller}/4) \quad (\text{Eq. 3.6})$
Width of impeller blade, ($W_{impeller}$), (m)	$W_{impeller} = (D_{impeller}/5) \quad (\text{Eq. 3.7})$
Number of baffles	3
Width of one baffle, (m)	$L_{baffle} = (D/10) \quad (\text{Eq. 3.8})$
Number of impellers	3
Number of impeller blades	6
Distance between each impeller, (m)	2.2
Shape factors	$S_1 = D_{impeller} / D \quad S_4 = W_{impeller} / D_{impeller}$ $S_2 = H_{impeller} / D \quad S_5 = L_{baffle} / D \quad (\text{Eq. 3.9})$ $S_3 = L_{impeller} / D_{impeller} \quad S_6 = L / D$
Tip velocity, (m/s)	$\pi \times D_{impeller} \times \text{Speed of impeller} \quad (\text{Eq. 3.10})$
Speed of impeller, (RPM)	$[\text{Tip velocity} / (\pi \times 2.2)] \times 60 \quad (\text{Eq. 3.11})$
Actual power required, (hp)	$((6 \times (D_{impeller})^3 \times (\text{Speed of impeller})^3 \times \rho) / g_c) / \text{impeller efficiency} \quad (\text{Eq. 3.12})$

The TS and VS contents of a substrate affect the functionality of both DF and AD. Changing the TS content of the substrate will result in variation in microbial morphology of DF and AD (Orhorhoro et al., 2017). The solids matrix for both fermentation and digestion process is shown in Fig. 3.18.

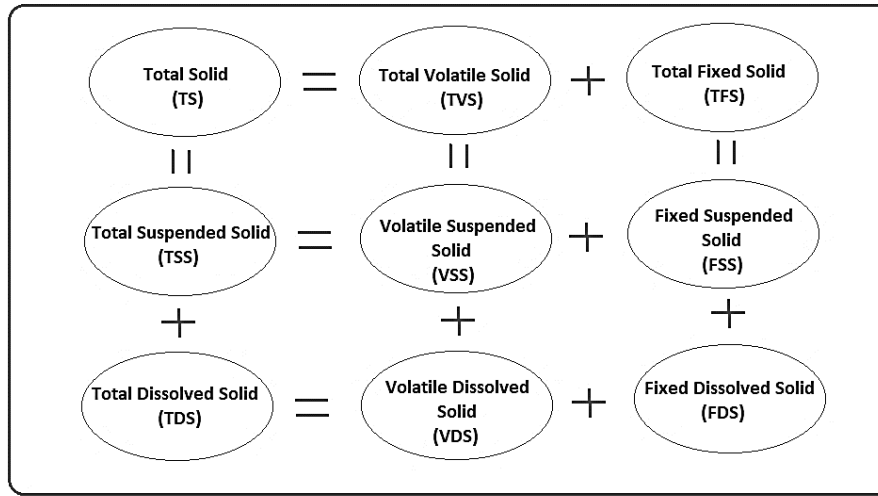


Fig. 3.18: Solids matrix.

Fig. 3.19 also shows the appropriate conditions (range of pH and HRT) for a two-stage DF+AD process to take place. The inhibition of the methanogenic activity can also be accomplished by monitoring the operating parameters such as pH, temperature (heat treatment of inoculum can inactivate hydrogenotrophic methanogens, enhance hydrogen producing bacteria, and select anaerobes that form spores.), OLR, or using additives (De Giannis et al., 2013).

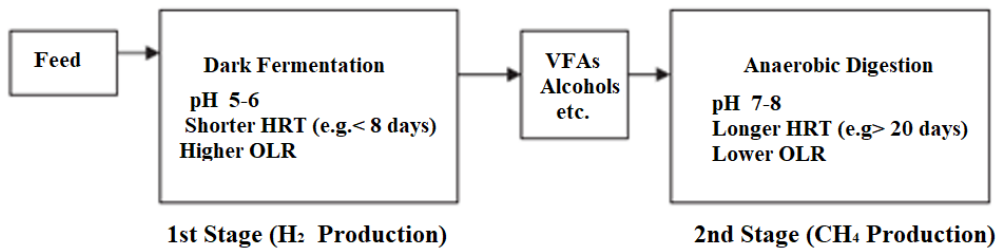


Fig. 3.19: Optimum operational condition for a two-stage DF+AD process.

The VS concentration in the bioreactor at the time t is calculated using Eq. 3.13:

$$C_t = C_o \cdot e^{-kt} \quad (\text{Eq. 3.13})$$

Where, C_t is the VS concentration in the reactor at time t (g/kg), C_o the VS concentration of the influent (g/kg), k the first order constant, (d^{-1}), and t the time (d). In this study C_o is the input and C_t is measured, k is calculated using Eq. 3.13.

θ is the OLR, (gVS/L d) and is calculated using Eq. 3.14:

$$\theta = \frac{k \cdot C_o \cdot C_t}{C_o - C_t} \quad (\text{Eq. 3.14})$$

Y is the biogas yield ($\text{m}^3/\text{kg VS}$) and is calculated by means of Eq. 3.15.

$$y = \frac{\mu \cdot k \cdot C_t}{\theta} \quad (\text{Eq. 3.15})$$

Where, μ is theoretical maximum biogas yield ($\text{m}^3/\text{kg VS}$).

G_{PR} is the gas production rate ($\text{m}^3/\text{m}^3\text{d}$) and is derived from Eq. 3.16.

$$G_{PR} = \theta \times y \quad (\text{Eq. 3.16})$$

Q_{biogas} is the biogas production volume (m^3/d) and is calculated using Eq. 3.17.

$$Q_{biogas} = y \times m \quad (\text{Eq. 3.17})$$

Where, m is the input mass flow rate to the bioreactor (kg/d).

Solis Retention Time (SRT) (d) is estimated as Eq. 3.18.

$$SRT = \frac{1}{k} \quad (\text{Eq. 3.18})$$

Amount of substrate is derived from Eq. 3.19.

$$\text{Amount of substrate} = \theta \times \text{HRT} \quad (\text{Eq. 3.19})$$

BOD is calculated using Eq. 3.20.

$$BOD = 0.6 \times TCOD \quad (\text{Eq. 3.20})$$

Where, $TCOD$ is the total chemical oxygen demand.

3.5.2.3 Gas separation efficiency

Purification of the biogas to remove contaminants is critical to maintain a high conversion rate of ammonia. The separation efficiency for the selected MFI, EMS and ITM membranes used as upgrading stages for ammonia synthesis will significantly affect the overall performance of the process. Since even trace amounts of hydrogen sulfide in the separated hydrogen from EMS directed to SOFC cause irreversible poisoning of the catalyst. This also applies to both MFI and ITM, trace amounts of CO_2 along with separated hydrogen from MFI which is directed to SSAS results in temporary poisoning of the catalyst and small amounts of oxygen along with the separated nitrogen from ITM which is directed to SSAS also cause irreversible poisoning of the catalyst. The objective of incorporating each of the afore-mentioned membranes into the process model was to achieve gas separation of $>99.99\%$ for the system to operate at its maximum performance, meaning, high conversion rate of biogas to ammonia. Therefore, the process design and all of the calculations are based on achieving the separation efficiency of $>99.99\%$, this is clearly demonstrated in the logical flow diagrams in Fig. 3.20-3.22. These figures show the algorithm and modelling approach implemented in VBA in order to solve the balances for the membrane modules. Through the use of VBA,

the system can be tailored and manipulated based on the system component design and desired production output (higher separation efficiency) compared to the physical setup of the process, detailed information on how the desired separation efficiency in each of the above-mentioned membranes is achieved can be found in the four excel files included in the supplemental materials. The results of modelling and simulation discussed in *Chapter 4* indicate that hydrogen and CO₂ from MFI membrane, nitrogen and oxygen from ITM, and hydrogen and sulfur from EMS can be effectively recovered from the gas mixture yielding purity levels of approximately 99.99% from one membrane/a number of membranes, further details can be found in Appendix A (VBA code). This was carried out using MOO of theoretical equations and/or parameters correlated to the above-mentioned membranes adopted from stated sources. The equations Higher gas separation performance could be achieved by adjusting various process parameters indicated as “input data” pertaining to each process component in the following logical flow diagrams. The high purity level was achieved without the need for incorporating a unit operation. However, higher gas separation through the use of a single membrane in real world operation is not realistic. Therefore, hybrid processes such as, membrane separation technology integrated with pressurized water scrubber, amine swing absorption, PSA or multi-membrane separation stages need to be incorporated. Although, this will not be applicable for the separation of hydrogen sulfide in EMS for the proposed waste to ammonia production process, as the amount of hydrogen sulfide produced in both technologies (Tech-1 and Tech-2) is minimal (about 4 kg/day), and the inclusion of an additional unit operation along with a membrane for the separation of approximately >0.0004 kg/d of unseparated hydrogen sulfide is unnecessary.

MFI modelling approach

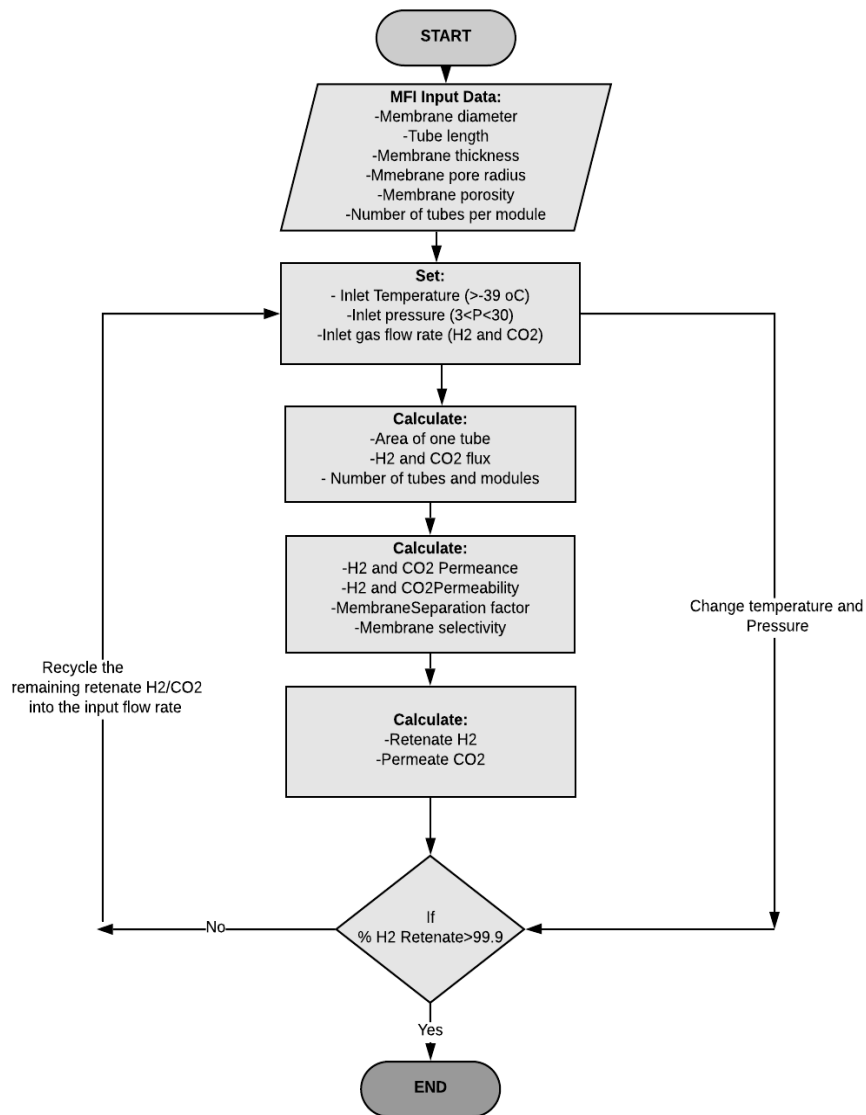


Fig. 3.20: Modelling approach flow diagram for MFI membrane.

The following equations were adopted from Korelskiy et al. (2015), Fouladvand (2016) and Shimonosono et al. (2016).

Kinetics of transport/ flux (J_i) of component i through membrane is formulated as Eq. 3.21.

$$J_i = \frac{F_i}{A} \quad (\text{Eq. 3.21})$$

Where, J_i is the flux, ($\text{mol. s}^{-1} \cdot \text{m}^{-2}$), F_i the molar flow, (mol. s^{-1}), and A the area, (m^2).

The permeance Ω_i of component I , is calculated using Eq. 3.22.

$$\rho_i = \frac{J_i}{\Delta P_i} \quad (\text{Eq. 3.22})$$

Where, ρ_i is the permeance, (mol. s⁻¹.m-2. Pa-1) and ΔP_i the partial pressure (Pa) difference of component i across the membrane.

The membrane selectivity $\alpha_{i/j}$ is estimated as shown in Eq. 3.23.

$$\alpha_{i/j} = \frac{\rho_i}{\rho_j} \quad (\text{Eq. 3.23})$$

Typically, the membrane performance is evaluated based on flux, permeance, and the separation factor.

The separation factor $\beta_{i/j}$ is calculated from Eq. 3.24:

$$\beta_{i/j} = \frac{(y_i/y_j)_{\text{Permeate}}}{(x_i/x_j)_{\text{feed}}} \quad (\text{Eq. 3.24})$$

Where, x and y are the concentrations (e.g., mole fractions or weight fractions) of the separated component i and j in the feed and permeate, respectively.

For calculating the Knudsen Number (KN)

The mechanism of gas flow is determined from the ratio of molecular mean free path of both H₂ and CO₂ to the pore size (Knudsen number). The mean free path is defined as Eq. 3.25:

$$\lambda = \frac{RT}{\pi N_A d_m p \sqrt{2}} \quad (\text{Eq. 3.25})$$

Where, R is the universal gas constant (atm m³/mol K), T the cell temperature (K), N_A is the Avogadro constant, d_m the diameter of the permeating molecule, p the pressure (atm).

Knudsen number is then calculated by dividing the molecular free path to the pore radius (H₂ and CO₂) from Eq. 3.26:

$$KN = \frac{\lambda}{2r} \quad (\text{Eq. 3.26})$$

Where, r is the pore radius. When $KN > 1$ the Poiseuille flow becomes dominate and when $KN < 1$ Knudsen diffusion is considered to become dominant. For this study with the given temperature and pressure KN was less than unity as a result, the Poiseuille flow becomes dominate.

When $KN > 1$ permeability coefficient of gas for the Knudsen equation is calculated using Eq. 3.27:

$$\alpha = \frac{2\epsilon r \bar{c}}{3RT} \quad (\text{Eq. 3.27})$$

\bar{c} is the average velocity of gas molecules and expressed as Eq. 3.28.

$$\bar{c} = \sqrt{\frac{8RT}{\pi M}} \quad (\text{Eq. 3.28})$$

Where, M is the molecular weight of the gas molecules.

The membrane selectivity

From Poiseuille equation permeability of component i ($\propto i$) is calculated as Eq. 3.29:

$$\alpha = \frac{\epsilon r^2 \bar{P}}{8RT\eta} \quad \text{(Eq. 3.29)}$$

Where, α is the permeability coefficient of gas, ϵ open porosity, r pore radius of a porous membrane (μm), η gas viscosity (CentiPoise), R gas constant ($8.314 \text{ J. mol}^{-1} \cdot \text{K}^{-1}$), T absolute temperature (K), \bar{P} average pressure between the inlet and outlet gases (atm).

By knowing the permeability of gas and multiplying it by the pressure gradient $\frac{\Delta P_i}{L}$ the gas flux is calculated as Eq. 3.30.

$$J_i = \alpha \frac{\Delta P_i}{L} \quad \text{(Eq. 3.30)}$$

The fraction of hydrogen gas at the outlet for the mixed gas is calculated as:

By calculating α for both CO_2 and H_2 , two fluxes are obtained by using the following Eq. 3.31. The fraction of outlet H_2 gas to the total CO_2 and H_2 gases for Poiseuille flow is:

$$F_P = \frac{J(\text{H}_2)}{J(\text{H}_2)+J(\text{CO}_2)} = \frac{\eta(\text{CO}_2)}{\eta(\text{CO}_2)+\eta(\text{H}_2)} \quad \text{(Eq. 3.31)}$$

If $\text{KN} > 1$ for Knudsen diffusion the following Eq. 3.32 is:

$$F_K = \frac{J(\text{H}_2)}{J(\text{H}_2)+J(\text{CO}_2)} = \frac{\bar{c}(\text{H}_2)}{\bar{c}(\text{H}_2)+\bar{c}(\text{CO}_2)} = \frac{\sqrt{M(\text{CO}_2)}}{\sqrt{M(\text{CO}_2)}+\sqrt{M(\text{H}_2)}} \quad \text{(Eq. 3.32)}$$

The mechanism of gas flow is determined from the ratio of molecular mean free path to the pore size (Knudsen number). The mean free path is defined as (Eq. 3.33):

$$\lambda = \frac{\eta}{0.499(P)\sqrt{\frac{8M}{\pi RT}}} \quad \text{(Eq. 3.33)}$$

The membrane selectivity which is generally defined as $f(i)$ is related to the F value according to the following equation, which is the ratio between the permeability coefficients of the major and minor permanent gases Eq. 3.34.

$$f(\text{H}_2) = \frac{\alpha(\text{H}_2)}{\alpha(\text{CO}_2)} = \frac{F(\text{H}_2)}{1-F(\text{H}_2)} = \frac{\bar{\Pi}_i}{\bar{\Pi}_j} \quad \text{(Eq. 3.34)}$$

Where, $\bar{\Pi}_i = \frac{J_i}{\Delta P_i}$ is defined as the permeance of the component through the membrane.

EMS modelling approach

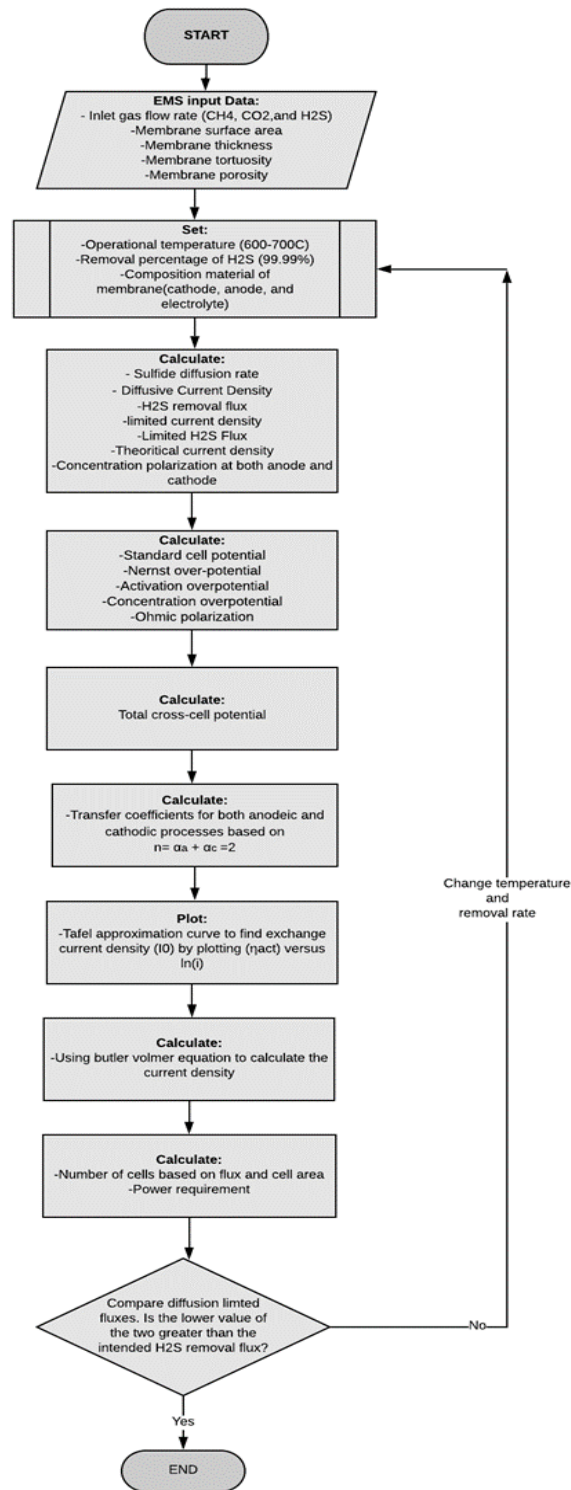
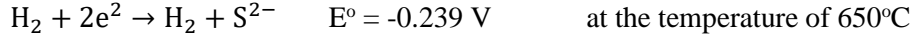


Fig. 3.21: Modelling approach flow diagram for EMS.

The following equations were adopted from Burke et al. (2004) and Winnick and Liu (2003).

The chemical reaction that takes place in this separation is as follows (Eq. 3.35).



$$E_{eq} = E^0 - \frac{RT}{nF} \ln \left\{ \frac{a_{\text{S}^{2-}}^{\text{cathode}} P_{\text{H}_2}^{\text{cathode}} P_{\text{S}_2}^{\frac{1}{2}}}{a_{\text{S}^{2-}}^{\text{anode}} P_{\text{H}_2\text{S}}^{\text{cathode}}} \right\} \quad (\text{Eq. 3.35})$$

Molar flux is attained from the diffusive flux of sulfide ions through the membrane and will be carried out through (Eq. 3.36).

$$\text{Molar Flux} = \frac{i_{\text{diffusion}}}{nF} = D_{\text{S}^{2-}\text{-electrolyte}} \frac{\varepsilon \rho_{\text{electrolyte}} C_{\text{S}^{2-}}^{\text{cath}}}{\tau x} \quad (\text{Eq. 3.36})$$

Where, $i_{\text{diffusion}}$ is the Diffusive Current Density, (A/cm²), n number of electrons transferred per mole reacted (2 mol⁻¹ in this reaction), F Faraday's constant (C), ε membrane porosity (72%), τ membrane tortuosity (3.6), $D_{\text{S}^{2-}\text{-electrolyte}}$ the diffusivity of sulfide ions in the electrolyte (1.0 x10⁻⁵ cm² s⁻¹), x membrane thickness (1.8 mm), $C_{\text{S}^{2-}}^{\text{cath}}$ the molar fraction of sulfide species at the cathode (1.47 x10⁻⁶), $\rho_{\text{electrolyte}}$ electrolyte molar density (5.450 mol/cm³).

Gas Mass Transfer Limitation

Flux of the of component i through membrane is formulated as Eq. 3.37.

$$\text{Flux} = \frac{i_L}{nF} = K_m \rho_{fg} \frac{(y_{\text{inlet}} - y_{\text{outlet}})}{\ln\left(\frac{y_{\text{inlet}}}{y_{\text{outlet}}}\right)} \quad (\text{Eq. 3.37})$$

Where, K_m is the mass transfer coefficient (~10-12 cm. s⁻¹), ρ_{fg} fuel gas molar density (5.45 mol/cm³), y_{inlet} the inlet mole fractions of H₂S (9.18 x10⁻⁸), y_{outlet} the outlet mole fractions of H₂S (4.33 x10⁻¹⁰), and i_L the mass transfer limited current density.

Minimum current required to remove all the H₂S is carried out through Eq.3.38 and 3.39 as follows:

$$i_{\text{theory}} = \frac{nF\dot{n}_{\text{H}_2\text{S}}}{A} \quad (\text{Eq. 3.38})$$

$$i_{\text{theory}} \approx nF \frac{P\dot{V}}{(R)(T)(A)} y_{\text{inlet},\text{H}_2\text{S}} \quad (\text{Eq. 3.39})$$

Where, $\dot{n}_{\text{H}_2\text{S}}$ is the molar flow rate of H₂S, (mol. s⁻¹), R the Universal gas constant (8.314 J/mol.K), A , the electrode area (7.9 cm²), T , the membrane's operational temperature (650°C +273.15= 923.15 K), P the operational pressure of membrane that drives the separation (1 atm), and \dot{V} the volumetric flow rate, (cm³/s).

The excess voltage required due to mass transport limitations in a membrane is the concentration polarization. The concentration polarization at both cathode and anode is carried out as shown in Eq. 3.40 and 3.41.

$$\eta_{conc,cathode} = \frac{RT}{nF} \ln \left(\frac{i_L - i}{i_L} \right) \quad (\text{Eq. 3.40})$$

$$\eta_{conc,anode} = \frac{RT}{nF} \ln \left(\frac{i_{diff} - i}{i_{diff}} \right) \quad (\text{Eq. 3.41})$$

Butler-Volmer equation is shown in Eq.3.42: The following equation relates the activation over-potential to the flux/current density.

$$i = i_0 \left\{ \exp \left(\alpha_a \frac{nF}{RT} \eta_{act,anode} \right) - \exp \left(\alpha_c \frac{nF}{RT} \eta_{act,cathode} \right) \right\} \quad (\text{Eq.3.42})$$

Where, α_a , α_c are the transfer coefficients for the anodic and cathodic processes respectively (1 Based on the set assumptions: $n = \alpha_a + \alpha_c = 2$), i_0 the exchange current density, and η_{act} the activation overpotential (-1.23V).

In order to solve the Butler-Volmer equation, a Tafel approximation was carried out based on Eq. 3.43. η_a is the activation overpotential (V), T is membrane's operational temperature (K), R is the universal gas constant (J/mol.K), F = Faraday's constant, α = the transfer coefficient, i_0 = the exchange current density, and i = the current density.

$$\eta_a = \frac{RT}{\alpha F} \ln \frac{i}{i_0} = \frac{RT}{\alpha F} \ln i_0 + \ln i \quad (\text{Eq. 3.43})$$

i versus η_a was plotted in order to find i_0 .

The total cell over-potential in this separation is carried out as Eq. 3.44:

$$E_{cell} = E_{eq} + \eta_{act} + \eta_{conc} + IR_{cell} \quad (\text{Eq. 3.44})$$

The required power for running this separation process is Eq. 3.45:

$$P = I A V \quad (\text{Eq. 3.45})$$

Where, P is the power (kW), I is the total current (A), (Area \times current density), and V the total voltage ($E_{cell} \times$ number of cells).

ITM modelling approach

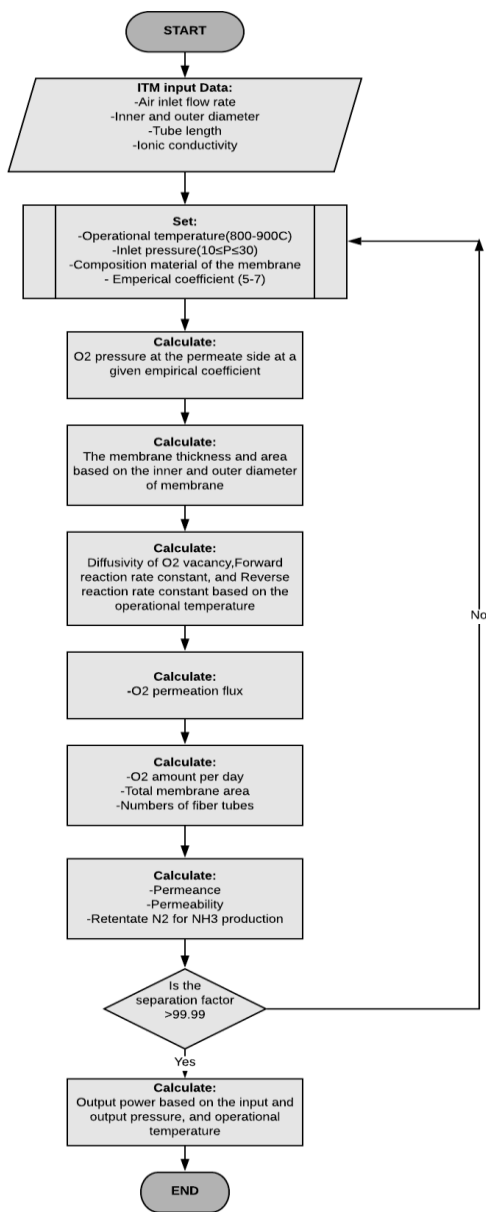


Fig. 3.22: Modelling approach flow diagram for ITM.

The following equations were adopted from Han et al. (2018) and Sun, Larpudomlert and Thepwatee (2011).

Ionic oxygen flux is calculated using Eq.3.46.

$$J_{O_2} = \frac{\sigma_i RT}{4Ln^2 F^2} \ln \left(\frac{P'_{O_2}}{P''_{O_2}} \right) \quad (\text{Eq. 3.46})$$

Where, J_{O_2} is the ionic oxygen flux (mol.cm⁻².s⁻¹), F is the Faraday's constant (96485 coulombs/mole), L the membrane thickness (mm), n the charge of carrier ($n = 2$), R the gas constant (8.314 J/K.mol), T is absolute temperature (K), σ_i the ionic conductivity, P'_{O_2} the oxygen pressure at the feed surface of the membrane, P''_{O_2} the oxygen pressure at the permeate surface of the membrane.

Oxygen permeation flux is obtained as Eq.3.47a and 3.47b:

$$J_{O_2} = \frac{K_r (P_{O_2}^{0.5} - P_{O_2}''^{0.5})}{R_o (P_{O_2}^{0.5}) + \frac{2k_f (R_o - R_{in}) (P'_{O_2} P''_{O_2})^{0.5}}{D_v} + \frac{R_m}{R_{in} (P'_{O_2})^{0.5}}} \quad (\text{Eq. 3.47a})$$

$$J_{O_2} = \frac{D_v k_r [(p'_{O_2})^{0.5} - (p''_{O_2})^{0.5}]}{2k_f t_m (p'_{O_2} p''_{O_2})^{0.5} + D_v (p'_{O_2})^{0.5} + (p''_{O_2})^{0.5}} \quad (\text{Eq. 3.47b})$$

Where, J_{O_2} is oxygen permeation flux (mol/ cm².s), k_r the reverse reaction rate, (mol/atm².s), k_f the forward reaction rate, (cm/atm^{0.5}. s), D_v is the diffusivity of oxygen vacancy, (cm²/s), R_o outer radius (mm), R_{in} inner radius (mm), R_m thickness (mm) are derived from Eq. 3.48- 3.51 respectively:

$$k_r = 2.07 \times 10^4 * e^{\left(\frac{-29023}{T} \right)} \quad (\text{Eq. 3.48})$$

$$k_f = 5.9 \times 10^6 * e^{\left(\frac{-27291}{T} \right)} \quad (\text{Eq. 3.49})$$

$$D_v = 1.58 \times 10^2 * e^{\left(\frac{-8852.5}{T} \right)} \quad (\text{Eq. 3.50})$$

$$R_m = \frac{(R_o - R_{in})}{\ln \left(\frac{R_o}{R_{in}} \right)} \quad (\text{Eq. 3.51})$$

Permeability is carried out through Eq. 3.52.

$$P_m = \frac{(J_{O_2}) l_m}{P_F - P_P} \quad (\text{Eq. 3.52})$$

Where, P_m is the permeability, l_m the thickness, P_F and P_P are the feed pressure and permeate pressure respectively.

Permeance is obtained using Eq. 3.53.

$$\bar{P}_M = \frac{P_m}{l_m} \quad (\text{Eq. 3.53})$$

Where, \bar{P}_M is the permeance.

Membrane thickness is carried out as Eq.3.54.

$$\delta = \frac{R_o - R_{in}}{\ln\left(\frac{R_o}{R_{in}}\right)} \quad (\text{Eq. 3.54})$$

Where, δ is the thickness (mm), R_o the outer radius (mm), and R_{in} the inner radius (mm).

Vacancy conductivity is estimated using Eq. 3.55.

$$\sigma_V = \frac{4F^2}{kT} C_v D_v \quad (\text{Eq. 3.55})$$

Where, σ_V is the ionic conductivity, k the Boltzmann constant, F Faraday constant, T absolute temperature, $C_v = \delta/V_m$ (Where V_m is the molar volume (m^3/mole)), and D_v diffusivity of oxygen vacancy (cm^2/s).

Cell pressure at the permeate side is Eq. 3.56.

$$P_{O_{2out}} = \frac{P_{feed} X_{feed}}{\pi} \quad (\text{Eq. 3.56})$$

Where, π is the empirical coefficient in the range of $5 \leq \pi \leq 7$, here it is assumed that π is 5.2.

Membrane area is obtained using Eq. 3.57.

$$UTA = 2\pi \frac{R_o}{1000} \frac{L}{100} \quad (\text{Eq. 3.57})$$

Where, UTA is the unit tube area (m^2), L is the tube length (m), and R_o is the outer diameter (mm).

Effect of temperature on oxygen permeation (Empirical Formula) Eq. 3.58.

$$J_o = e^{-12.794388 + \frac{-7012.019}{T} + 1.0115107 \ln(T)} \quad (\text{Eq. 3.58})$$

Effect of temperature on oxygen production (Empirical Formula) Eq. 3.59.

$$J_o = e^{13.072706 + \frac{-7242.7553}{T} + 0.78088907 \ln(T)} \quad (\text{Eq. 3.59})$$

CH₄-assisted SOFEC modelling approach

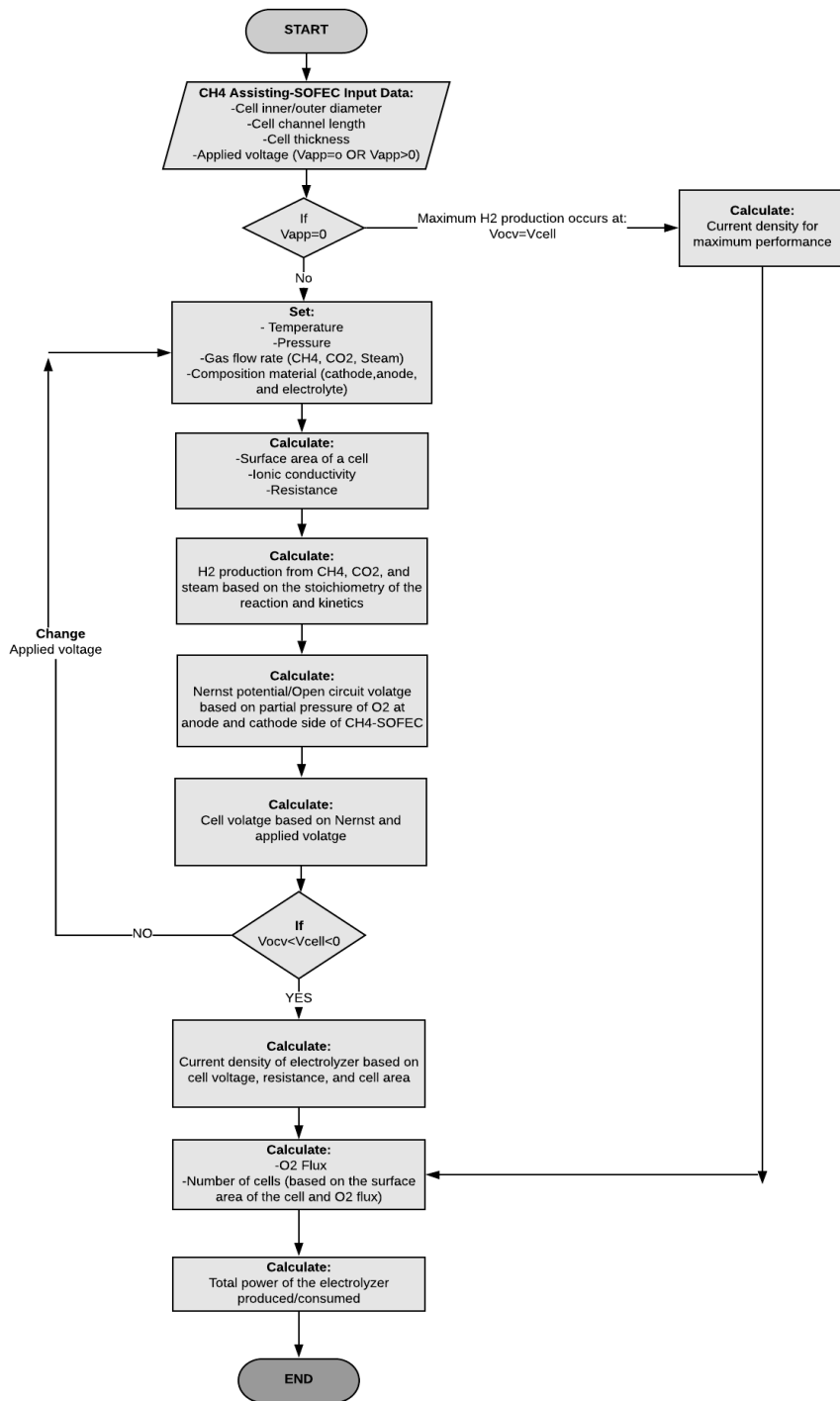


Fig. 3.23: Modelling approach flow diagram for CH₄ assisted-SOFEC.

The following equations were adopted from Xu et al. (2016), Wijers (2011) and Gross (2008).

Membrane separation is calculated using Eq. 3.60:

$$N_i = \frac{D_i}{L}(C_{i0} - C_{iL}) \quad \text{(Eq. 3.60)}$$

Where, N_i is the flux (mol O²/cm².s), D_i diffusivity (cm²/s), L membrane thickness (cm), and C_{iL} and C_{i0} are concentrations in the membrane interfaces (mol O²/cm³).

Current density is calculated using Eq. 3.61:

$$i = \frac{(E_{OCV} - E_{OP})\sigma}{L} \quad \text{(Eq. 3.61)}$$

Where, E_{OCV} is the open circuit voltage (V), E_{OP} operating voltage (V), σ ionic conductivity (1/Ω.cm), and L thickness of membrane (cm).

The area of micro tube is calculated through Eq. 3.62.

$$A_m = \frac{\pi(D_o - D_i)L}{\ln\left(\frac{D_o}{D_i}\right)} \quad \text{(Eq. 3.62)}$$

Where, A_m is the area of micro tube (m²), D_o , D_i are the outer and inner diameters respectively (m), and L the length of tube (m).

The active area of cell is calculated through Eq. 3.63.

$$A_{cell} = 2 \pi r_{in} L_{cell} \quad \text{(Eq. 3.63)}$$

Where, A_{cell} is the active area of cell (m²), r_{in} the inner radius (m), and L_{cell} the activate length (m).

The electrolyzer voltage is calculated using Eq. 3.64:

$$V = i.RA \quad \text{(Eq. 3.64)}$$

Where, V is voltage (Ω.C/s), i current density (C/cm².s), RA area-specific resistance (Ω. cm²).

The oxygen ion flux is derived from Eq. 3.65a and Eq. 3.65b:

$$N_{O^{2-}} = \frac{i}{nF} \quad \text{(Eq. 3.65a)}$$

$$N_{O^{2-}} = \frac{\sigma}{L.nF}(E_{OCV} - E_{OP}) \quad \text{(Eq. 3.65b)}$$

Where, $N_{O^{2-}}$ is the flux (mol O²/cm².s), i current density (C/cm².s), n mole of electrons passed through the membrane, F Faraday constant 96485 (C/mol.e⁻).

SSAS modelling approach

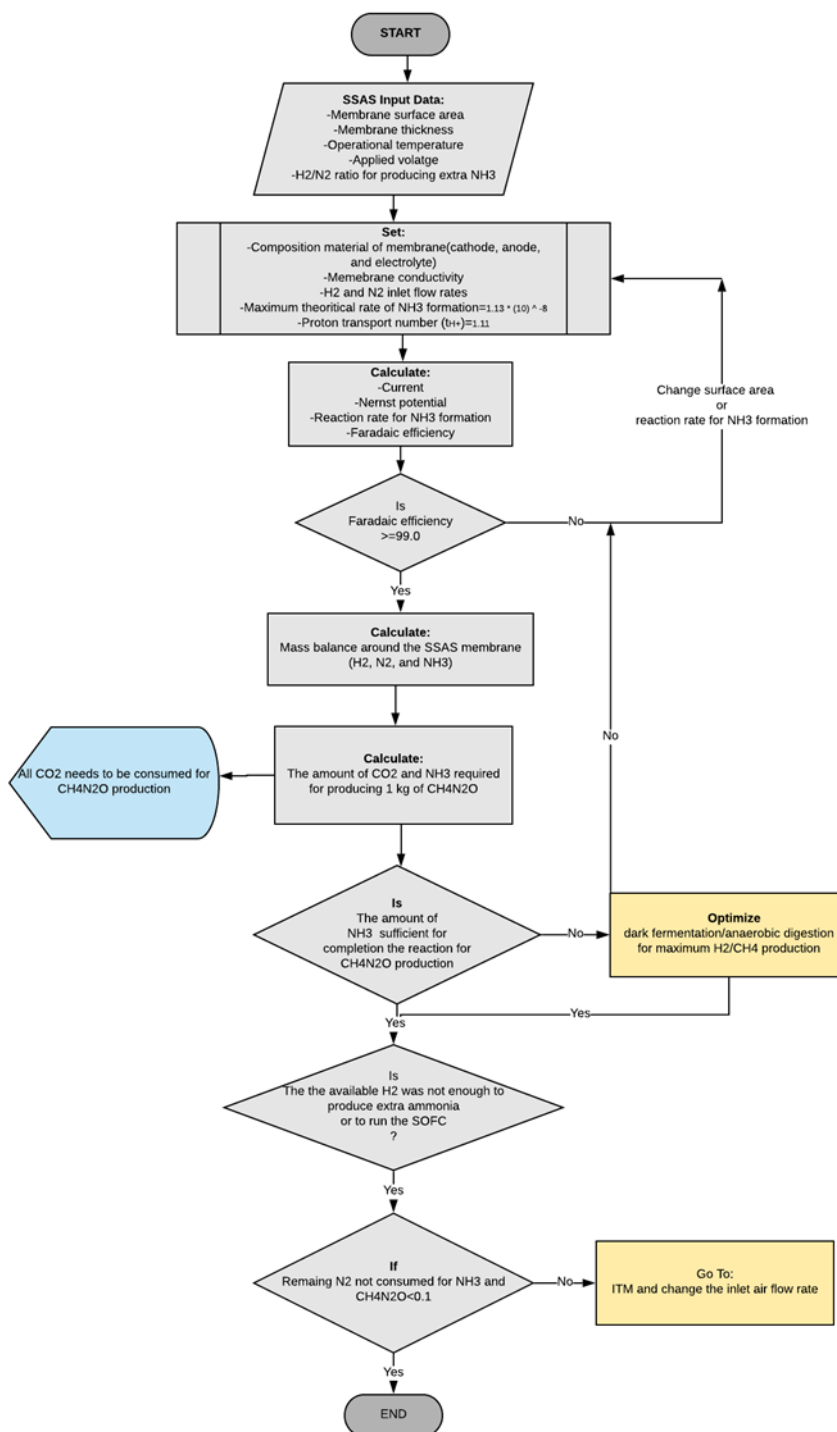


Fig. 3.24: Modelling approach flow diagram for SSAS membrane.

The following equations were adopted from Xu et al. (2009) and Garagounis et al. (2014).

The specific area resistance of membrane is derived from Eq. 3.66.

$$\bar{R}_{int} = \frac{\delta}{\sigma} \quad (\text{Eq. 3.66})$$

Where, \bar{R}_{int} is the specific area resistance (Ω), δ electrolyte thickness, and σ ionic conductivity.

Standard emf of the cell is obtained using Eq. 3.67.

$$E_0 = \frac{\Delta G_{rxn}^0}{6F} \quad (\text{Eq. 3.67})$$

Where, E_0 is the standard emf of the cell (V), and ΔG_{rxn}^0 Gibbs free energy (KJ/mol).

Nernst voltage is calculated using Eq. 3.68.

$$E_{ner} = E_0 + \frac{RT}{6F} \ln \left(\frac{P_{N_2} P_{H_2}^3}{P_{NH_3}^2} \right) \quad (\text{Eq. 3.68})$$

Where, E_{ner} is the Nernst voltage (V), R gas constant $8.314 \text{ (JK}^{-1}\text{mol}^{-1}\text{)}$, T cell temperature (K), P_{N_2} , P_{H_2} , and P_{NH_3} are pressures of nitrogen, hydrogen, and ammonia (atm).

The required cell voltage is carried out through Eq. 3.69.

$$E_C = E_{ner} + E_{app} \quad (\text{Eq. 3.69})$$

Where, E_C is the required cell voltage (V) and E_{app} the applied voltage (V).

Ammonia reaction rate is derived from Eq. 3.70.

$$r_{NH_3} = -\frac{2}{3} \left(\frac{E_{ner} - E_{cell}}{(\delta/\sigma)6F} \right) \quad (\text{Eq. 3.70})$$

Where, r_{NH_3} is the ammonia reaction rate ($\text{mol/cm}^2\cdot\text{s}$).

The cell current density is estimated from Eq. 3.71.

$$i_{cell} = \frac{(E_{ner} - E_{cell})}{\bar{R}_{int}} \quad (\text{Eq. 3.71})$$

Where, i_{cell} is the cell current density ($\text{A}\cdot\text{cm}^{-2}$) and E_{cell} is the applied voltage (V).

There is a proportional relation between reaction rate and cell current density as shown in Eq. 3.72 (Total current per unit cell area):

$$\frac{i_{cell}}{2F} = -r_{H_2} = r_{NH_3} \quad (\text{Eq. 3.72})$$

Where, r_{H_2} is the hydrogen reaction rate (mol/cm².s).

Exchange current density is calculated through Eq. 3.73.

$$i_0 = 2Fr_{NH_3} \quad (\text{Eq. 3.73})$$

i_0 is the exchange current density (C/cm².s).

Faradaic efficiency is estimated through Eq. 3.74.

$$FE = \frac{3F.r_{max}.A}{I.t_H^+} \times 100 \quad (\text{Eq. 3.74})$$

Where, FE is the Faradaic efficiency (%), A the surface area of membrane (cm²), I the current (A), t_H^+ the proton (H⁺) transport number (1.07) at a given r_{max} (1.13×10⁻⁸ mol.s⁻¹.cm⁻²). This maximum reaction rate is based on the study conducted by Xu et al. (2009).

SOFC modelling approach

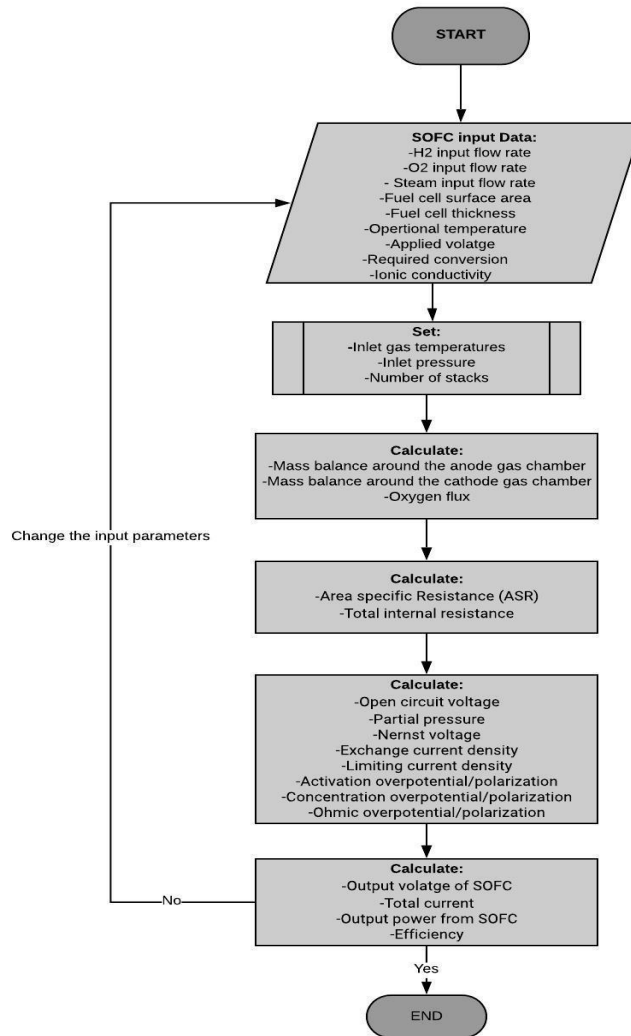


Fig. 3.25: Modelling approach flow diagram for SOFC.

The following equations were adopted from Ugartemendia, Ostolaza and Zubia (2013) and Chmielewski (2008).

There is a proportional relation between reaction rate and cell current density as shown in Eq. 3.75 (Total current per unit cell area):

$$\frac{i_{cell}}{2F} = -r_{H_2} = r_{H_2O} = -2r_{O_2} \quad (\text{Eq. 3.75})$$

Standard cell potential is estimated using Eq. 3.76.

$$E_0 = \frac{\Delta G_{rxn}^0}{2F} \quad (\text{Eq. 3.76})$$

Nernst voltage is calculated using Eq. 3.77.

$$E_{ner} = E_0 + \frac{RT}{2F} \ln \left(\frac{P_{H_2} P_{O_2}^{1/2}}{P_{H_2O}} \right) \quad (\text{Eq. 3.77})$$

H₂ reaction rate is estimated through Eq. 3.78.

$$-r_{H_2} = \frac{\left(E_0 + \frac{RT}{2F} \ln \left(\frac{P_{H_2} P_{O_2}^{1/2}}{P_{H_2O}} \right) - E_{cell} \right)}{\left(\frac{\theta}{\sigma} \right) 2F} \quad (\text{Eq. 3.78})$$

Activation overpotential is calculated using Eq. 3.79.

$$E_{ACT} = \frac{RT}{\beta F} \text{Sinh}^{-1} \left(\frac{i}{2i_0} \right) \quad (\text{Eq. 3.79})$$

Where, E_{ACT} is the activation overpotential (V), i the current density (kA cm⁻²), i_0 the exchange current density (kA cm⁻²), and β charge transfer coefficient.

Exchange current density is calculated as Eq. 3.80.

$$i_0 = A \exp \left(\frac{E_{ACT}}{RT} \right) \quad (\text{Eq. 3.80})$$

Where, i_0 is the exchange current density (kA cm⁻²), E_{ACT} the activation energy of electrochemical reaction (J mol⁻¹), and A the area of cell (m²).

Ohmic polarization is calculated using **Eq. 3.81**.

$$\eta_{ohm} = IR_{ohm} \quad (\text{Eq. 3.81})$$

Where, η_{ohm} is the total voltage drop of a fuel cell due to ohmic polarization (V), I total current throughout the fuel cell (A), and R_{ohm} —the electrical resistance of the fuel cell.

Urea production process (Snamprogetti process) modelling approach

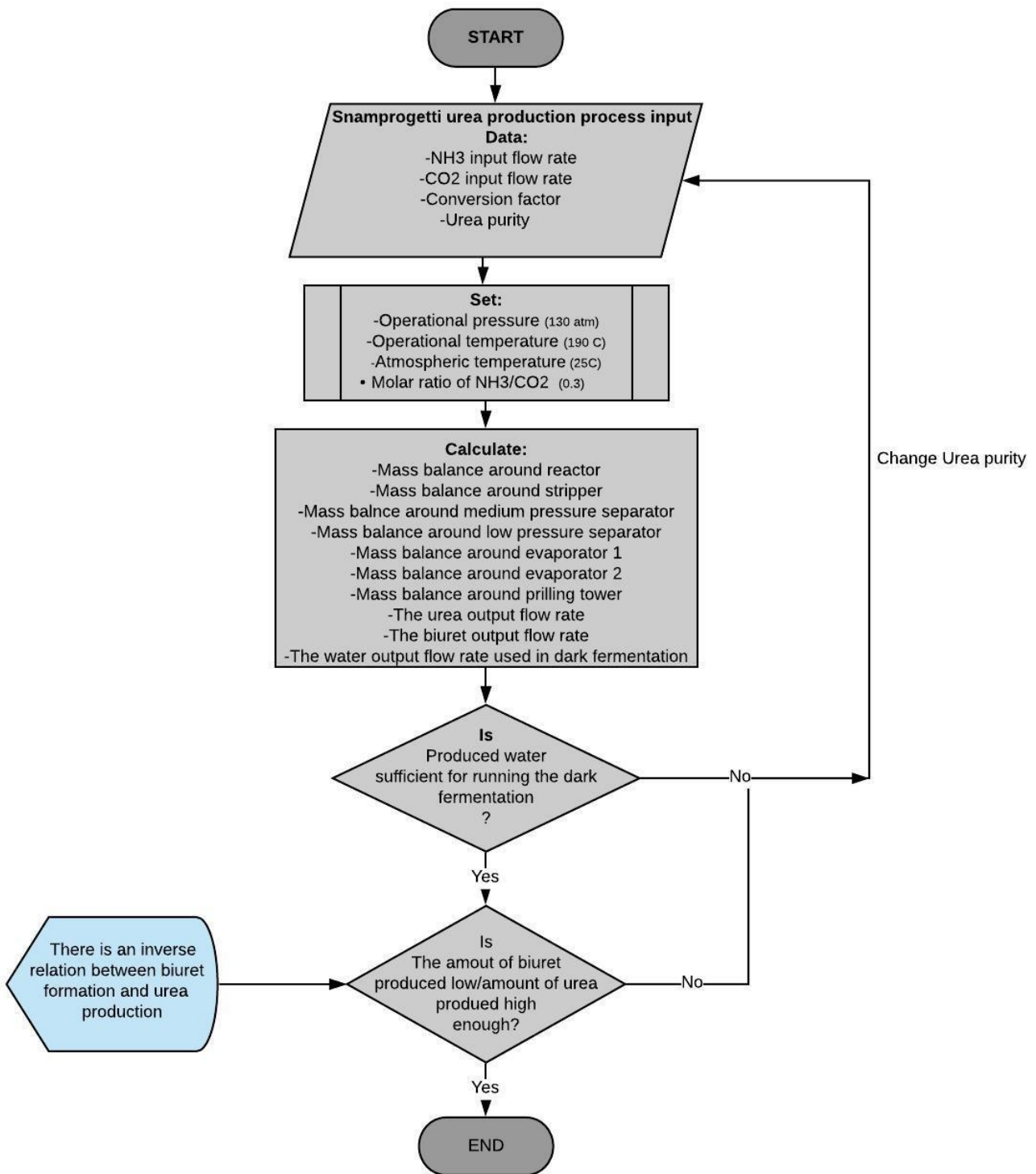
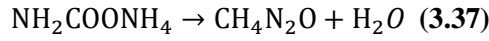


Fig. 3.26: Modelling approach flow diagram for urea production through Snamprogetti process.

The following equations were adopted from Li (2013) and Bhaskar and Chandra Das (2007).

The chemical reaction for the urea production is as follows (3.36 and 3.37):



By combining the conversion of the above reactions an overall conversion is derived as stated by, Li, (2013) (3.82, 3.83, and 3.84):

$$\text{Reaction1: } \varepsilon_1 = \frac{F_{\text{carbamate}} + F_{\text{urea}}}{F_{\text{carbamate}}^0 + F_{\text{urea}}^0 + F_{\text{CO}_2}^0} \quad (\text{Eq. 3.82})$$

$$\text{Reaction2: } \varepsilon_2 = \frac{F_{\text{urea}}}{F_{\text{carbamate}} + F_{\text{urea}}} \quad (\text{Eq. 3.83})$$

$$\text{Overall: } \varepsilon = \frac{F_{\text{urea}}}{F_{\text{carbamate}}^0 + F_{\text{urea}}^0 + F_{\text{CO}_2}^0} \quad (\text{Eq. 3.84})$$

Ammonia feed ratio and water ratio are assumed to be a and b respectively (3.85 and 3.86) and the overall conversion as expressed by Li, (2013) is:

$$a = \frac{F_{\text{NH}_3}^0}{F_{\text{carbamate}}^0 + F_{\text{urea}}^0 + F_{\text{CO}_2}^0} \quad (\text{Eq. 3.85})$$

$$b = \frac{F_{\text{H}_2\text{O}}^0}{F_{\text{carbamate}}^0 + F_{\text{urea}}^0 + F_{\text{CO}_2}^0} \quad (\text{Eq. 3.86})$$

$$F_{\text{Total}}^0 = F_{\text{NH}_3}^0 + F_{\text{carbamate}}^0 + F_{\text{urea}}^0 + F_{\text{CO}_2}^0 + F_{\text{H}_2\text{O}}^0 \quad (\text{Eq. 3.87})$$

$$F_{\text{carbamate}} = \varepsilon_1 - \varepsilon (F_{\text{carbamate}}^0 + F_{\text{urea}}^0 + F_{\text{CO}_2}^0)$$

$$F_{\text{urea}} = \varepsilon (F_{\text{carbamate}}^0 + F_{\text{urea}}^0 + F_{\text{CO}_2}^0)$$

$$F_{\text{NH}_3} = a - 2\varepsilon_1 (F_{\text{carbamate}}^0 + F_{\text{urea}}^0 + F_{\text{CO}_2}^0)$$

$$F_{\text{CO}_2} = 1 - \varepsilon_1 (F_{\text{carbamate}}^0 + F_{\text{urea}}^0 + F_{\text{CO}_2}^0)$$

$$F_{\text{H}_2\text{O}} = b + \varepsilon (F_{\text{carbamate}}^0 + F_{\text{urea}}^0 + F_{\text{CO}_2}^0)$$

$$F_N = (1 + a + b - 2\varepsilon_1 + \varepsilon) \quad (\text{Eq. 3.88})$$

The mole fractions of each component will be defined as (3.89, 3.90, 3.91, 3.92, and 3.93):

$$X_{\text{carbamate}} = \frac{\varepsilon_1 - \varepsilon}{F_N} \quad (\text{Eq. 3.89})$$

$$X_{\text{urea}} = \frac{\varepsilon}{F_N} \quad (\text{Eq. 3.90})$$

$$X_{\text{NH}_3} = \frac{a - \varepsilon_1}{F_N} \quad (\text{Eq. 3.91})$$

$$X_{\text{CO}_2} = \frac{1 - \varepsilon_1}{F_N} \quad (\text{Eq. 3.92})$$

$$X_{\text{H}_2\text{O}} = \frac{b + \varepsilon}{F_N} \quad (\text{Eq. 3.93})$$

The reactions taking place in urea reactor are derived through Eq. 3.94, Eq. 3.95, and Eq. 3.96.

$$r_{\text{CO}_2} = -k_{1F} [C_{\text{NH}_3}]^2 [C_{\text{O}_2}] + k_{1R} [C_{\text{carbamate}}] \quad (\text{Eq. 3.94})$$

$$= -k_{1F} \left([C_{\text{NH}_3}]^2 [C_{\text{O}_2}] - \frac{[C_{\text{carbamate}}]}{k_1} \right)$$

$$r_{\text{carbamate}} = k_{1F} [C_{\text{NH}_3}]^2 [C_{\text{O}_2}] - k_{1R} [C_{\text{carbamate}}] - k_{2F} [C_{\text{carbamate}}] + k_{2R} [C_{\text{urea}}] [C_{\text{H}_2\text{O}}] \quad (\text{Eq. 3.95})$$

$$= k_{1F} \left([C_{\text{NH}_3}]^2 [C_{\text{O}_2}] - \frac{[C_{\text{carbamate}}]}{k_1} \right) - \left([C_{\text{carbamate}}] - \frac{[C_{\text{urea}}] [C_{\text{H}_2\text{O}}]}{k_2} \right)$$

$$r_{\text{urea}} = k_{2F} [C_{\text{carbamate}}] - k_{2R} [C_{\text{urea}}] [C_{\text{H}_2\text{O}}] \quad (\text{Eq. 3.96})$$

$$= k_{2F} \left([C_{\text{carbamate}}] - \frac{[C_{\text{urea}}] [C_{\text{H}_2\text{O}}]}{k_2} \right)$$

The volume of the reactor is derived using the following equation (Eq. 3.97):

$$\frac{dF_{\text{urea}}}{dV} = r_{\text{urea}} = k_{2F} \left([C_{\text{carbamate}}] - \frac{[C_{\text{urea}}] [C_{\text{H}_2\text{O}}]}{k_2} \right) \quad (\text{Eq. 3.97})$$

Conclusion

In this work, the technology sets were assessed based on SDP to emphasize GHG mitigation (CO₂ utilization) and waste utilization. In addition to the integration of CO₂ conversion into product, the SDP approach led to the use of emerging and novel membranes which are a critical component of the waste-to-ammonia and urea processes. These membranes provide more efficient resource and space utilization while enabling the viable utilization of food, human and CO₂ waste streams. In accordance to the set assumptions, multiple configurations of the core, waste-based processes were modelled in VBA software, linked to several carbon capture/utilization options in order to create multiple green ammonia and green ammonia + urea production processes.

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Chapter 4

Results and Discussion for The Modelling and Simulation

This chapter includes a discussion of the results obtained from the process modelled in VBA software. The results include, mass and energy balance, model validation, sensitivity analysis, and a comparison of the two technologies and seven scenarios with SMR and water electrolysis coupled with Haber-Bosch process powered by renewable technologies. Finally, assessing the significance of a waste-based process such as the green ammonia technology developed here, instead of degradation of FW openly in landfills.

This chapter was drafted based on the publication submitted to the frontiers in energy research journal:

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4. Results and discussion

4.1 Input and output data associated with DF coupled with AD and AD-only (Technology-1 and Technology-2)

Initially, FW is diluted with water before being mixed with BW. A portion (approximately 90%) of this water is the byproduct of the urea production plant and the remaining 10% comes from the reclaimed water (moisture content of the sludge) resulting from AD separated in the filter press.

The calculations for each processing unit (bioreactors, membranes, electrolyzer, fuel cell, and the urea production plant) in the proposed ammonia production process is based on 20 TPD of input waste with a dilution rate of 2.5 and FW to BW ratio of 1.

4.1.1 Mass Balance

4.1.1.1 Bioreactors

Technology-1: Modelling results of ammonia production through a two-stage DF coupled with AD

Input and output waste compositions to and from DF and AD along with the gas/biogas specifications, yields, and the output composition of H₂ and CO₂, CH₄, H₂S, etc. are shown in Table 4.1. The composition of the gas stream from DF is based on a H₂ content of 58.7%. If the ratio of H₂/CO₂ is $\geq 58.7\%$, the proposed production process produces both steam and power for SOFC, excess NH₃, and urea. When the ratio of H₂/CO₂ $\leq 58.7\%$, the only output product is urea.

The biogas composition from AD is based on a CH₄ content of 81.5%, which is a controllable aspect of the proposed process. If the ratio of CH₄/CO₂ is $\geq 81.5\%$ the proposed production process produces both steam and power for SOFC, excess NH₃, and urea. With the ratio of CH₄/CO₂ $\leq 81.5\%$ the only output product is urea.

Technology-2: Modelling results of ammonia production through AD-only

Input and output waste compositions to and from AD along with the biogas specifications, yields, and the output composition of biogas are shown in Table 4.1.

The biogas composition from AD is based on a CH₄ content of 81.5%. If the ratio of CH₄/CO₂ $\geq 75\%$, the proposed production process produces both steam and power for SOFC, excess NH₃, and urea. When the ratio of CH₄/CO₂ $\leq 75\%$ the only output product is urea.

Table 4.1: Input data to DF+AD (Technology-1) and AD-only (Technology-2) process along with their specifications.

Tech-1			Tech-2		
Inputs	Values	Units	Inputs	Values	Units
Input FW specifications			Input FW specifications		
FW input flow rate	10,000	kg/day	FW input flow rate	10,000	kg/day
Dilution water ratio	2.50	-	Dilution water ratio	2.50	-
Water flow rate	25,000	kg/day	Water flow rate	25,000	kg/day
FW to BW ratio	1	-	FW to BW ratio	1	-
BW flow rate (after dilution)	10,000	kg/day	BW flow rate (after dilution)	10,000	kg/day
Volumetric flow rate of FW	77.262	m ³ /day	Volumetric flow rate of FW	77.262	m ³ /day
TS content of FW	38,010	%	TS content of FW	38,010	%
VS content of FW	35,719	%	VS content of FW	35,719	%
TCOD of FW	10,523	%	TCOD of FW	10,523	%
SCOD of FW	4,740	%	SCOD of FW	4,740	%
TKN of FW	0.538	%	TKN of FW	0.538	%
Carbohydrate content of FW	8.136	%	Carbohydrate content of FW	8.136	%
Potential of Hydrogen (pH)	6	-	pH	6	-
Input BW specifications			Input BW specifications		
Volumetric flow rate of BW	10	m ³ /day	Volumetric flow rate of BW	10	m ³ /day
TS content of BW	4.5	%	TS content of BW	4.5	%
VS content of BW	2,950	%	VS content of BW	2,950	%
TCOD of BW	5.7	%	TCOD of BW	5.7	%
SCOD of BW	3,560	%	SCOD of BW	3,560	%
TKN of FW	0.320	%	TKN of FW	0.320	%
Carbohydrate content of FW	0.085	%	Carbohydrate content of FW	0.085	%
pH	6.6	-	pH	6.6	-
Input waste specifications			Input waste specifications		
Total mass flow rate	45,000	kg/day	Total mass flow rate	45,000	kg/day
Total volumetric flow rate	57.08	m ³ /day	Total volumetric flow rate	57.08	m ³ /day
TS content of input waste	11,229	%	TS content of input waste	11,229	%
VS content of input waste	9,429	%	VS content of input waste	9,429	%
VS/TS	0.840	-	VS/TS	0.840	-
TCOD of input waste	12,700	%	TCOD of input waste	12.7	%
SCOD of input waste	5,250	%	SCOD of input waste	5,250	%
Density of FW	453	kg/m ³	Density of FW	453	kg/m ³

Density of BW	1000	kg/m ³	Density of BW	1000	kg/m ³
Density of waste mixture (FW and BW)	788.436	kg/m ³	Density of waste mixture (FW and BW)	788.436	kg/m ³
Dark fermentation bioreactor specifications			Anaerobic digestion bioreactor specifications		
First order rate constant K_H (<1)	0.385	day ⁻¹	First order rate constant K_M (<1)	0.144	day ⁻¹
Hydraulic Retention Time (HRT)	2	day	Hydraulic Retention Time (HRT)	16	day
OLR	36.310	gVS/L.day	OLR	0.497	gVS/L.day
Waste inlet temperature	55	°C	Waste inlet temperature	35	°C
Waste inlet pressure	1	atm	Waste inlet pressure	1	atm
Ratio of microorganism (In/Out)	0.68	-	First order rate constant K_M (<1)	0.144	day ⁻¹
BOD	7.620		Hydraulic Retention Time (HRT)	16	day
Anaerobic digestion bioreactor specifications			Conversion factor of anaerobic digestion only		
First order rate constant K_M (<1)	0.101	day ⁻¹	Conversion factor (with recycling)	0.988	-
Hydraulic Retention Time (HRT)	16	day	Conversion factor (without recycling)	0.720	-
OLR	0.497	gVS/L.day	Inoculum tank specifications		
Waste inlet temperature	35	°C	Density of effluent	788.435	kg/m ³
Waste inlet pressure	1	atm	Time	7	day
Conversion factor of the two-stage dark fermentation coupled with anaerobic digestion			Impeller speed	108.51	RPM
Conversion factor (with recycling)	0.990	-	Impeller power	916.33	HP
Conversion factor (without recycling)	0.770	-	Agitation Velocity	6	m/s
Inoculum tank specifications			Impeller Diameter	1.06	m
Density of effluent	788.435	kg/m ³	Diameter of Tank	3.170	m
Time	7	day	Height of Tank	6.339	m
Impeller speed	108.51	RPM	Number of tanks	10	N ^o
Impeller power	8145.13	HP	Recycle rate/tank	0.2	m ³ /s
Agitation Velocity	6	m/s			
Impeller Diameter	1.06	m			
Diameter of Tank	3.170	m			
Height of Tank	6.339	m			
Number of tanks	10	N ^o			
Recycle rate/tank	0.2	m ³ /s			

Input and output waste compositions to and from DF and AD along with the biogas specifications, yields, and the output composition of H₂ and CO₂, CH₄, H₂S, etc., produced compost, effluent specifications from AD including the sludge composition, removed components (the removed VS from waste), DF and AD specifications (SRT, OLR, theoretical biogas yield, digester height, diameter, input gas flow rates for both MFI (from DF) and EMS (from AD) are presented in Table 4.2.

Table 4.2: Input and output waste composition, biogas specifications, produced compost, yields, and output composition of biogas fed to membranes (MFI and EMS) from both DF and AD for both technologies.

Tech-1														
Waste input to DF			Effluent specifications from DF			DF specifications								
Waste specifications	(g/l) / (kg/m ³)	%	Waste specifications	(g/l) / (kg/m ³)	%	Bioreactor volume		118.14	m ³					
TS	112.29	11.229	TS	53.78	5.379	Solids Retention Time (SRT)		2.60	day					
VS	94.30	9.429	VS	47.146	4.715	OLR		36.31	kgVS/m ³ .day					
TCOD	127	12.7	TCOD	45.72	4.572	Theoretical biogas yield		0.70	m ³ /kgVS					
SCOD	52.5	5.250	SCOD	18.89	1.888	Bioreactor diameter		4.22	m					
TVFA	5.8	0.580	TVFA	8.90	0.889	Bioreactor height		8.444	m					
Biogas specifications			Biogas yield from DF			Biogas output composition from DF to MFI								
Biogas production rate		7.04	m ³ /m ³ .day	H ₂	0.114	m ³ /kgVS		H ₂	58.7	%				
Biogas volumetric flow rate		8,724.90	m ³ /day	CO ₂	0.080	m ³ /kgVS		CO ₂	41.3	%				
Biogas yield		0.194	m ³ /kgVS	Total	0.194	m³/kgVS		Total	100	%				
Stage 2														
Effluent specifications from AD		(g/l) / (kg/m ³)	%	Removed components (%)		AD specifications								
TS		30.02	3.002	VS	89	Digester volume		410.94	m ³		CH ₄	14,794.50	kg/day	
VS		9.43	0.943	Digested tank		SRT		9.94	day		CO ₂	9,220.23	kg/day	
TCOD		8.68	0.869	TS (recycled %)	1.78	OLR		1.19	gVS/l.day		H ₂ S	3.87	kg/day	
TVFA		4.44	0.445	TS (for compost %)	1.22	Theoretical biogas yield		0.80	m ³ /kgVS		NH ₃	3.86	kg/day	
TS recycled		17.79	1.779	Recycled (m ³ /day)	114.15	Digester diameter		6.7	m		Total	24,022.46	kg/day	
Digester height						Digester height		13.4	m					
Biogas yield from AD			Biogas output composition yields from AD			Biogas output composition from AD to EMS			Biogas output flowrate from AD to EMS					
Gas production rate		0.762	m ³ /m ³ .d	CH ₄	0.524	m ³ /kgVS		CH ₄	81.5	%		CH ₄	23,577.577	m ³ /day
Biogas volumetric flow rate		2.89E+04	m ³ /day	CO ₂	0.119	m ³ /kgVS		CO ₂	18.470	%		CO ₂	5,349.072	m ³ /day
Biogas yield		0.643	m ³ /kgVS	H ₂ S	6.429E-05	m ³ /kgVS		H ₂ S	0.010	%		H ₂ S	2.893	m ³ /day
Produced compost			NH ₃	1.286E-04	m ³ /kgVS		NH ₃	0.020	%		NH ₃	5.786	m ³ /day	
127.138		kg/day												
Digested tank (kg/day)														
Recycled	4,429.910	Discharged	10,336.457	Total	0.643	m³/kgVS		Total	100	%		Total	28,935.328	m³/day
Tech-2														
Waste input to AD			AD effluent specifications			AD specifications								
Waste specifications	(g/l) / (kg/m ³)	%	Waste specifications	(g/l) / (kg/m ³)	%	Bioreactor volume		1050.18	m ³					
TS	112.289	11.230	TS	30.020	3.002	SRT		6.95	day					
VS	94.291	9.429	VS	9.429	0.943	OLR		1.51	kgVS/m ³ .day					
TCOD	127	12.7	TCOD	8.687	0.869	Theoretical biogas yield		0.804	m ³ /kgVS					
SCOD	52.5	5.250	SCOD	4.445	0.445	Bioreactor diameter		8.75	m					
TVFA	5.8	0.580	TVFA	17.7898	1.779	Bioreactor height		17.49	m					
Biogas specifications			Removed components (%)		Biogas output composition from anaerobic digestion to EMS									
Biogas production rate		1.090	m ³ /m ³ .day	VS	84.8	CH ₄		16,643.806	kg/day		81.5	%		
Biogas volumetric flow rate		32,545.735	m ³ /day			CO ₂		10,372.767	kg/day		18.470	%		
Biogas yield		0.723	m ³ /kgVS	TS (recycled %)	1.779	H ₂ S		4.352	kg/day		0.010	%		
Produced compost				TS (for compost %)	1.223	NH ₃		4.3473	kg/day		0.020	%		
154.762		kg/day		Recycled (m ³ /day)	114.15	Total		27,025.273	kg/day		100	%		

The maximum volume of each digester is 25 m³. From this amount the number of fermenters is 21 and digester 16 for the waste flow rate of 45,000 kg/day. The specifications of the impeller and shape factor of the agitator for both fermenter and digester are shown in Table 4.3. These specifications include, height from bottom of vessel, impeller blade length and width, speed, power, efficiency, number of impellers and impeller blades, width and height of baffles, corrosion allowance, etc. The calculations are based on the impeller efficiency of 85% for both fermenter and digester. Agitation velocity is assumed to be 2 m/s for the fermenter and 5m/s for the digester. Number of baffles is set to be 4 for the fermenter and 6 for the digester. Number of impellers are 2 for the fermenter and 3 for the digester, the number of impeller blades is 6 for both bioreactors.

Table 4.3: The specifications of impellers and baffles along with shape factor of the agitator for the fermenter and anaerobic digester for both technologies.

Tech-1		Tech-2		Units
Number of Digester in parallel	3	12	26	N ^o
Impeller design				
Specifications	Values-DF	Values-AD	Values-AD-only	Units
Input Feed	43,378.511	249,783.521	249,783.521	mol/day
Conversion rate	0.5	0.8	0.8	
Impeller Diameter	1.407	2.234	2.915	m
Impeller height from bottom of Vessel	1.407	2.234	2.915	m
Impeller Blade Length	0.352	0.558	0.729	m
Impeller Blade Width	0.281	0.447	0.583	m
Number of Impeller	2	3	3	N ^o
Number of Impeller Blades	6	6	6	N ^o
Agitation Velocity	2	5	5	m/s
Impeller Speed	27.156	42.768	32.774	RPM
Impeller Power	3.5	826.931	1,056.141	HP
Impeller Efficiency	85	85	85	%
Power according to Efficiency	2.98	702.89	897.72	HP
Number of Baffles	4	6	6	N ^o
Width of Baffle	0.422	0.670	0.875	m
Height of Baffle	8.059	13.404	17.491	m
Corrosion Allowance	0.002	0.002	0.002	m
Static Pressure	0.370	0	0.766	atm.
Operational Pressure	0.0144	0.014	0.014	atm.
Maximum allowance pressure	0.384	0.014	0.781	atm.
Shape factor of agitator				
Specifications	Values	Values	Values	Units
Shape Factor 1	0.333	0.333	0.333	m
Shape Factor 2	0.333	0.333	0.333	m
Shape Factor 3	0.250	0.250	0.250	m
Shape Factor 4	0.2	0.2	0.2	m
Shape Factor 5	0.1	0.1	0.1	m
Shape Factor 6	2	2	2	m

Anaerobic digester storage tank

The specifications of the storage tank following after AD for both technologies is shown in Table 4.4.

Table 4.4: The specifications of the storage tank following AD for both technologies.

Storage Tank			
	Tech-1	Tech-2	Units
Number of Tanks	1	1	N°
Diameter of Tank	1.909	2.038	m
Height of Tank	3.818	4.077	m
Recycle Rate /Tank	0.033	0.033	m ³ /s

4.1.1.2 Input and output data associated with EMS

The input and output data from the modelling in VBA for EMS along with its characteristics are presented in Table 4.5. i versus η_a was plotted in order to find i_o at the intersection of (i) axis, as shown in Fig. 4.1. i_o was found to be $\sim 4.5 \text{ mA/cm}^2$.

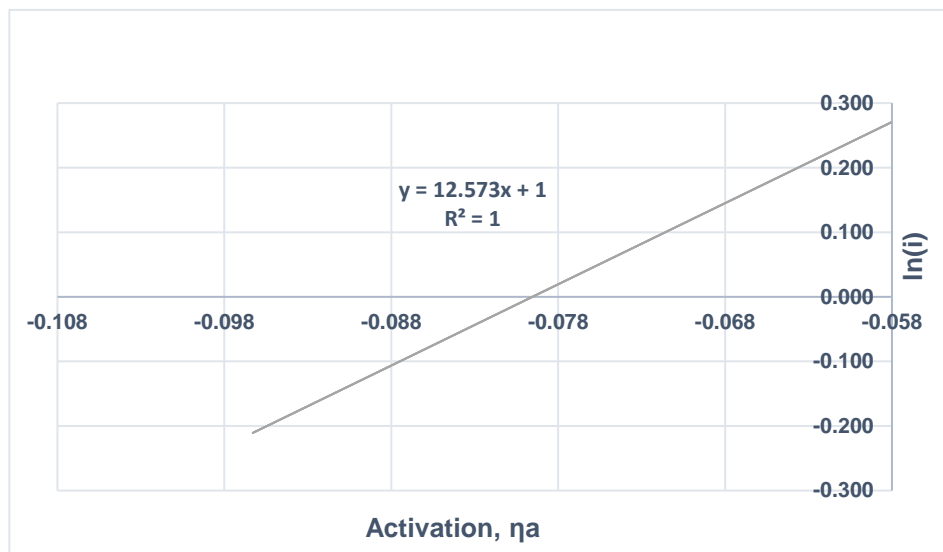


Fig. 4.1: A sample plot of η_a versus $\ln(i)$ to find i_o at the intersection of (i) axis.

Table 4.5: The specifications of the inlet biogas to EMS from AD, membrane specifications, and Tafel approximation results.

Membrane Inputs	Values Tech-1	Values Tech-2	Units
CH ₄ input flow rate	14794.494	16,643.806	kg/day
CO ₂ input flow rate	9220.237	10,372.767	kg/day
H ₂ S input flow rate	3.87E	4.35E	kg/day
NH ₃ input flow rate	3.86E	4.35E	kg/day
Biogas inlet temperature	35	35	°C
Biogas inlet pressure	1	1	atm.
Nitrogen flow rate used as sweep gas	28935.327	27,025.273	kg/day
Nitrogen inlet temperature	850	850	°C
Membrane Specifications			
Membrane operational temperature	650	650	°C
Membrane operational pressure	1	1.00	atm.
Membrane tortuosity (τ)	3.6	3.6	τ
Membrane thickness (δ)	0.90	0.90	mm
Membrane surface area	400	400	cm ²
Membrane porosity (ϵ)	36	36	%
Mass transfer coefficient (K_m)	11	11	cm/s
Electrolyte diffusivity	1.00E-05	1.00E-05	cm ² /s
Electrolyte average density	5.450	5.450	mole/cm ³
Applied voltage	0.75	0.75	volt
Tafel Approximations Results			
Activation η_a /Cells	3.960E-01	3.960E-01	volt
Activation current density/Cells	2.719	2.719	mA/cm ²
Applied current density/Cells	0.0187	1.871E-02	mA/ cm ²
Conductivity	20	20	S/cm
Resistance	1.930E-07	3.960E-01	Ω

The output specifications of EMS membrane include, S₂, CH₄, CO₂, H₂, and NH₃ output flow rate, maximum H₂S removal flux, current, total voltage per cell, total cell voltage, cell power, required area, and number of cells is shown in Table 4.6. The results were also tested for high H₂S concentrations, operating at a lower temperature of 600°C with the same optimized membrane specifications as shown in Table 4.5. The results indicate that at higher current efficiencies the same removal efficiency of approximately 99.99% was achieved.

Table 4.6: The effluent specifications of EMS.

Membrane Outputs	Values Tech-1	Values Tech-2	Units
S ₂ output flow rate	3.641	4.096	kg/day
(N ₂ +S ₂) output flow rate	24,026.106	27,029.369	kg/day
CH ₄ output flow rate	14,794.494	16,643.806	kg/day
CO ₂ output flow rate	9,220.237	10,372.767	kg/day
H ₂ output flow rate	0.227	0.256	kg/day
NH ₃ output flow rate	3.864	4.347	kg/day
Maximum H ₂ S removal flux	9.70E-08	9.70181E-08	gm/cm ² .s
Current	10,904.253	12,267.285	A
Total voltage/Cell	2.526	2.731	V
Total cells voltage	147.244	179.054	V
Cell area	23,310.156	26,223.926	cm ²
Cell Power	1,605.593	2,196.510	kW
Number of cells	58	66	N ^o

4.1.1.3 Input and output data associated with MFI

The input and output data from the modelling in VBA for MFI along with its characteristics are presented in Table 4.7 and 4.8 respectively. Membrane specifications include: Operational temperature and pressure, outlet pressure, number of tubes, tube length and area, porosity, pore radius, membrane diameter and thickness. The output specifications of MFI membrane also include, permeate and retentate CO₂, permeate and retentate H₂, CO₂ and H₂ permeance, CO₂ and H₂ permeability, CO₂ and H₂ flux, separation factor, selectivity, required area, and number of membrane modules. Table 4.7 and 4.8 are not applicable for technology-2.

The separation efficiency of hydrogen from the biogas stream at the temperature of -39°C and inlet pressure of 20 atm is 99.965%. In this operational condition the selectivity of the membrane is said to be 237.485 and the separation factor is 118.69, this is shown in Table 4.8 along with the effluent specifications of MFI membrane. However, by increasing the pressure to 29 atm, the CO_2 separation will increase to 99.99%. The results show that at different temperature ranges the permeance of CO_2 was high and superior to that of hydrogen. This is due to the fact that the adsorption of CO_2 is higher than H_2 in the membrane, thus, blocking the transport of H_2 and making MFI membrane CO_2 -selective.

Table 4.7: The specifications of the inlet biogas from DF and the MFI membrane.

Membrane Inputs	Values	Units
	Tech-1	
H_2 input flow rate	529.465	kg/day
CO_2 input flow rate	8,195.434	kg/day
Inlet biogas temperature	55	$^{\circ}\text{C}$
Inlet biogas pressure	1	atm.
Membrane Specifications		
Membrane operational temperature (maximum -39)	-39.00	$^{\circ}\text{C}$
Inlet operational pressure ($3 < P \leq 30$)	20	atm.
Outlet pressure (fixed at 1 atm)	1	atm.
Tube area	1.57	cm^2
Membrane diameter	5	mm
Membrane Thickness (δ)	25	μm
Porosity (ϵ)	50	%
Pore radius	0.2	μm
Number of Tubes / Module	20	N°
Tube Length	0.010	m

Table 4.8: The effluent specifications of MFI membrane.

Membrane Outputs	Values	Units
	Tech-1	
Permeate CO_2	8,192.579	kg/day
Retentate CO_2	2.855	kg/day
Retentate H_2	529.281	kg/day
Permeate H_2	0.184	kg/day
CO_2 flux	3.649E-05	mol/s.cm^2
H_2 flux	3.682E-12	mol/s.m^2
Permeance (CO_2)	1.104E-09	$\text{mol/s.cm}^2.\text{atm}$
Permeance (H_2)	4.650E-12	$\text{mol/s.cm}^2.\text{atm}$
CO_2 Permeability	2.761E-11	mol/s.cm.atm
H_2 Permeability	1.163E-13	mol/s.cm.atm

Separation Factor	118.69	-
H ₂ % in Retentate	99.965	%
Number of tubes	1,739	N ^o
Required area	2,732	cm ²
N ^o of modules	87	N ^o
Selectivity	237.485	-

The optimum condition for the separation of H₂ and CO₂ from DF (applies to Technology-1)

The correlation between operational pressure variation to selectivity and separation factor in an MFI membrane is shown in Fig. 4.2. Increasing the operational pressure will result in an increase in selectivity and a decrease in the separation factor. The low separation factor is probably a result of a low CO₂/H₂ adsorption selectivity.

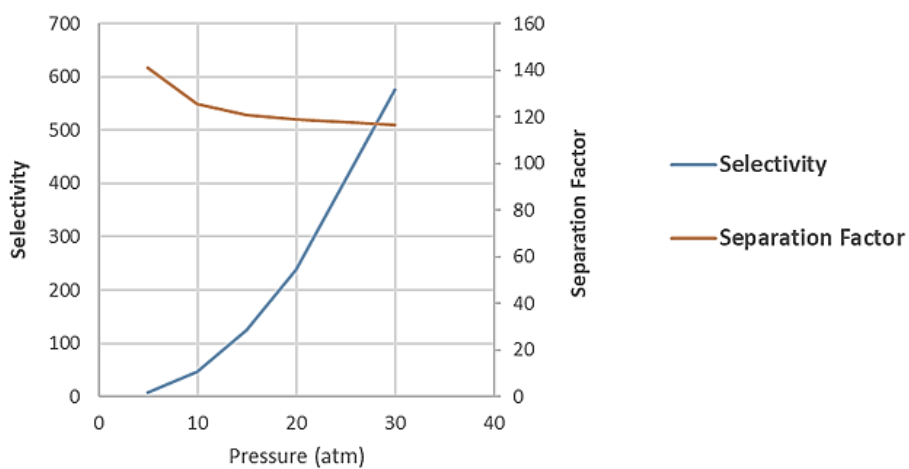


Fig. 4.2: The correlation between operational pressure variation to selectivity and separation factor for MFI membrane.

4.1.1.4 Input and output data associated with ITM

The input and output data from the modelling in VBA for ITM along with its characteristics are presented in Table 4.9 and 4.10 respectively. Table 4.9 and 4.10 are comprised of different specifications of ITM including, diffusivity of oxygen vacancy, forward and reverse reaction rate, oxygen permeation flux, nitrogen and oxygen output flow rates, required cell area, number of tubes and modules, membrane thickness, permeance, permeability, conductivity, voltage per tube, current, and resistance, oxygen and nitrogen pressure at the permeate and retentate side. The oxygen permeate pressure control, cell temperature and pressure operate in a specific range and were obtained from literature data such as Han et al. (2018) and Sun, Larpudomlert and Thepwater (2011) and the values were selected specifically based on the design constraints. The air flow rate (oxygen and nitrogen flow rates) changes based on the amount of ammonia produced, while the inner and outer radius, and tube length of the membrane are also subject to change accordingly. Changing each of the mentioned input parameters will result in different output values. The separation efficiency of oxygen from air stream in ITM is dependent on the pressure difference at feed side and the permeate side. For achieving a separation efficiency of 99.999% at the temperature of 800°C, the inlet pressure is set to 10 atm

and the permeate pressure is calculated as: $P_{O_{2out}} = \frac{P_{feed}X_{feed}}{\pi}$, $5 < \pi < 7$. π is the empirical coefficient which is assumed to be 7. Using this equation and empirical coefficient of 7 the pressure at permeate side is said to be 0.3 atm. The output from ITM can be separated into two streams. The resulting oxygen is routed to SOFC, while the nitrogen is divided into two streams: One stream enters the EMS as the sweep gas and the other stream enters the SSAS to produce ammonia.

Table 4.9: The specifications of ITM and the inlet air stream.

Membrane Inputs	Values Tech-1	Values Tech-2	Values
Air input flow rate	77,231.010	83,061.427	kg/day
O ₂ flow rate	16,218.51	17,442.90	kg/day
N ₂ flow rate	61,012.50	65,618.53	kg/day
Inlet temperature	800.00	800	°C
Inlet pressure	1	1	atm.
Membrane Specifications			
Membrane operational temperature (800 ≤ T ≤ 950)	850	850	°C
Cell pressure (10 ≤ P ≤ 30)	10	10	atm.
Outer radius	10	10	mm
Inner radius	0.115	0.115	mm
Tube length	20	20	cm
Membrane area/unit tube	27.82	27.818	m ² /u.t
Number of tubes / numbers of module	20	20	N°
O₂ at the permeate side			
Constant numbers: (5 ≤ π ≤ 7)	7	7	cnt.
Available nitrogen flow rate			
Nitrogen for SSAS	36,989.94	38,593.16	kg/day
Nitrogen for EMS	24,022.46	27,025.27	kg/day

Table 4.10: The effluent specifications of ITM.

Membrane Outputs	Values Tech-1	Values Tech-2	Units
Diffusivity of oxygen vacancy	5.958E-06	5.959E-06	cm ² /s
Forward reaction rate	0.0000165	1.647E-05	cm ² /atm ^{0.5} .s
Reverse reaction rate	5.778E-07	5.778E-07	mol/atm ^{0.5} .s
O ₂ permeation flux	1.680E-07	1.679E-07	mol/ cm ² .s
N ₂ input flow rate	61,012.498	65,618.527	kg/day
Oxygen input flow rate	16,218.512	17,442.9	kg/day
N ₂ output flow rate	61,012.406	65,618.436	kg/day
O ₂ output flow rate	16,218.488	17,442.875	kg/day
Required cell area	3.493	3.757	m ²
Number of tubes	2.781	2.991	N°
Number of modules	139	150	N°
Membrane thickness (δ)	2.214	2.214	mm
Oxygen pressure (at the permeate side)	0.3	0.3	atm
N ₂ pressure (at retentate)	10	10	atm
Permeance	1.731E-08	1.731E-08	mol/cm ² .s.atm
Permeability	3.832E-09	3.832E-09	mol/cm.s.atm
Voltage/Tubes	0.044	133.073	V
Conductivity	1.691E-01	1.691E-01	S/cm
Total resistance	5.206E	5.599E	Ohm
Total power	79.7058	99.154	kW

4.1.1.5 Input and output data associated with CH₄ assisted-SOFEC

The input and output data from the modelling in VBA for CH₄ assisted-SOFEC along with its characteristics are presented in Table 4.11 and 4.12 respectively. The inlet gas stream is comprised of CH₄, CO₂, H₂, and NH₃. While the output stream is comprised of, separated CO₂, H₂, and water. Table 4.11 and 4.12 are comprised of different specifications of CH₄ assisted-SOFEC including, inner and outer diameter, cell thickness, channel length, active surface area per cell, Nernst, applied and open circuit voltage, current density, O₂ ion flux, ionic conductivity, resistance, number of cells, power at input, operational pressure and temperature. The ionic conductivity, cell temperature and pressure operate in a specific range and were obtained from literature data such as Luo et al. (2014) and Xu et al. (2016) and the values were selected specifically based on the design constraints. The CH₄ assisted-

SOFEC input flow rates (methane and carbon dioxide flow rates) change based on the amount of biogas produced from AD, while the inner and outer radius, tube length, and cell thickness, and operational temperature of the membrane are subject to change accordingly. Changing each of the mentioned input parameters will result in different output values. The output from CH₄ assisted-SOFEC can be separated into two streams. The resulting hydrogen is routed to SSAS, while the produced CO₂ is compressed, cooled, and liquefied, then either discharged directly, captured and injected into the ground, or sold commercially.

Table 4.11: Input data to CH₄ assisted-SOFEC.

Electrolyzer Inputs	Values Tech-1	Values Tech-2	Units
CH ₄ input flow rate	14,794.494	16,643.806	kg/day
CO ₂ input flow rate	9,220.237	10,372.767	kg/day
H ₂ input flow rate	2.276E-01	2.560E-01	kg/day
NH ₃ input flow rate	3.86	4.347	kg/day
Inlet pressure	1	1	atm.
Gas input flow rate (Port-1)	24,018.823	27,021.176	kg/day
Steam Temperature	974.821	974.821	°C
Electrolyzer Specifications			
Electrolyzer operational temperature	850	850	°C
Electrolyzer operational pressure	1	1	atm.
Ionic conductivity	0.0148	0.0148	S/cm
Cell thickness (δ)	796	796	µm
Outer diameter	50	50	mm
Inner diameter	49.5	49.5	mm
Channel length	800	800	mm
Active surface area/cell	251.2	251.2	cm ² /cell
Applied voltage	0.150	0.150	V
Total current density	495.700	495.700	Amp/m ²
Power at Input (1)	-825.957	-929.202	kW

Table 4.12: Output data from CH₄ assisted-SOFEC.

Electrolyzer Outputs	Values Tech-1	Values Tech-2	Units
H ₂ output flow rate (Port-4)	7,397.475	8,322.159	kg/day
CO ₂ output flow rate (Port-2)	49,905.097	56,143.234	kg/day
H ₂ O input flow rate (Port-2)	0.6199	0.6199	kg/day
H ₂ O input flow rate (Port-3)	33,287.6123	37,448.5638	kg/day
H ₂ O (Steam total Aout)	33,286.992	37,447.9439	kg/day
Ionic conductivity of Ni	20,736.68	20,736.68	S/cm
Ionic conductivity of LSM	150,838.84	150,838.84	S/cm
Ionic conductivity of SeSz	0.060	0.060	S/cm
Ionic conductivity of ICYSZ	0.035	0.035	S/cm
O ₂ ion flux	1.41E-06	1.41E-06	mol O ₂ -/cm ² .s
Open circuit voltage	0.8320	0.832	V
Nernst voltage	0.416	0.416	V
Maximum current density	1550.435	1550.435	Amp/m ²
Required surface area	251.2	251.2	cm ² /cell
Number of cells	60,408	67,960	No
Resistance	0.0213	0.0213	Ω
Total Power	513.027	577.156	kW
Heat Loss			
Heat in	3,433.093	3,862.229	kW
Heat out	1,155.914	1,300.404	kW
Heat loss	2,277.178	2,561.826	kW

4.1.1.6 Input and output data associated with SSAS

The input and output data resulting from the modelling in VBA for SSAS along with its characteristics are presented in Table 4.13 and 4.14 respectively. The SSAS specifications include, the membrane's operational temperature and pressure, conductivity, thickness, surface area, current density, and applied voltage. The electrode conductivity and inlet temperature were obtained from literature data such as Garagounis et al. (2014) and the values were selected specifically based on the design constraints. The surface area and thickness of the membrane are also subject to

change (Xu et al., 2009). This membrane operates at a temperature of 80 °C and at atmospheric pressure. By changing the mentioned values in the input parameters, the following output results were obtained. For producing approximately 4,500 kg/day of ammonia per day through technology-1, 36,971.854 kg/day of nitrogen and 7,922.540 kg/day of hydrogen are required. For the production of about 4,700 kg/day of ammonia through technology-2, 35,727.512 kg/day of nitrogen and 7,655.895 kg/day of hydrogen are needed.

Table 4.13: Input data to SSAS.

Membrane Inputs	Values Tech-1	Values Tech-2	Units
N ₂ input flow rate	36,989.94	38,593.162	kg/day
N ₂ inlet temperature	850	850	°C
N ₂ inlet pressure	10	10	atm
H ₂ input flow rate	7,926.815	7,655.895	kg/day
H ₂ inlet temperature	790.64	850	°C
H ₂ inlet pressure	1	1	atm
Membrane Specifications			
Membrane inlet temperature	80	80	°C
Membrane inlet pressure	1	1	atm
Electrode Conductivity (σ)	0.036	0.036	1/cm.ohm
Membrane surface area	1.951	1.951	cm ²
Membrane thickness (δ)	0.010	0.010	cm

Table 4.14: Output data to SSAS.

Membrane Outputs	Values Tech-1	Values Tech-2	Units
Produced NH ₃	44,893.66	46,863.125	kg/day
Available H ₂ for SOFC	0.4	61.406	kg/day
N ₂ output flow rate	0.001	0.001	kg/day
Maximum Reaction Rate/Electrode	1.13E-08	1.13E-08	mol/s.cm ²
Actual reaction rate	3.080E-06	3.080E-06	mol/s.cm ²
Required area	9.927E+06	1.036E+07	cm ²
Number of cells	509	531	N ^o
Current	0.00597	0.00597	A
Total voltage	152.183	158.777	V
Faradaic efficiency	99.9	99.9	%
Heat Loss			
Heat in	628.981	660.222	kW
Heat out	240.881	254.918	kW
Heat loss	388.100	405.305	kW

4.1.1.7 Input and output data associated with SOFC

The input and output data resulting from the modelling in VBA for SOFC along with its characteristics are presented in Table 4.15 and 4.16 respectively. Cell temperature, ionic conductivity, and applied voltage were obtained from literature data such as Ramadhani et al. (2017) and the values were selected specifically based on the design constraints. The cell area and thickness of the membrane are also subject to change. By changing the mentioned values in the input parameters, the following output results were obtained. 61.406 kg/day of hydrogen is required to produce 46.528kW power through technology-2, this hydrogen is the result of the separation of hydrogen sulfide in the EMS.

Table 4.15: Input data to SOFC.

Fuel cell Inputs	Values Tech-1	Values Tech-2	Units
H ₂ input flow rate	0.394	61.406	kg/day
O ₂ input flow rate	2.680	417.566	kg/day
Inlet pressure	1	1	atm
H ₂ inlet temperature	790.633	850	°C
O ₂ inlet temperature	850	850	°C
Fuel cell specifications			
Cell temperature	1000	1000	°C
Cell pressure	1	1	atm
Ionic conductivity (σ)	0.05	0.05	1/cm. ohm
Electrolyte thickness (δ)	200	200	μ m
Cell area	1000	1000	cm ²
Number of fuel cells / Stack	100	100	N ^o
Applied voltage	0.75	0.75	V
Heat loss			
Heat in	232.294	263.779	kW
Heat out	118.686	127.646	kW
Heat loss	113.497	118.998	kW

Table 4.16: Output data from SOFC.

Fuel cell Outputs	Values Tech-1	Values Tech-2	Units
H ₂ output flow rate	5.913E-02	9.211E+00	kg/day
H ₂ O output flow rate	3.064	469.762	kg/day
O ₂ output flow rate	2.680	417.566	kg/day
Fuel Cell Specifications			
Total number of cells	3	157	N ^o
Number of stacks	1	2	N ^o
O ₂ flux	3.16E-07	9.64E-07	mol/s.cm ²
Total voltage	2.37	125.07	V
Total cell current density	2.37	372.012	Amp/cm ²
Resistance of system	59.847	63.837	Ω
Nernst voltage (E_{Nernst})	0.798	0.798	V
Open circuit voltage (E_{ocv})	0.919	0.919	V
Output power	0.289	46.528	kW

4.1.1.8 Input and output data associated with urea production through Snamprogetti process (Scenario ii)

The input data for urea production through Snamprogetti process resulting from the modelling in VBA for both technologies is presented in Table 4.17. The output results (urea production process) from technology-1 and technology-2 are shown in Table 4.18 and 4.19 respectively.

Table 4.17: Input data for urea production through Snamprogetti process for both technologies.

Urea process Inputs	Values Tech-1	Values Tech-2	Units
Inlet pressure	130	130	atm
Temperature	190	190	°C
Urea purity level	98.9	98.9	%
Required NH ₃ + recycled	45,636.37	44,101.14	kg/day
Required CO ₂ + recycled	59,058.83	57,072.06	kg/day
Produced biuret	440.090	425.284	kg/day
Produced output water	23,730.334	22,175.718	kg/day

Table 4.18: Mass balance results around each processing unit associated with urea production for technology-1.

MASS BALANCE													
REACTOR MASS BALANCE + recycling					STRIPPER MASS BALANCE				MEDIUM PRESSURE SEPARATOR				
REACTOR PERFORMANCE.(% UREA OUT)					100% SEPARATION OF CARBAMATE				PERFORM.(% NH ₃ &CO ₂ OUT)				
COMPO.		% with no recycling*	OUT Kg/day	%	IN Kg/day	%	OUT Kg/day	%with recycling*	IN Kg/day	% With recycling	OUT Kg/day	OUT with no *Recycling	% Without recycling
NH ₃	45,636.372	43.590	574.636	0.247	574.636	0.247	574.636	0.549	574.636	0.549	287.318	287.318	0.276
CO ₂	59,058.834	56.410	649.647	0.279	649.647	0.279	649.647	0.621	649.647	0.621	324.824	324.824	0.312
CAR. REC.	128,058.221		128,058.221	55.019	128,058.221	55.019	128,058.221						
UREA			79,136.165	34.000	79,136.165	34.000	79,136.165	75.587	79,136.165	75.587	79,136.165	79,136.165	76.032
H ₂ O			23,894.667	10.266	23,894.667	10.266	23,894.667	22.823	23,894.667	22.823	23,894.667	23,894.667	22.957
BIURET			440.090	0.189	440.090	0.189	440.090	0.420	440.090	0.420	440.090	440.090	0.423
TOTAL*	104,695.206	100.000					104,695.206					104,083.065	
TOTAL	232,753.428	100.000	232,753.428	100.000	232,753.428	100.000	232,753.428	100.000	104,695.206	100.000	104,695.206		100.000
CARBAMATE 100% RECYCLED					128058.221				No Rx. (% SEPARATION OF NH ₃ & CO ₂)				
LOW PRESSURE SEPARATOR					EVAPORATOR-1				EVAPORATOR-2				
ALL NH ₃ and CO ₂ RECYCLED					PERFORM.(%UREA OUT)				PERFORM.(%UREA OUT)				
Kg/day	IN Kg/day	%	OUT Kg/day	%with no recycling*	IN Kg/day	%	OUT Kg/day	% with no recycling*	IN Kg/day	%	OUT Kg/day	OUT Kg/day	% without recycling*
NH ₃	287.318	0.276	287.318	0.290	0.290		0.290		0.290				
CO ₂	324.824	0.312	324.824										
ERROR N=0	79,136.165	76.032	79,136.165	76.482	79,136.165	76.482	79,136.165	76.110	79,136.165	76.110	79,136.165	79,136.165	98.277
H ₂ O	23,894.667	22.957	23,894.667	23.093	23,894.667	23.093	11,473.846	12.602	11,473.846	11.035	946.975	946.975	1.176
BIURET	440.090	0.423	440.090	0.425	440.090	0.425	440.090	0.483	440.090	0.423	440.090	440.090	0.547
H ₂ O rec.*							11,473.846				11,473.846		
TOTAL	104,083.065	100.000	103,470.923	100.000	103,470.923	100.000	102,523.948	89.195	103,976.042	87.568	80,523.230	80,523.230	100.000
PRILLING TOWER					PERFORM.(%UREA OUT)								
Kg/day	IN Kg/day	%	VAPOR OUT H ₂ O	OUT LIQUID	% without recycling*								
UREA	79,136.165	98.277	79,136.165	79,136.165	98.478								
H ₂ O	946.975	1.176		782.642	0.974								
BIURET	440.090	0.547	440.090	440.090	0.548								
TOTAL*				80,358.897									
TOTAL	80,523.230	100.000	79,576.255	80,358.897	100.000								

Table 4.19: Mass balance results around each processing unit associated with urea production for technology-2.

MASS BALANCE																		
REACTOR MASS BALANCE + recycling					STRIPPER MASS BALANCE					MEDIUM PRESSURE SEPARATOR								
REACTOR PERFORMANCE.(% UREA OUT)					34.000	100% SEPARATION OF CARBAMATE					PERFORM.(% NH ₃ &CO ₂ OUT)					50.000		
COMPO.	Kg/day	% with no recycling*	OUT Kg/day	%	IN Kg/day	%	OUT Kg/day	%with recycling*	IN Kg/day	% With recycling	OUT Kg/day	OUT with no *Recycling	% Without recycling					
NH ₃ (l)	44,101.136	43.590	555.305	0.247	555.305	0.247	555.305	0.549	555.305	0.549	277.653	277.653	0.276					
CO ₂ (g)	57,072.058	56.410	627.793	0.279	627.793	0.279	627.793	0.621	627.793	0.621	313.896	313.896	0.312					
CAR. REC.	123,750.262		123,750.262	55.019	123,750.262	55.019	123,750.262											
UREA			76,473.975	34.000	76,473.975	34.000	76,473.975	75.587	76,473.975	75.587	76,473.975	76,473.975	76.032					
H ₂ O			23,090.836	10.266	23,090.836	10.266	23,090.836	22.823	23,090.836	22.823	23,090.836	23,090.836	22.957					
BIURET			425.285	0.189	425.285	0.189	425.285	0.420	425.285	0.420	425.285	425.285	0.423					
TOTAL*	101,173.194	100.000	224,923.456		101,173.194		224,923.456	100.000	101,173.194	100.000	101,173.194	100,581.645						
TOTAL	224,923.456	100.000	224,923.456	100.000	224,923.456	100.000	224,923.456	100.000	224,923.456	100.000	224,923.456	100,581.645	100.000					
CARBAMATE 100% RECYCLED					No Rx. (% SEPARATION OF NH ₃ & CO ₂)													
LOW PRESSURE SEPARATOR					EVAPORATOR-1					EVAPORATOR-2								
ALL NH ₃ and CO ₂ RECYCLED					PERFORM.(%UREA OUT)					76.110	A	PERFORM.(%UREA OUT)					97.800	B
Kg/day	IN Kg/day	%	OUT Kg/day	%with no recycling*	IN Kg/day	%	OUT Kg/day	% with no recycling*	IN Kg/day	%	OUT Kg/day	OUT Kg/day	% without recycling*					
NH ₃	277.653	0.276	277.653	0.280	0.280		0.280		0.280		0.280							
CO ₂	313.896	0.312	313.896															
ERROR N=0	76,473.975	76.032	76,473.975	76.482	76,473.975	76.482	76,473.975	76.110	76,473.975	76.110	76,473.975	76,473.975	98.277					
H ₂ O	23,090.836	22.957	23,090.836	23.093	23,090.836	23.093	11,087.859	12.602	11,087.859	11.035	11,087.859	915.118	1.176					
BIURET	425.285	0.423	425.285	0.425	425.285	0.425	425.285	0.483	425.285	0.423	425.285	425.285	0.547					
H ₂ O rec.*							11,087.859				11,087.859							
TOTAL	100,581.645	100.000	99,990.096	100.000	99,990.096	100.000	99,074.978	89.195	100,478.222	87.568	87,987.119	77,814.378	100.000					
PRILLING TOWER																		
PERFORM.(%UREA OUT)					98.000	C												
Kg/day	IN Kg/day	%	VAPOR OUT H ₂ O	OUT LIQUID	% without recycling*													
UREA	76,473.975	98.277	76,473.975	76,473.975	98.478													
H ₂ O	915.118	1.176		756.313	0.974													
BIURET	425.285	0.547	425.285	425.285	0.548													
TOTAL*				77,655.573														
TOTAL	77,814.378	100.000	76,899.260	77,655.573	100.000													

Effect of urea purity on biuret and output water from urea production process

Increasing the urea purity will result in an increase in the output water and a decrease in the amount of biuret formation, as shown in Fig. 4.3.

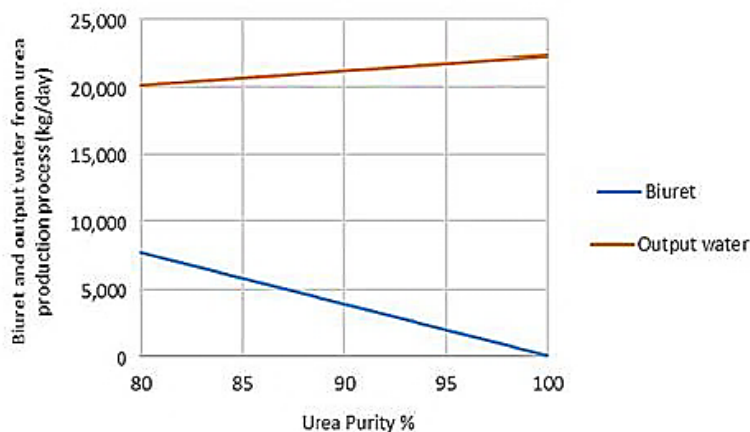


Fig. 4.3: The effect of urea purity on the amount of biuret and output water from the urea production process.

4.1.2 Energy balance results

4.1.2.1 a. Energy balance results of ammonia production through a two-stage DF coupled with AD

The energy draw is driven primarily by the urea production process, which accounts for approximately 93% of the total energy consumed (Fig. 4.4(a)). This is followed by the energy loss (6.04 MW), power required for supplying steam (5.2 MW), and driving the impellers. Other energy uses are much smaller; indeed, the next highest energy use is the air compressor (COMP-2) with 1.72 MW. This process is designed with renewable electricity supply (solar/wind).

The energy production and consumption for the two-stage process as shown in Sankey diagram (Fig. 4.4(a)) is calculated based on Eq. 4.2 and 4.3.

The required power for running the membranes is carried out using Eq. 4.1:

$$P = I A V \quad (\text{Eq. 4.1})$$

Where, P is the power (kW), I is the total current (A), ($\text{Area} \times \text{current density}$), and V the total voltage ($E_{\text{cell}} \times \text{number of cell}$).

$$\text{Energy Consumed} = \text{HEX-(1,5,6,7,8,9,10,13,14,15)} + \text{COMP-(1,2,3,4,5,7,8)} + \text{Required Steam} + \text{Impellers} + \text{Pumps} + \text{Filter Press} + \text{Refrigeration} + \text{Blower} + P_{\text{EMS} + \text{CH}_4 \text{ assisted-SOFEC} + \text{SSAS} + \text{UREA}} + \text{Heat loss} + \text{Energy loss} \quad (\text{Eq. 4.2})$$

$$\text{Energy Produced} = \text{HEX-(2,3,4,11,12)} + \text{COND-(1,2,3)} + P_{\text{ITM} + \text{SOFC}} + \text{Turbine} \quad (\text{Eq. 4.3})$$

4.1.2.2 b. Energy balance results of ammonia production through AD-only

As with the two-stage configuration, urea production is the largest energy user (Fig. 4.4(b)), accounting for 85% of the energy draw. This is followed by the power required for driving the impellers (7.11 MW), energy loss (6.85 MW), and power required for supplying steam (2.64 MW) as shown in Fig. 4.4(b). Other energy uses are smaller, the next highest energy use is the required power for the EMS with 2.19 MW. The source of this electricity is renewable energy sources (solar/wind).

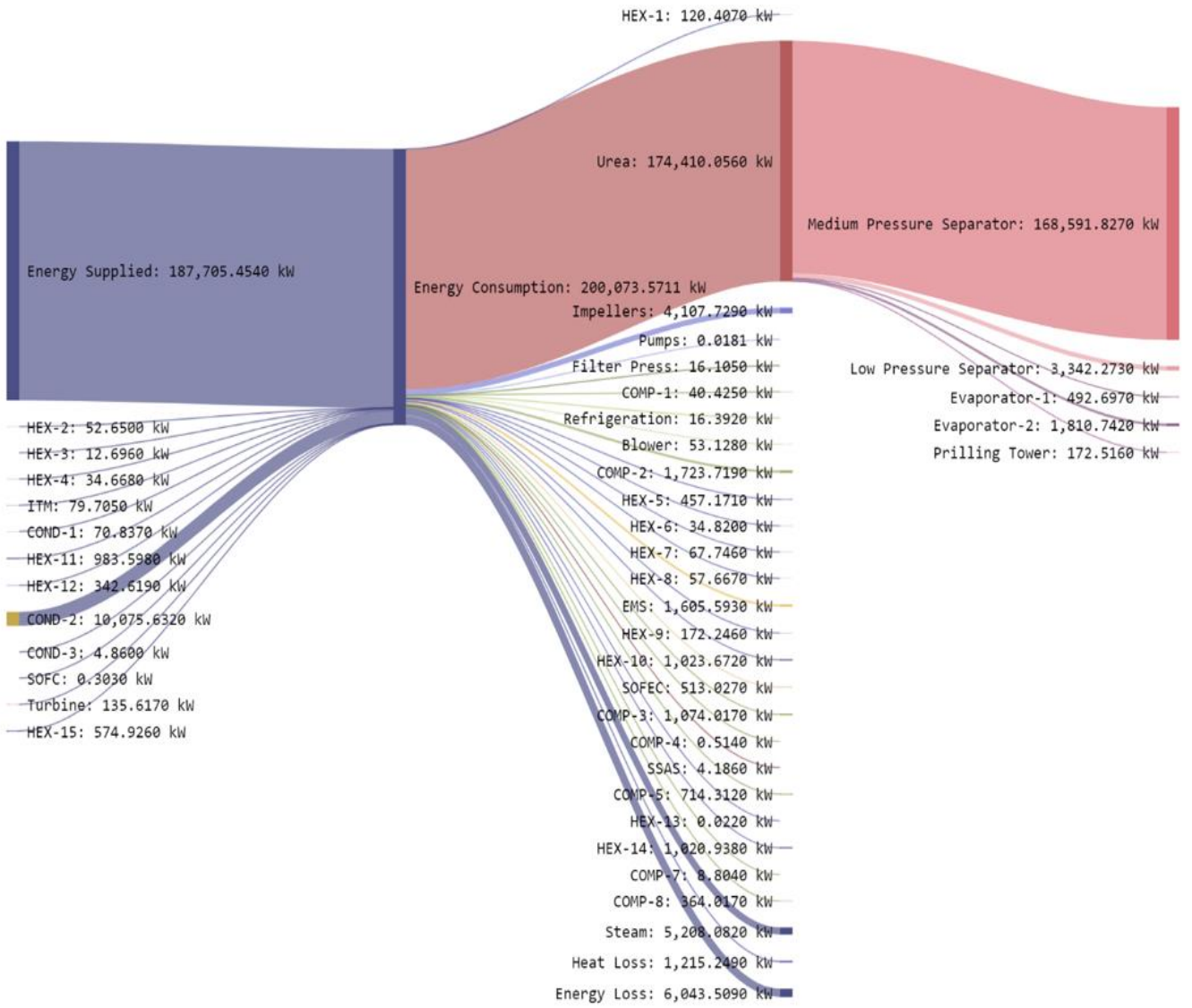
The energy draw in this process (AD-only) is about 8% lower than the two-stage due to higher NH_3 production. This is due to higher NH_3 yields driven by increased CO_2 production resulting from the incorporation of DF. With AD-only, the energy draw goes up due to higher H_2S handling by the EMS when DF is not used.

The energy production and consumption for the AD-only process as shown in Sankey diagram (Fig. 4.4(b)) is calculated based on Eq. 4.4 and 4.5.

$$\text{Energy Consumed} = \text{HEX-(1,3,4,5,6,7,8,11,12)} + \text{COMP-(1,2,3,4,5,6)} + \text{Required Steam} + \text{Impellers} + \text{Pumps} + \text{Filter Press} + \text{Blower} + P_{\text{EMS} + \text{CH}_4 \text{ assisted-SOFEC} + \text{SSAS} + \text{UREA}} + \text{Heat loss} + \text{Energy loss} \quad (\text{Eq. 4.4})$$

$$\text{Energy Produced} = \text{HEX-(2,9,10,13)} + \text{COND-(1,2,3)} + P_{\text{ITM} + \text{SOFC}} + \text{Turbine} \quad (\text{Eq. 4.5})$$

(a)



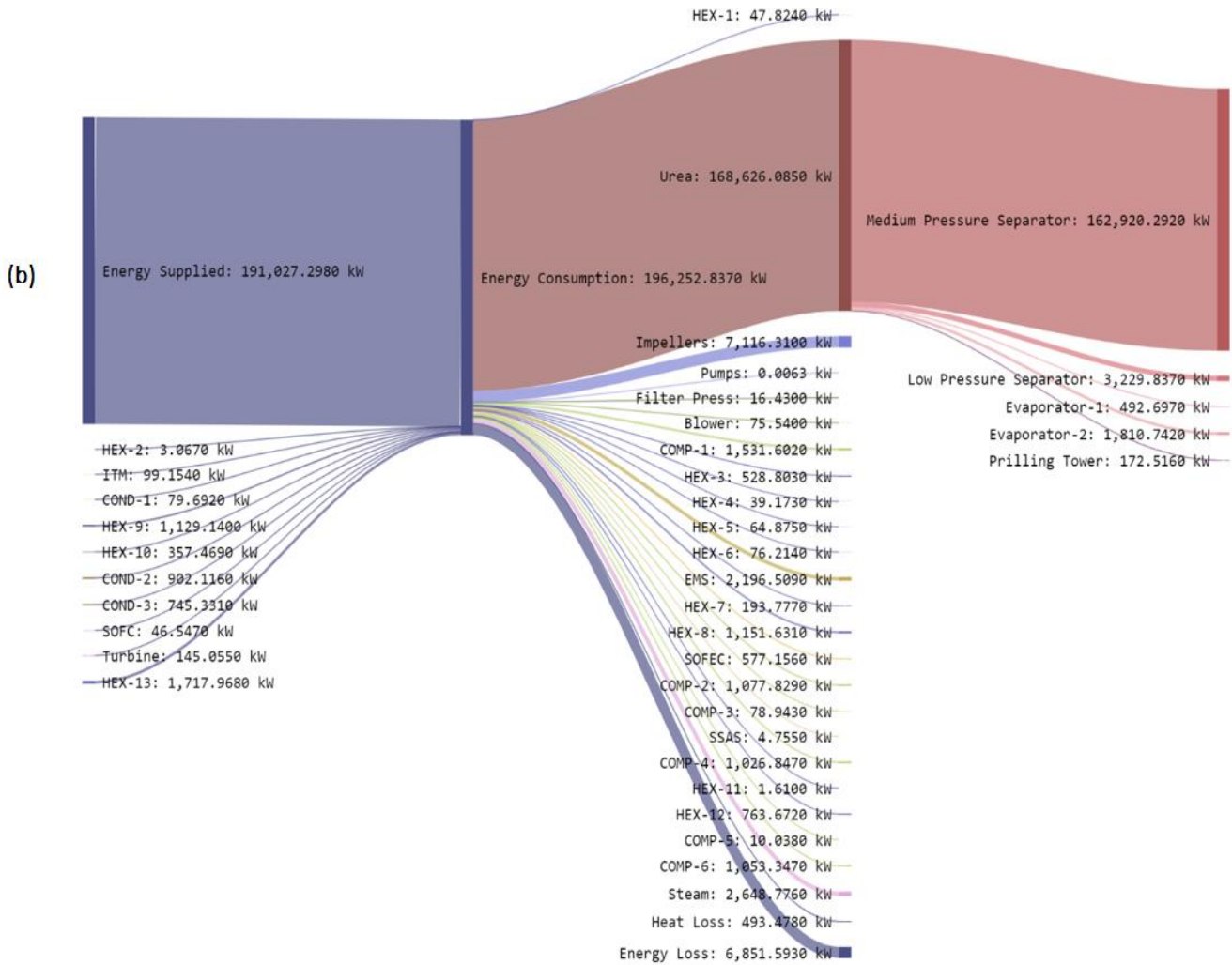


Fig. 4.4: Energy flows in the proposed ammonia production through, (a) two-stage DF+AD (Based on Fig. 3.14 (a)) and (b) AD-only process (Based on Fig. 3.15 (a)).

4.1.3 Model Validation

To validate the written VBA computer code, or in other words to test the accuracy of the modelled process, the code for each processing unit/component was initially written separately, considering that each component operates independently. Once each section of the process was thoroughly tested, the independent sections were connected in order to obtain the entire developed integrated waste-to-ammonia/waste-to-ammonia-urea process. Experimental data from the literature was used to validate each simulated model. The model tuning parameters important for each processing unit can be found in Table 4.20. There is a small difference between the modelling results due to different process conditions (e.g., in MFI where the inlet CO₂/H₂ gas ratios differ from the proposed process) and between the proposed theoretical process and experimental results. This small difference between the literature data and the proposed process confirms that the developed model was correctly implemented and can give accurate steady-state results.

Table 4.20: Model validation of processing units incorporated into the modelled process.

Model validation					
DF+AD				Unit	
Tested parameters (FW+BW)	Paudel et al. (2017)		Proposed process		
TS/VS _{OUT-mix}	0.84		0.837	%	
Maximum assessed production yield (DF)	0.3		0.2	m ³ H ₂ /kg VS	
OLR _{DF}	34.8		36.309	g VS/L. d	
Maximum assessed production yield (AD)	0.72		0.642	m ³ CH ₄ /kg VS	
OLR _{AD}	1.24		1.185	g VS/L. d	
Operational parameters					
Temperature	DF: 37	AD: 37	DF: 35	AD:55	°C
Pressure	1		1		atm
HRT	24	480	24.33	384	hr
Volume (DF/AD)	0.25		0.25		m ³
pH	5.0–5.5	7–7.5	5.5	6.5	
EMS					
Tested parameters					
	Winnick and Liu (2003)		Proposed process		Unit
Maximum H ₂ S removal flux	1.1E-06		1.126E-06		gmol H ₂ S min ⁻¹
Operational parameters					
Operating temperature	650		650		°C
Pressure	1		1		atm
Thickness	20		20		cm
Area of each cell	1		1		m ²
Number of cells	160		160		N ^o
MFI					
Tested parameters					
	Korelskiy et al. (2015)		Proposed process		Unit
CO ₂ Pemance	2E-07		1.678E-07		mol.m ⁻² .s ⁻¹ .Pa ⁻¹
CO ₂ /H ₂ separation factor	202		200		-
CO ₂ /H ₂ membrane selectivity	258		236.5		-
Operational parameters					
Temperature	-38		-38		°C
Pressure	9		19		atm
Thickness	0.5		0.5		µm
ITM					
Tested parameters					
	Hong, Kirchen and Ghoniem (2012)		Proposed process		Unit
Oxygen permeation flux	3E-07		2.891E-07		mol/cm ² .s
Operational parameters					
Temperature	907.35		907.35		°C
Pressure at permeate side	0.18		0.18		atm
Channel length	1		1		mm
Channel height from membrane to inlet (feed)	50.8		50.8		mm
Channel height from membrane to inlet (sweep)	25.4		25.4		mm
SOFEC					
Tested parameters					
	Xu et al. (2016)		Proposed process		Unit
Current density	2,000		1,996.33		A/m ²
Applied cell potential	0.7		0.7		V
Operational parameters					
Cell temperature	750		750		°C
Pressure	1		1		atm
Electrolyte membrane thickness	796		796		µm
Inner diameter	3		3		mm
Outer diameter	5		5		mm
Channel length	70		70		mm
SOFC					
Tested parameters					
	Ugartemendia, Ostolaza and Zubia (2013)		Proposed process		Unit
Total current density	146.76		146.76		A/cm ²
Cell voltage	0.72		0.672		V
Power density	105		98.62		mW/cm ²
Operational parameters					
Cell temperature	1000		1000		°C
Pressure	1		1		atm
Diameter	2.2		2.2		cm
Active length	150		150		cm
Number of cells in series/stack	364		364		N ^o
Fuel utilization	85		85		%
SSAS					
Tested parameters					
	Xu et al. (2009)		Proposed process		Unit
Theoretical rate of ammonia production	2.35 × 10 ⁻⁸		2.52 × 10 ⁻⁸		mol·cm ⁻² ·s ⁻¹
Efficiency	90.4		93.2		%
Operational parameters					
Cell temperature	80		80		°C
Pressure	1		1		atm
thickness	0.1		0.1		cm

4.1.4 Sensitivity analysis results

The sensitivity analysis examines the dependency in the output parameters of the proposed model (such as, gas and biogas production, output flow rate of ammonia, urea, and water, number of cells and output power for membranes, energy demand, power from SOFC, water consumption, and energy consumption) and the identifiability and significance of the input parameters involved (such as, waste compositions, substrate concentrations, input air flow rates, recirculation rate, urea purity, and different dilution ratios). The effects of changing the important input parameters on the output parameters are shown in Table 4.21-4.25 and Fig. 4.5 -4.7.

The results of the sensitivity analysis are based on changes to the input waste and the effect on hydrogen flow rate from DFB, methane flow rate from ADB, air flow rate to ITM, produced ammonia and urea, total CO₂ produced, power from SOFC, and required power for running the production process which are shown in Table 4.21. All of the results are based on the ratio of 1.1 for FW/BW and 2.5 for dilution water. The results indicate that for both technologies, the modelled system is sensitive to the power required for running the proposed production process followed by the amount of urea produced.

Table 4.21: Sensitivity analysis results for both technologies based on changes to input waste.

Tech-1								
Input waste flow rate (kg/d)	Hydrogen flow rate from DFB (kg/d)	Methane flow rate from ADB (kg/d)	Input air flow rate to ITM (kg/d)	Ammonia output flow rate from SSAS (kg/d)	Urea output flow rate from Snamprogetti process (kg/d)	SOFC power output (kW)	Total power required for running the process (kW)	Total CO ₂ produced (kg/d)
562.500	6.618	184.931	965.510	0.284	989.203	0.004	6,018.005	623.814
1,125	13.237	369.862	1,930.900	0.567	1,978.405	0.008	8,222.752	1,247.628
2,250	26.473	739.725	3,861.670	1.135	3,956.809	0.015	12,637.463	2,495.255
4,500	52.947	1,479.450	7,723.210	2.269	7,913.617	0.030	21,495.758	4,990.510
9,000	105.893	2,958.899	15,446.300	4.539	15,827.234	0.061	39,327.528	9,981.020
13,500	158.840	4,438.348	23,169.390	6.808	23,740.850	0.091	57,316.718	14,971.529
18,000	211.786	5,917.798	30,892.480	9.077	31,654.467	0.121	75,434.655	19,962.039
22,500	264.733	7,397.247	38,615.570	11.346	39,568.083	0.152	93,694.324	24,952.549
27,000	317.679	8,876.697	46,338.660	13.616	47,481.699	0.182	112,084.397	29,943.058
31,500	370.626	10,356.146	54,061.740	15.885	55,395.316	0.213	130,769.752	34,933.568
36,000	423.572	11,835.596	61,784.827	18.154	63,308.932	0.243	149,553.794	39,924.078
40,500	476.519	13,315.045	69,507.920	20.424	71,222.549	0.273	168,528.114	44,914.587
45,000	529.465	14,794.494	77,231.010	22.693	79,136.165	0.304	187,705.455	49,905.097
90,000	1,058.930	29,588.989	154,461.900	45.386	158,272.330	0.607	393,023.226	99,810.194
Tech-2								
562.500	104.027	208.048	1,038.390	43.496	955.925	0.572	4,822.746	701.791
1,125	208.054	416.095	2,076.660	86.993	1,911.850	1.154	7,071.360	1,403.581
2,250	416.108	832.190	4,153.190	173.986	3,823.699	2.318	11,451.404	2,807.162
4,500	832.216	1,664.381	8,306.250	347.972	7,647.398	4.646	20,259.221	5,614.324
9,000	1,664.432	3,328.761	16,612.380	695.944	15,294.795	9.302	38,121.209	11,228.647
13,500	2,496.648	4,993.142	24,918.520	1,043.915	22,942.193	13.957	56,245.450	16,842.971
18,000	3,328.864	6,657.523	33,224.650	1,391.887	30,589.590	18.613	74,609.868	22,457.294
22,500	4,161.080	8,321.903	41,530.780	1,739.859	38,236.9878	23.269	93,265.586	28,071.617
27,000	4,993.295	9,986.284	49,836.910	2,087.830	45,884.385	27.925	112,228.502	33,685.941
31,500	5,825.511	11,650.664	58,143.040	2,435.802	53,531.783	32.580	131,452.696	39,300.264
36,000	6,657.727	13,315.045	66,449.170	2,783.774	61,179.180	37.236	150,977.926	44,914.587
40,500	7,489.943	14,979.426	74,755.300	3,131.746	68,826.578	41.892	170,816.866	50,528.911
45,000	8,322.159	16,643.806	83,061.427	3,479.717	76,473.975	46.548	191,027.299	56,143.234
90,000	16,644.318	33,287.612	166,122.740	6,959.435	152,947.950	93.105	414,036.832	112,286.468

The results of the sensitivity analysis are based on the changes to input air flow rate, the effect on the number of tubes and cells in ITM and EMS respectively, total cell voltage from ITM, and current, total voltage, and total power required for EMS which are shown in Table 4.22. The results indicate that for both technologies, the modelled system is most sensitive to the total power required for EMS followed by EMS voltage.

Table 4.22: Sensitivity analysis results for both technologies based on changes to input air flow rate.

Tech-1						
ITM			EMS			
Input air flow rate (kg/day)	Number of tubes (N°)	Voltage (volt)	Current (Amp)	Voltage (volt)	Total power required (kW)	Number of cells (N°)
965.510	2	1.547	187.116	0.919	0.172	1
1,930.900	3	3.093	272.606	1.3578	0.370	1
3,861.670	7	6.186	545.212	2.834	1.545	3
7,723.210	14	12.373	1,090.425	6.1459	6.702	6
15,446.300	28	24.747	2,180.851	14.1981	30.964	12
23,169.390	42	37.120	3,271.276	24.1567	79.023	17
30,892.480	56	49.493	4,361.702	36.0217	157.116	23
38,615.570	70	61.866	5,452.127	49.7930	271.478	29
46,338.660	83	74.239	6,542.552	65.4706	428.345	35
54,061.740	97	86.612	7,632.978	83.0546	633.954	41
61,784.827	111	98.985	8,723.403	102.5449	894.541	47
69,507.920	125	111.359	9,813.829	123.9416	1,216.342	52
77,231.010	139	123.732	10,904.254	147.2446	1,605.593	58
Tech-2						
1,038.390	2	1.664	187.1159	0.919	0.172	1
2,076.660	4	3.327	306.6822	1.536	0.471	2
4,153.190	7	6.654	613.3644	3.222	1.977	3
8,306.250	15	13.307	1,226.7287	7.048	8.646	7
16,612.380	30	26.615	2,453.4572	16.509	40.504	13
24,918.520	45	39.922	3,680.1858	28.383	104.454	20
33,224.650	60	53.229	4,906.9143	42.669	209.373	26
41,530.780	75	66.536	6,133.6429	59.368	364.143	33
49,836.910	90	79.844	7,360.3715	78.480	577.641	39
58,143.040	105	93.151	8,587.1000	100.004	858.748	46
66,449.170	120	106.458	9,813.8286	123.942	1,216.342	52
74,755.300	135	119.765	11,040.5572	150.292	1,659.303	59
83,061.427	150	133.073	12,267.2857	179.054	2,196.510	66

The results of the sensitivity analysis are based on changes to recirculation rate from a base rate of 30% and the effect on the total power required, conversion factor of the reactors, and the amount of produced compost which are shown in Table 4.23. The results indicate that for both technologies, the modelled system is most sensitive to the conversion factor of the reactors followed by the amount of produced compost and almost insensitive to changes in the power required for operating the process.

Table 4.23: Sensitivity analysis results for both technologies based on changes to recirculation rate.

Recirculation rate (%)	Tech-1			Tech-2		
	Total power required for running the process	Conversion factor of the reactors	Compost output flow rate	Total power required	Conversion factor of the reactors	Compost output flow rate
%	kW	-	kg/day	kW	-	kg/day
20	187,700.084	0.737	145.301	191,019.0207	0.680	176.871
30	187,705.455	0.770	127.138	191,027.299	0.720	154.762
40	187,710.746	0.803	108.976	191,035.495	0.760	132.653
50	187,715.933	0.836	90.813	191,043.579	0.800	110.545

The results of the sensitivity analysis are based on changes to urea purity and the effect on the amount of produced biuret and water for the mixing tank which are shown in Table 4.24. The results indicate that for both technologies, the modelled system is most sensitive to produced biuret formation followed by water from the urea production process to the mixing tank.

Table 4.24: Sensitivity analysis results for both technologies based on changes to urea purity.

Urea Purity	Tech-1		Tech-2	
	Biuret output flow rate	Water output flow rate for the mixing tank	Biuret output flow rate	Water output flow rate for the mixing tank
%	kg/day	kg/day	kg/day	kg/day
80	8,001.635	21,851.295	7,732.455	20,149.209
98.5	600.123	23,690.566	579.934	22,132.829
98.9	440.090	23,730.334	425.285	22,175.718
99.990	40.008	23,829.754	38.662	22,292.590

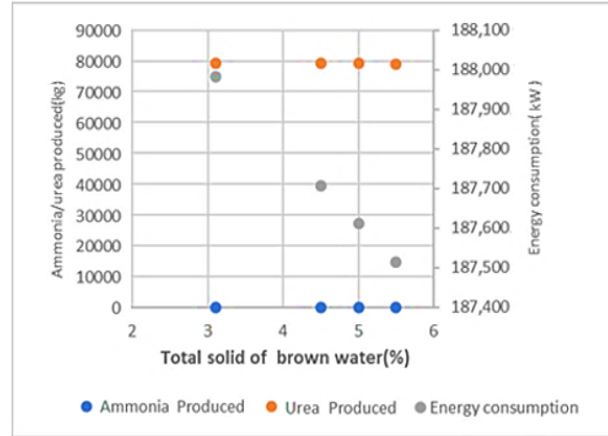
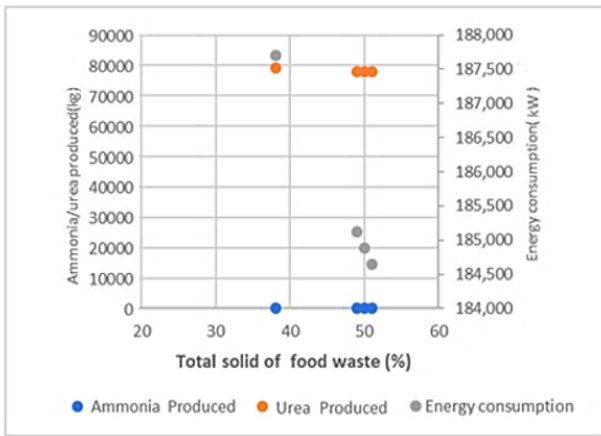
The results of the sensitivity analysis are based on changes to H₂/N₂ ratio from a base rate of 1.1 and the effect on the amount of produced ammonia, power from SOFC and the power required for operating the process which are shown in Table 4.25. The results indicate that for both technologies, the modelled system is most sensitive to power from SOFC followed by the ammonia output flow rate.

Table 4.25: Sensitivity analysis results for both technologies based on changes to H₂/N₂ ratio.

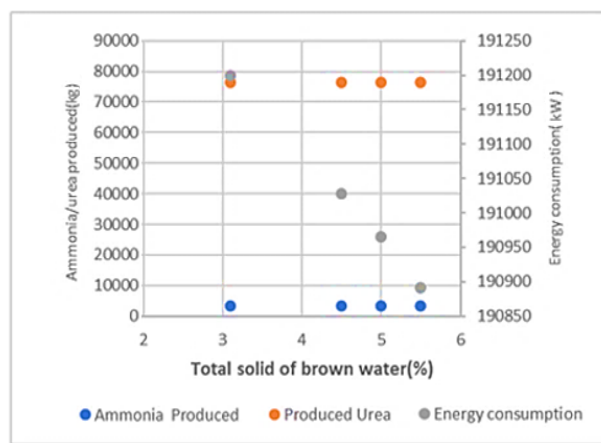
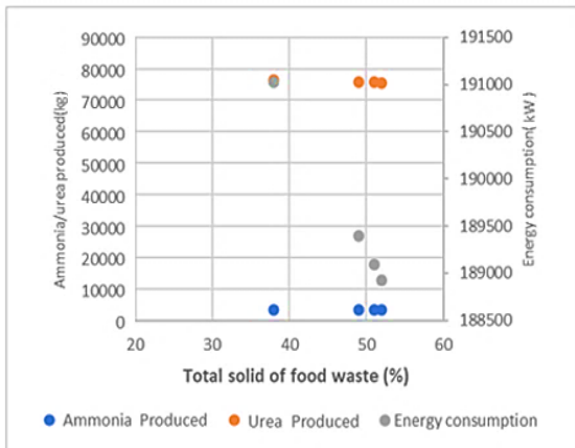
H ₂ /N ₂	Tech-1			Tech-2		
	Ammonia output flow rate	SOFC power output	Total power required for running the process	Ammonia output flow rate	SOFC power output	Total power required for running the process
Ratio	kg/day	kW	kW	kg/day	kW	kW
1.1	22.693	0.304	187,705.455	3,479.718	46.548	191,027.299
4.9	5.706	2.977	187,705.045	874.969	456.555	190,839.030
5.9	4.767	3.125	187,705.023	730.976	479.220	190,828.792
6.9	4.093	3.231	187,705.005	627.680	495.480	190,821.458
7.9	3.587	3.311	187,704.995	549.963	507.713	190,815.946
8.9	3.191	3.373	187,704.985	489.370	517.251	190,811.653
9.9	2.875	3.423	187,704.978	440.805	524.895	190,808.213

The TS and VS contents of a substrate affect the functionality of both DF and AD. Changing the TS content of the substrate will result in variations in microbial morphology of DF and AD (Orhorhoro et al., 2017).

Changing the TS of FW and BW for a two-stage DF+AD leads to changes in energy consumption. Sensitivity analysis has been conducted in order to assess how the above-mentioned functionalities respond to changes in these and other key parameters, and how much variability in these streams may matter to the process conditions, yields, and outputs. By keeping the VS of FW and BW parameters fixed throughout the sensitivity analysis, the following results were obtained as shown in Fig. 4.5. The energy consumption of the two-stage DF+AD process (1) is approximately 1.7% higher than the AD-only process (2). As the TS of FW and BW goes up, the energy consumption of both processes (1) and (2) drops significantly due to lower gas/biogas production.



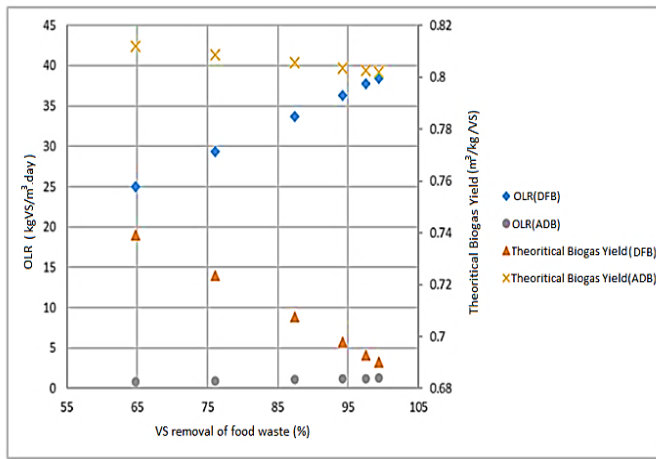
1) Dark fermentation coupled with anaerobic digestion process for scenario-1 (ammonia and urea production)



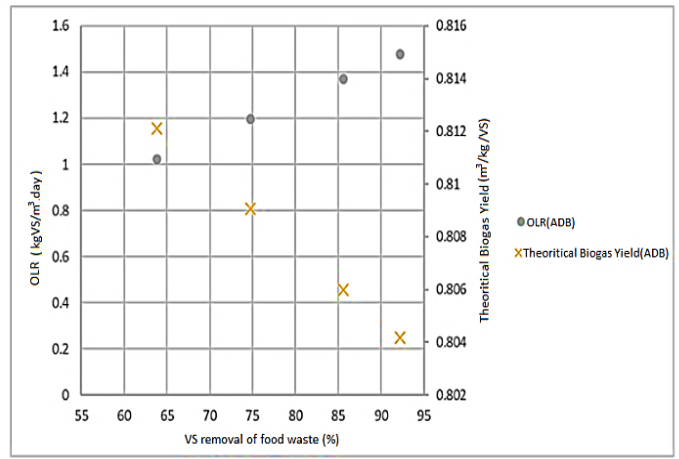
2) Anaerobic digestion process for scenario-1 (ammonia and urea production)

Fig. 4.5: A comparison of the two proposed technologies for ammonia production in terms of energy consumption, ammonia, and urea produced at different TS of FW and BW in a 20 TPD facility for (1) two stage DF+AD (2) AD-only process.

Variations on the VS removal of FW have a more significant impact on the two-stage DF+AD process (1) on OLR and the theoretical biogas yields compared to the AD-only process (2). This effect becomes more evident by varying the VS removal of FW compared to BW as shown in Fig. 4.6.



1) Dark fermentation coupled with anaerobic digestion process



2) Anaerobic digestion process

Fig. 4.6: The effects of VS removal on both OLR and theoretical biogas yields for (1) two stage DF+AD and (2) AD-only process.

For the AD-only process (2), increasing the ratio of FW/BW results in a decrease in the produced hydrogen, ammonia, urea, and compost. However, the decrease in urea production is sharper than in the other process outputs. When the ratio of FW/BW is 0.5 the optimum production yields were achieved. Conversely, for the two stage DF+AD process (1), the ammonia production yield goes up when the ratio of FW/BW increases. This is due to higher CO₂ production resulting from the presence of DF in the proposed process based on the modelling method described in the logical flow diagram which can be found in Fig. 3.13. Increasing the dilution rate will result in an increase in compost and methane production in both processes. An increase in methane production will in turn result in higher ammonia and urea production (Fig. 4.7).

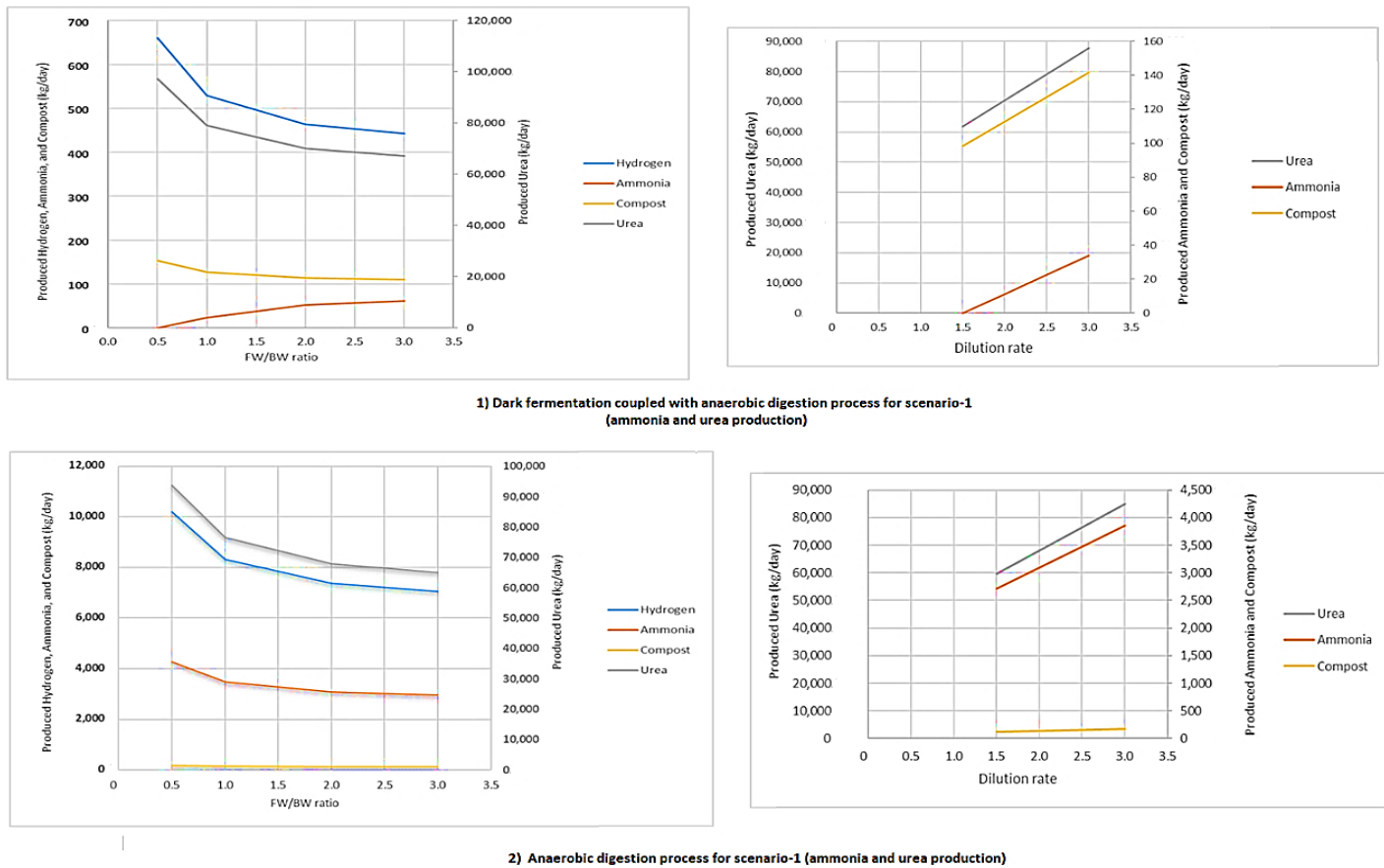


Fig. 4.7: The effect of FW/BW ratio and dilution rate on produced hydrogen, ammonia, urea, and compost for both (1) two stage DF+AD and (2) AD-only process.

4.1.5 A comparison of total daily production and consumption results for the two technologies and seven scenarios

The highest ammonia yields are obtained from AD, which produces about 6.5 times that of the two-stage process. However, the two-stage process makes more urea in urea-producing configurations. This is due to the higher production volume of CO₂ with the incorporation of the DF process. Based on Table 4.26 (a) the two-stage process consumes less energy and water compared to the AD-only. The AD-only produces about 3.5% less CO₂ compared to the two-stage process. Colors ranging from green towards yellow and red represent increasing values as shown in Tables 4.26 (a) and (b).

Although all calculations for the proposed processes are carried out on the basis of per kg NH₃ produced, a comparison needs to be conducted for per kg-N basis, since in each of the two technologies when using scenario ii, both urea and ammonia are produced. Table 4.26 (b) shows the efficiencies of different proposed processes per kg-N basis. The AD-only process is superior to the two-stage in terms of the CO₂ emitted/kg-N with 1.455 compared to 1.571. The water usage/kg-N through AD-only is lower compared to the two-stage except in the case where urea is produced with 0.902 compared to 0.973 for AD-only process. The energy consumption (MW/kg-N) for the two-stage process is lower than the AD-only except in the case where urea is produced with 5.087MW compared to 4.961MW for the AD-only process.

Table 4.26: A comparison of the modelling results of the proposed processes for a 20 TPD waste facility in terms of CO₂ emissions, water and energy consumption (a) daily basis and (b) per kg utilized-N.

(a)

Technology	Units	Two-stage DF coupled with AD with urea production and with SOFC	Two-stage DF coupled with AD without urea production and without SOFC	Two-stage DF coupled with AD with urea production and without SOFC	Two-stage DF coupled with AD without urea production and with SOFC	Two-stage DF coupled with AD with CCS and with SOFC	Two-stage DF coupled with AD with CCS without SOFC	Two-stage DF coupled with AD with CCU	AD with urea production and with SOFC	AD without urea production and without SOFC	AD with urea production and without SOFC	AD without urea production and with SOFC	AD with CCS with SOFC	AD with CCS without SOFC	AD with CCU
Carbon Dioxide Produced	kg	Traces	58.10	Traces	58.10	58.10	58.10	58.10	Traces	56.14	Traces	56.14	56.14	56.14	56.14
Water consumption	kg	33.28	48.07	33.28	48.07	48.07	48.07	48.07	37.44	50.02	37.44	50.02	50.02	50.02	50.02
Energy consumption	MW	187.70	13.22	187.70	13.22	187.70	13.50	13.5	191.02	21.13	191.07	21.08	22.10	22.15	22.08

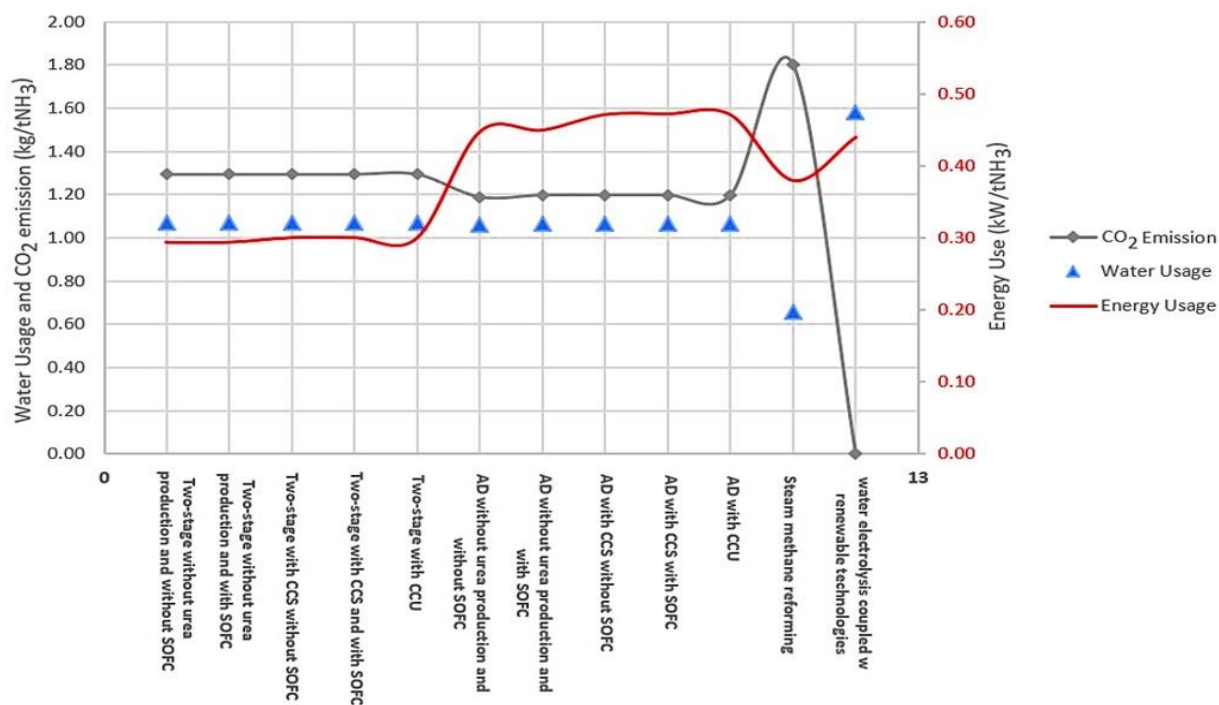
Low Mid range High

(b)

Technology	Two-stage DF coupled with AD with urea production and with SOFC	Two-stage DF coupled with AD without urea production and without SOFC	Two-stage DF coupled with AD with urea production and without SOFC	Two-stage DF coupled with AD without urea production and with SOFC	Two-stage DF coupled with AD with CCS and with SOFC	Two-stage DF coupled with AD with CCS without SOFC	Two-stage DF coupled with AD with CCU	AD with urea production and with SOFC	AD without urea production and without SOFC	AD with urea production and without SOFC	AD without urea production and with SOFC	AD with CCS with SOFC	AD with CCS without SOFC	AD with CCU
CO ₂ emitted/kgN	Traces	1.571	Traces	1.571	1.571	1.571	1.571	Traces	1.444	Traces	1.455	1.455	1.455	1.455
Water usage/kgN	0.902	1.3	0.902	1.3	1.3	1.3	1.3	0.973	1.287	0.965	1.296	1.296	1.296	1.296
Energy consumption MW/kgN	5.087	0.358	5.087	0.358	0.365	0.365	0.365	4.961	0.544	4.926	0.546	0.573	0.574	0.572

4.1.5.1 A comparison of the proposed processes with currently available ammonia technologies in use

A comparison of the proposed ammonia production process with conventional methods (SMR and water electrolysis coupled with H-B process) in terms of water usage kg/tNH₃, CO₂ emissions kg/tNH₃, and energy consumption kW/tNH₃ at steady state condition is shown in Fig. 4.8. This figure shows that the proposed ammonia process through a two-stage DF+AD both with and without the incorporation of SOFC is the most efficient in terms of water consumption compared to other technologies. The consumption rate for water electrolysis is approximately 82% higher than SMR-H-B which uses 0.66 kgH₂O/tNH₃. In terms of CO₂ emissions, this process is similar to water electrolysis, assuming that both processes are powered by renewable technologies. However, the energy consumption of water electrolysis is (0.44 kW/tNH₃) which is approximately 15% higher than SMR-H-B and approximately 41% higher than the two-stage process and about 6% lower than the AD-only process.



*Cited from: (Pfromm, 2017)

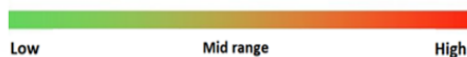


Fig. 4.8: A comparison of different proposed ammonia production processes with conventional methods in terms of CO₂ emissions, water and energy usage.

A study conducted by Morgan (2013), also shows that for the production of 300 TPD of ammonia, 476 TPD of distilled water through desalination is required. Through this study, 53.3 TPD of hydrogen is produced from water electrolysis powered by offshore wind. The ratio of the treated water required per tonne of ammonia (excluding the water needed for the cooling tower) is approximately 1.6. This figure is similar to the water electrolysis coupled with Haber-Bosch powered by renewable technologies shown in Fig. 4.8. However, the energy consumption in Morgan’s study using desalination is almost 13% higher than the water electrolysis assessed in Fig. 4.8 which is 0.49 kW/tNH₃. The energy consumption for desalination is almost 33% lower than the air separation unit in the study. This shows that the use of desalination systems is not as energy intensive as water electrolysis, however, it must be stated that from an environmental perspective it is detrimental to ocean biodiversity and marine life (Morgan, 2013; Peterson, 2017).-If environmental factors are not taken into account, the incorporation of desalination with water electrolysis for ammonia production would be an appealing option.

4.1.6 The significance of the proposed waste-based process

A particular benefit of a waste-based process such as the green ammonia technology developed here is the potential to avoid methane that could have been released from uncontained degradation of waste. The potential GHG

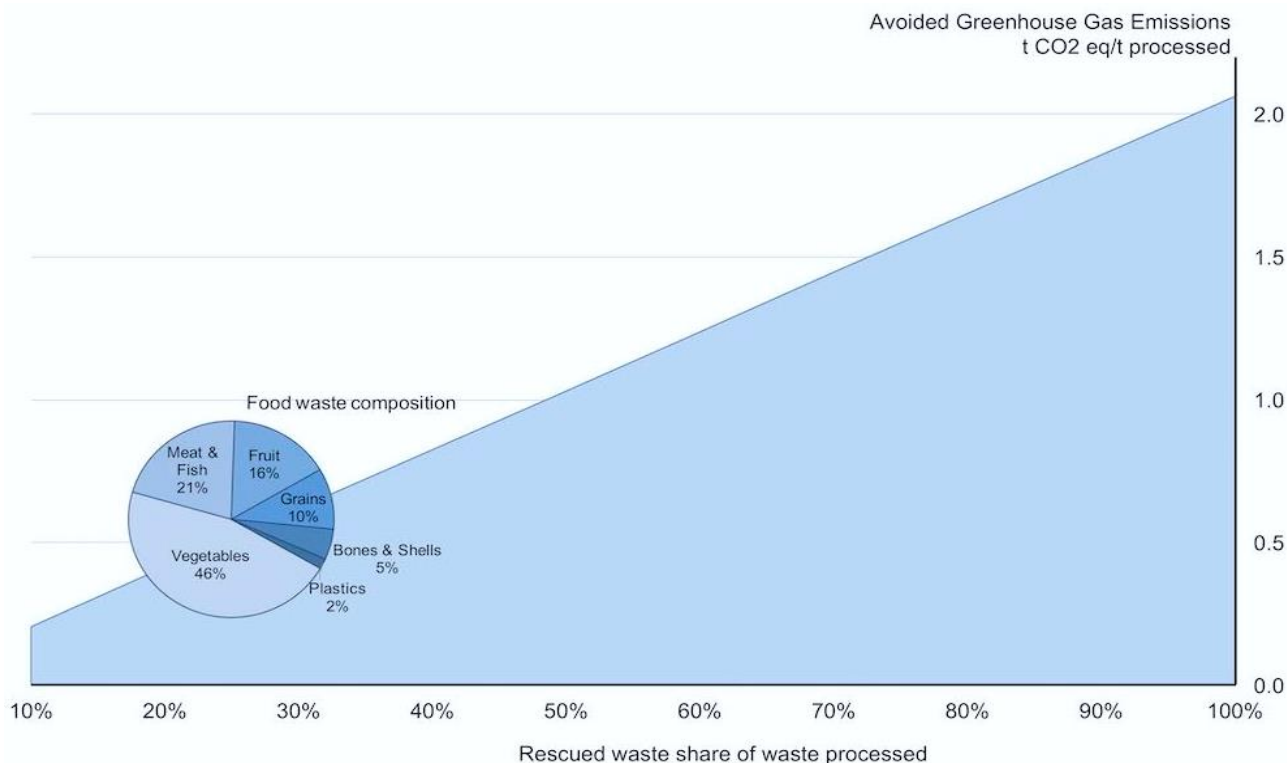


Fig. 4.9: Carbon dioxide mitigation potential per tonne processed FW as a function of fraction diverted into various processes instead of landfilling, calculated with WBCSD’s Food Loss and Waste Value Calculator (Quantis 2019) with composition of FW (vegetables, meat and fish, fruit, grains, bones and shells, and plastics) selected to assess the avoided emissions throughout this study (FW composition for South East Asia (Paudel et al., 2017)).

mitigation benefit with the technology depending on how much of the processed waste was diverted from uncontained degradation is illustrated in Fig. 4.9. About 74 kg of CH₄ is released with open degradation of a tonne of FW comprised of about half vegetable and a quarter meat wastes (Quantis, 2019). If 10% of each tonne of processed FW resulted from diversion, that would avoid releasing about 7.4 kg CH₄ or 200 kg CO₂ eq; at 50% rescued material that grows to nearly 1 kg of CO₂ eq /kg FW processed and at 90%, almost 1.85 kg CO₂ eq /kg FW would be prevented from directly reaching the atmosphere.

4.1.6.1 GHG mitigation by diverting different fractions of FW into the modelled process

Assuming 10%, 33%, 50%, and 100% of the FW is directed into the proposed process instead of degrading openly in landfills, this will prevent the release of about 5,159.06, 17,024.91, 25,795.32, and 51,590.64 kg CO₂ eq respectively from directly reaching the atmosphere, which results from the open decomposition of FW (Fig. 4.10).

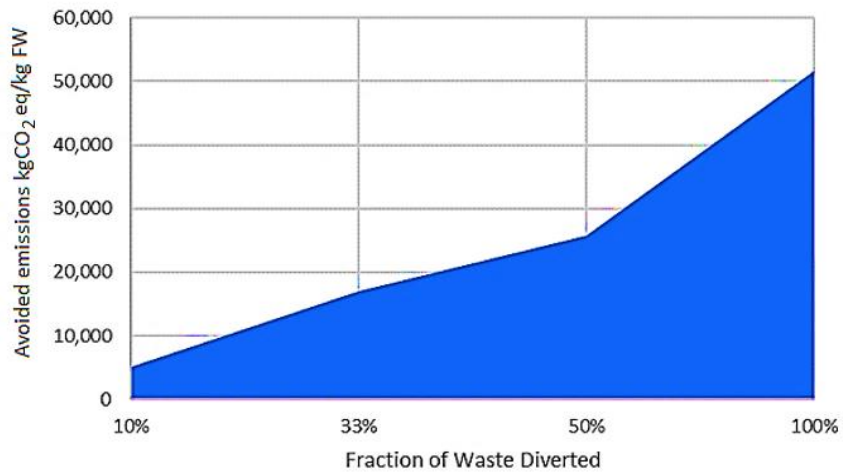


Fig. 4.10: Carbon dioxide mitigation by diverting different fractions of FW into the proposed process.

Conclusion

The results indicate that among the proposed technologies, the AD-only is the most efficient for GHG emissions, while the two-stage DF+AD process requires less energy per kgNH₃ basis. When comparing the proposed ammonia processes to the literature data, water electrolysis powered by renewable technologies is the best of all processes in terms of GHG emissions, while steam reforming coupled with H-B has the lowest water consumption of all the processes mentioned.

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Chapter 5

Methods and Tools for The Life Cycle Assessment

This chapter focuses on the rationale behind choosing the methods employed for the cradle-to-gate LCA and an overview of the goal and scope, system boundary, software evaluation, allocation, cut offs, life cycle inventory, facility siting, library processes, data quality and uncertainty, and sensitivity analysis.

This chapter was drafted based on the publication submitted to the journal of cleaner production:

Ghavam, S., Taylor, C.M. and Styring, P., (2021). The life cycle environmental impacts of a novel sustainable ammonia production process from food waste and brown water. *Journal of Cleaner Production* [online]. 320, 128776. [Viewed 22 September 2021]. Available from: <https://doi.org/10.1016/j.jclepro.2021.128776>.

5. Environmental impact assessment using life cycle assessment techniques

5.1 Methods

5.1.1 Life cycle assessment

LCA is a primary technique used to support decision-making for sustainable design in production. This study presents a cradle-to-gate comparative LCA of a waste management facility for ammonia production. This comparative LCA considers relative environmental impacts in the areas of global warming, water scarcity, human health, ecosystems, and resource use, as well as human toxicity, acidification potential, eutrophication, depletion of abiotic resources, ozone depletion, and terrestrial ecotoxicity. For two configurations and four scenarios, life cycle inventories were developed based on computational modelling and design decisions discussed in *Chapter 3*. Biogenic CO₂ was used in all calculations (contribution, uncertainty, and sensitivity analyses). The ISO 14040 (ISO, 2006) and ISO 14044 (ISO, 2009) standards offer direction on the LCA framework which is comprised of the following four main stages (Fig. 5.1).

- i) Defining the goal and the scope of the LCA
- ii) Gathering and keeping a list of energy and mass inputs/outputs throughout all relevant life cycle stages
- iii) Assessing relevant environmental impacts that are related to the life cycle inputs and outputs
- iv) Finally, interpreting the results, that will lead to a decision based on the data obtained from previous stage and improving the results

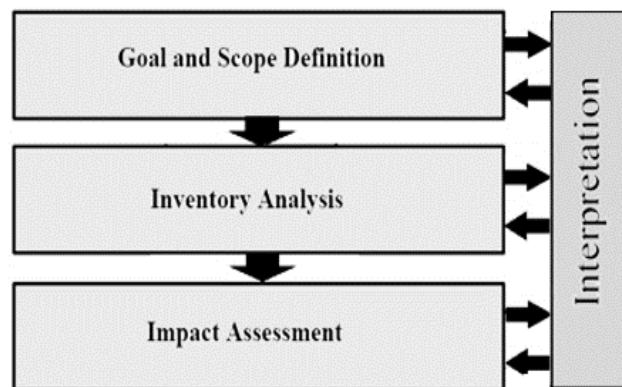


Fig. 5.1: The framework of a life cycle analysis.

5.1.1.1 Goal and scope definition

Goal definition defines the objectives of the study, the intended applications, the target audience, and the key stakeholders. The scope definition, in turn, defines the Functional Unit (FU), system boundaries, impact assessment methods, allocation, and cut-off criteria, Life cycle inventory, assumptions, and limitations.

The goals/objectives of this study are:

- i) To determine the environmental impacts of the proposed ammonia production processes and whether they can compete with other existing ammonia production technologies on a full life cycle environmental impact basis.
- ii) To investigate the use of LCA and LCT early in the green design process.

The system boundaries of an LCA define what processes are included or excluded in the studied system. The overall scope of this attributional LCA is cradle-to-gate, meaning it includes all stages from raw material extraction through the ammonia production facility, but does not include subsequent “downstream” storage, transportation, distribution, consumption, and end-of-life fate of the product. The system boundary for this study is illustrated in Fig. 5.2. The processes considered within the system boundaries in this cradle-to-gate LCA are grouped into four stages: (1) BW and FW transportation to the proposed ammonia process site; (2) Ammonia production process; (3) CO₂ handling; and (4) Depending on the source of power (solar, wind, or grid) the extra electricity produced will be sold to the grid. Fig. 5.3 illustrates the black box shown in Fig. 5.2.

The primary FU used in this analysis is 1 kg of NH₃. Impacts were also assessed on a urea production basis, in which a FU of 1 kg urea is considered, as well as on the basis of total nutrient N (kg urea-N + kg NH₃-N) (further information can be found in *Chapter 6*).

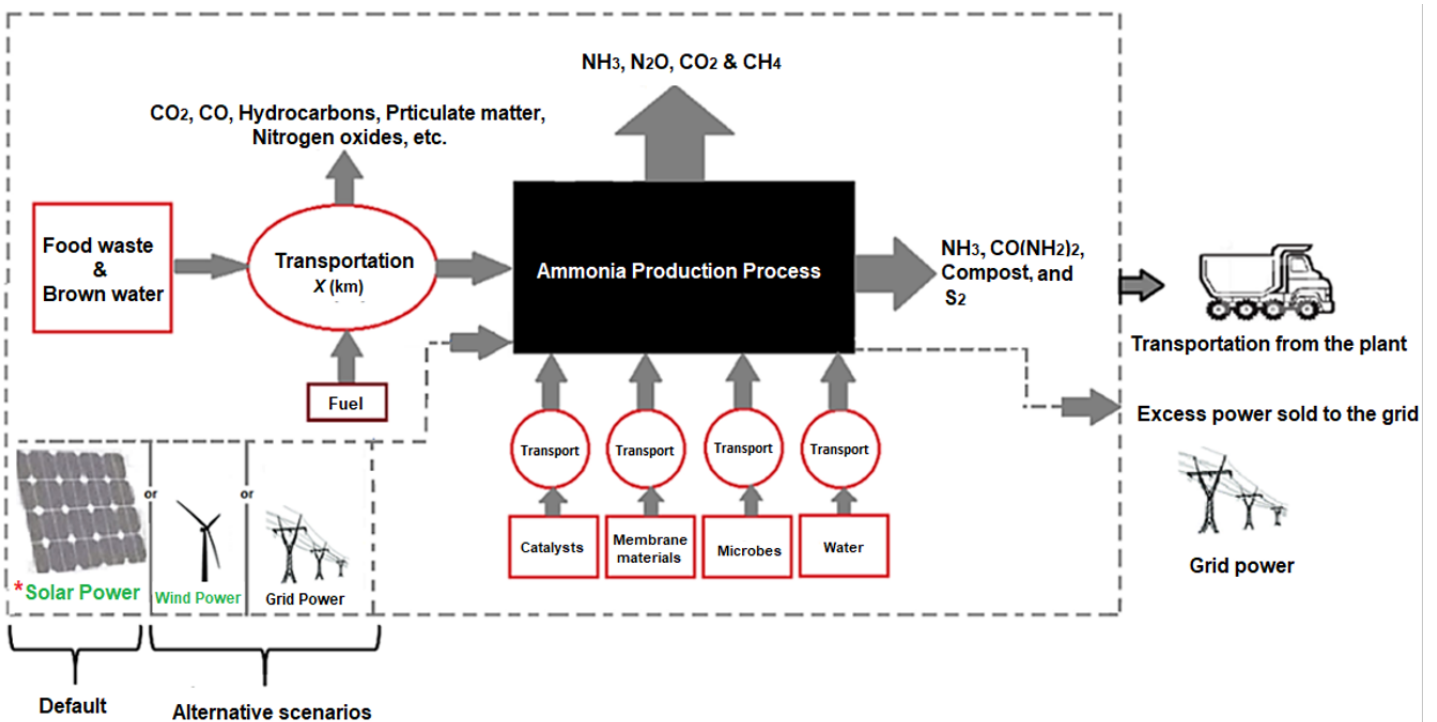


Fig. 5.2: System boundary for the cradle-to-gate LCA for this study’s green ammonia and ammonia+urea production from waste (for a detailed description of the ammonia production process shown in the black box refer to Fig.5.3).

Depending on the scenario configuration assessed in section 3 of *Chapter 3*, the process configuration and computational model behaviour changes. Additionally, since electricity is an important contributor to impact, an

alternative configuration option where the SOFC is used was also modelled (assessed in *Chapter 6*, section 6.2.1.2). The technology and the technology modelling are described in detail in *Chapter 3 and 4*. In general terms, the process configurations are shown in Fig. 5.3. The elements that differ in each scenario are shown in cream colour and the fixed elements are in white (Fig. 5.3). The impacts from three selected sources of energy, solar, wind, and grid were assessed, however, solar is the default primary source, the rationale behind choosing it is discussed in *Geographic location assessment of the proposed ammonia plant* section.

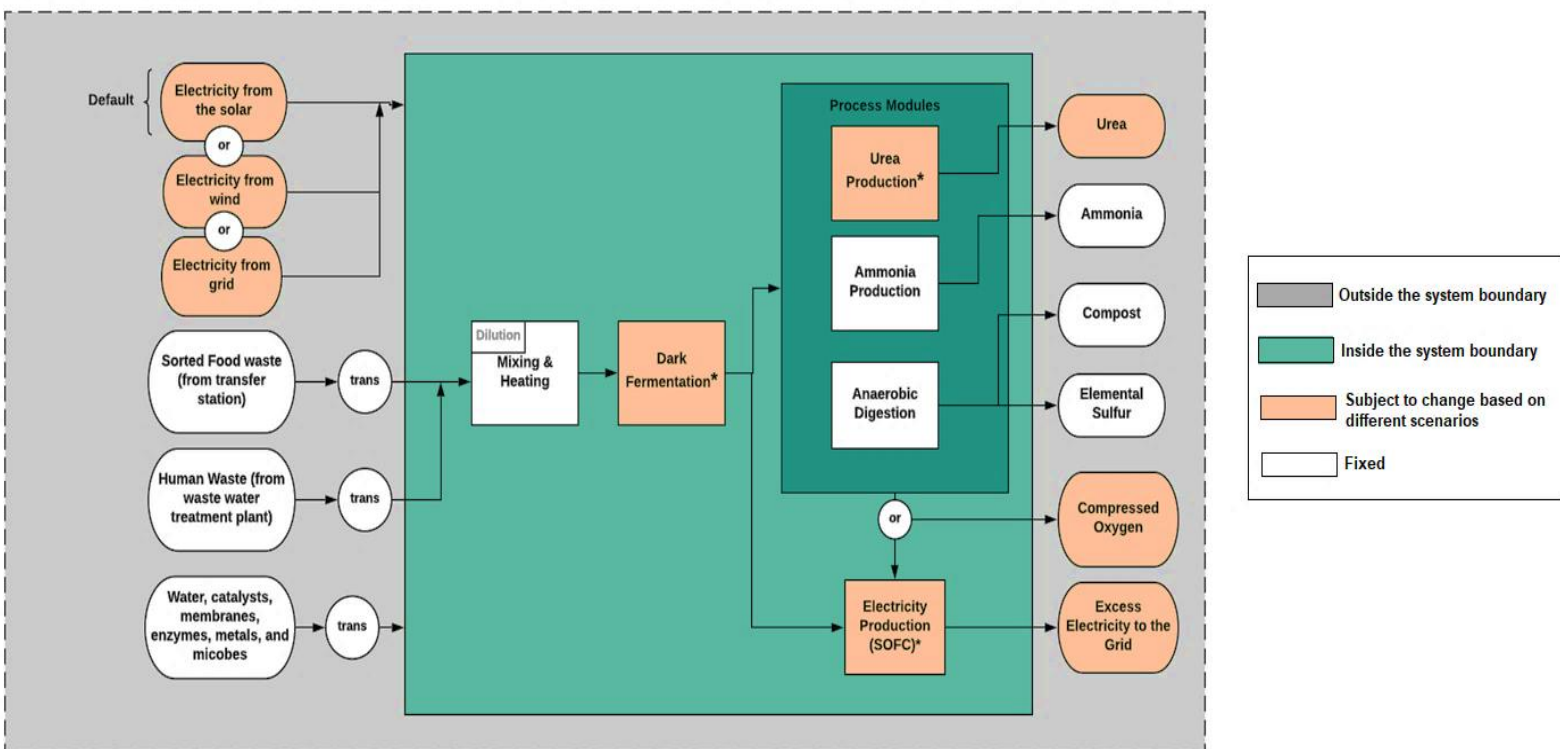


Fig. 5.3: A schematic of the proposed ammonia production process (Description of the black box in Fig. 5.2).

5.1.1.2 Selecting the appropriate software

Depending on the chosen LCA approach, there are software tools to calculate the GWP and GHG emissions, such as GaBi, SimaPro, Open LCA, Athena Eco Calculator, and eTool. The two most adopted tools which are suitable for this research are SimaPro and GaBi software. Each include extensive databases that allow users to compare the environmental impacts arising from different scenarios (GOGA, 2016).

GaBi

GaBi software is one of the most widely adopted LCA tools and is available in various versions. In addition to carrying out an LCA, GaBi software assists in providing data⁴. All LCA associated data is ISO 14040/44 compliant. This software has different databases which cover many areas. Both the USLCI and ELCD databases are available in GaBi. Additionally, GaBi has access to the lower priced ecoinvent database (Howe, Pepke and Fernholz, 2017).

⁴ Data is accessed via Think step, an international company focusing on sustainability on multiple levels.

SimaPro

SimaPro is an LCA software solution which provides an understanding for generating sustainable values. This software, includes many standard impact assessment methods where each method is comprised of several impact categories. Similar to GaBi software, SimaPro is one of the most widely adopted LCA tools which is available in different versions. SimPro’s database is more comprehensive when compared to other LCA software such as GaBi. It is comprised of ecoinvent, USLCI, ELCD, Agri-footprint, and many other databases (Howe, Pepke and Fernholz, 2017; SimaPro, 2015).

5.1.1.3 Impact assessment methods

Life cycle inventory models for ammonia / ammonia +urea production at the defined scale in each scenario were developed and assessed using SimaPro 9.0.0.49 PhD version, developed by PRÉ Consultants, the Netherlands (Oele, Dolfing Fanous and PRÉ Sustainability, 2020) (Sample of inventory processes for DF+AD for both scenarios set ii and iii are provided in Appendix B). The inventories are detailed in section 5.1.1.6. Secondary data is drawn from the widely-used ecoinvent library (version 3.6) (Wernet et al., 2016). Comparison processes are drawn from both ecoinvent v3.6 and Agri-footprint v4 (Durlinger et al., 2017). The impact assessment methods used are the Intergovernmental Panel on Climate Change (IPCC) Global Warming Potential (GWP, 100 years) {2013} (IPCC 2013), ReCiPe 2016 endpoint (H) (Huijbregts et al., 2017), water scarcity (AWARE) (Boulay et al., 2018), and CML 2001 (Guinée et al., 2002).

The selected impact categories and corresponding methods and units are shown in Table 5.1. The CML 2001 and Eco-indicator 99 methods from the superseded impact categories were used for the purpose of comparing with literature data.

Table 5.1: The selected impact categories and corresponding methods and units.

Impact Category	Method	Units
Human Health (Damage)	ReCiPe World Endpoint (H)	DALY
Ecosystem (Damage)	ReCiPe World Endpoint (H)	Species.yr
Resources (Damage)	ReCiPe World Endpoint (H)	USD 2013 (\$)
GHG emissions /GWP ₁₀₀	IPCC 2013 GWP 100a V1.03	kg CO ₂ eq.
GHG emissions /GWP _{biogenic}	Greenhouse Gas Protocol V1.02	kg CO ₂ eq.
Water foot-print	AWARE (water scarcity)	m ³
Used for comparison to prior literature		
GHG emissions	CML 2001 (All impacts)	kg CO ₂ eq.
Abiotic depletion	CML 2001 (All impacts)	kg Sb eq.
Human toxicity	CML 2001 (All impacts)	kg 1,4-DB eq.
Human Health	Eco-indicator 99	DALY
Ecosystem Quality	Eco-indicator 99	PDF [*] m ² yr
Resources	Eco-indicator 99	MJ surplus

According to the IPCC, CO₂ emissions from biogenic sources should not be included in national GHG inventories, as these emissions are counted in the Agriculture, Forestry and Other Land-Use (AFOLU) sectors (Liu et al., 2017). Therefore, bioenergy is considered a carbon neutral source of energy as a replacement for fossil fuels. This convention is followed (a GWP of zero) when assessing the Global Warming Impact (GWI) of biogenic CO₂ emissions in the LCA. However more recent studies indicate that the CO₂ emissions from biomass combustion will remain in the atmosphere for years, as a result, to assess the GWP of biogenic CO₂, a GWP_{biogenic} metric has been used. According to Liu et al. (2017) “when the biogenic CO₂ emission is multiplied by a nonzero GWP_{biogenic} factor,

higher GHG emissions were anticipated in the LCA case study”. The inclusion of biogenic emissions using the GHG Protocol impact assessment method version 1.02, which includes fossil, biogenic, land, uptake, and transformation emissions individually to incorporate biogenic CO₂ have been thus assessed (for detailed calculations for each CO₂ fate, refer to *Chapter 6*, Tables 6.4 and 6.5 (IPCC, 2008).

5.1.1.4 Allocation

In cases where a process produces more than one product, allocation of flows and emissions associated with the co-product system is needed. ISO guidance is to avoid allocation where possible by using system expansion where reasonable and to compare to an alternative allocation method where allocation is used. In keeping with the ISO standards (ISO, 2006; ISO, 2009), system expansion was used to account for all non-urea coproducts throughout. There is a large disparity in production volumes (urea dwarfs the primary ammonia production volume), in cases where the urea co-product comes from the waste CO₂ stream. As for the multi-product systems, those making urea along with ammonia, the impacts were allocated in keeping with ISO 14044:2016 recommendations (ISO, 2009). This was done through: System expansion with urea as an avoided product for cases where ammonia is the primary focus; and based on mass to allow comparison of the combined system on a nitrogen content basis and the effect of allocation. Since the production volumes of urea are so much higher than that of ammonia in the co-production cases, mass allocation between the two was used for the primary analysis and avoided product considered in the sensitivity analysis. The allocation types used and % table of allocation shares are shown in Table 5.2.

Table 5.2: Allocation types used and % table of allocation shares.

	AD	DF+AD
Urea producing processes		
Allocation Case 1: Mass allocation		
Ammonia	4.72 % by mass	0.0312 % by mass
Urea	95.3 % by mass	99.968 % by mass
Allocation Case 2: System expansion		
Ammonia	100%	
Urea	Avoided product	
All processes		
Sulfur (S ₂)	Avoided product	Avoided product
Compost	Avoided product	Avoided product
Oxygen (O ₂) (l)	Avoided product	Avoided product

For scenario ii (those producing urea), the effect of allocation is also evaluated, with three alternatives: Mass allocation, avoided product, and the unallocated process per tonne of processed input waste. All mentioned scenarios have three energy supply options comprised of solar (base case), grid, and wind. The afore-mentioned four carbon-fate scenarios and their permutations (72 in total) are then compared with each other and with other ammonia production processes (partial oxidation, cocamide diethanolamine production, and steam reforming). Fig. 5.4 illustrates all permutations of this proposed process.

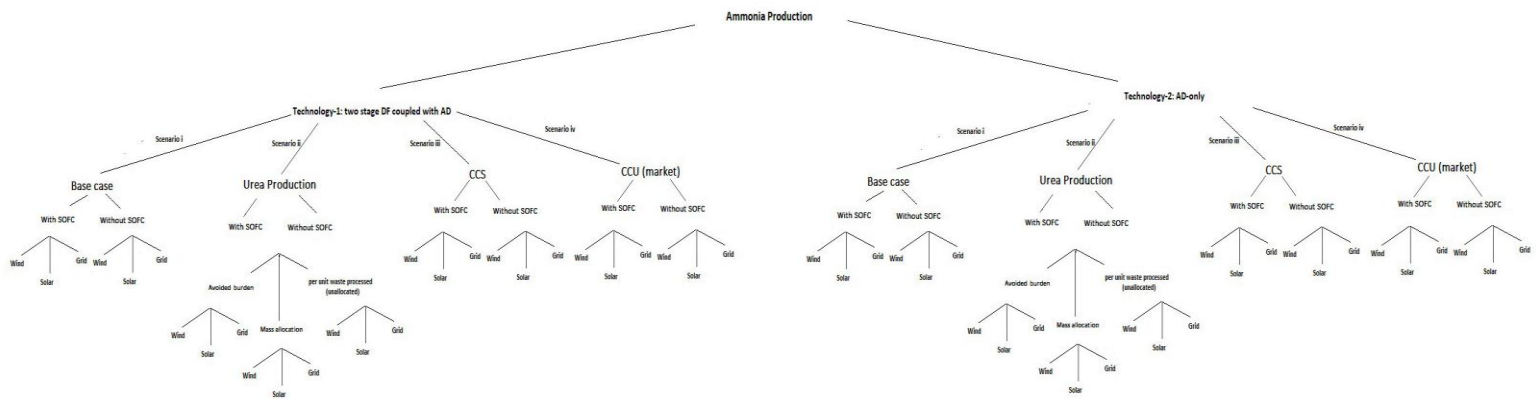


Fig. 5.4: All scenarios and permutations of the proposed process.

5.1.1.5 Cut-Offs

While conducting an LCA, cut-off criteria are used frequently to select the processes and flows in the system boundary by excluding processes from the study that are below the thresholds for mass, energy, and/or environmental relevance. In this case, given the simplicity of the modelled process, cut-off was not needed, although, as the results demonstrate (*Chapter 6*), factors such as membrane constituents, would fall below the threshold.

Excluded processes in the LCA model are: Waste collection prior to transport to facility, packaging of delivered membranes, disposal of spent membranes, if any, secondary treatment of the biuret byproduct, capital equipment (including membrane scaffolding), infrastructure, maintenance, and chemical usage to help maintain the biological culture.

5.1.1.6 Life cycle inventory

Process operating parameters and yields are taken from the technology model and simulations for the four scenario sets of technologies and set out in Table 5.3 derived from *Chapter 4*. The results presented here (Table 5.3) are based on the calculations for 20 TPD of input waste (FW and BW) (Detailed input and output parameters used in SimaPro are provided in Appendix B). This value is calculated to roughly represent the size of a mid-size city such as Bakersfield, California, although other scaling can be evaluated with the implemented model (siting is discussed further in *Geographic location assessment of the proposed ammonia plant* section) (Brown, 2018). Leakage, as in other methane and natural gas systems, has a high environmental impact on the process. Therefore, the processes are modelled with and without the impact from leakage, using values from USEPA (U.S. EPA, 2001; U.S. EPA, 2021) and California Air Resources Board (CARB) (CARB, 2017). Membrane components are represented using proxy background data, refer to *Chapter 6*, section 6.2.1.1. Table 5.3 also provides the electricity inventory for the studied technologies. The effect of SOFC on energy demand is negligible. The technology configuration with the lowest energy intensity (two-stage) consumes about 41% less energy than water electrolysis coupled with H-B and approximately 27% lower energy than SMR coupled with H-B per kg NH₃.

Table 5.3: Material inventory for assessed processes, per tonne of processed input waste.

Process data	Values				Units	Notes		
	CCU-Urea		No CCU-Urea					
	AD	DF+AD	AD	DF+AD				
Inputs								
Total waste	1	1	1	1	tonne			
Food waste	0.5	0.5	0.5	0.5	tonne	Main Feedstock		
Brown water	0.5	0.5	0.5	0.5	tonne	Main Feedstock		
NaOH	0	0.3711	0	0.3711	tonne	Added for pH balance (pH target: 5.5), based on De Gioannis et al. (2013)		
Dilution water	0.1411	0.0634	1.25	1.25	tonne	Water used for feedstock dilution		
Deionized (DI) water	1.872	1.664	1.872	1.664	tonne	DI water used for SOFEC		
Outputs								
Ammonia (default)	0.1739	0.00113	2.343	2.246	tonne	Primary product in default configurations		
Ammonia (without SOFC)	0.1913	0.00124	2.360	2.246	tonne	Primary product in process configurations without SOFC		
Urea	3.823	3.956	0	0	tonne	Main Product		
Compost	0.0077	0.00635	0.0077	0.00635	tonne	By-product		
Sulfur	0.0002	0.00018	0.0002	0.00018	tonne	By-product		
Direct emissions								
CO ₂	0	0	2.807	2.495	tonne	Direct emission from SOFEC, applicable for Base case only		
leakage rates								
CH ₄	1.5	1.5	1.5	1.5	%	Based on Odeh (2019)		
CO ₂	1	1	1	1	%	Based on the modifications made on the U.S. EPA (2021)		
NH ₃	1	1	1	1	%	Based on the modifications made on the U.S. EPA (2001)		
N ₂ O	0.5	0.5	0.5	0.5	%	From nitrogen in waste CARB (2017)		
Transport								
FW distance	24.9+/-10%	24.9+/-10%	24.9+/-10%	24.9+/-10%	km	Distance travelled from collection facility to the plant		
BW distance	45.4+/-10%	45.4+/-10%	45.4+/-10%	45.4+/-10%	km	Distance travelled from collection facility to the plant		
Energy demand (kWh)								
	CCU-Urea		CCU-market		No CCU-Urea (Base Case)		CCS	
	AD	DF+AD	AD	DF+AD	AD	DF+AD	AD	DF+AD
SOFEC configurations (default)	9.551	9.385	1.104	0.674	1.054	0.661	1.107	0.675
Configurations without SOFC	9.553	9.385	1.106	0.674	1.056	0.661	1.106	0.675
Labels for configurations included in study	CCU-Urea: AD CCU-Urea: AD no SOFC	CCU-Urea: DF+AD CCU-Urea: DF+AD no SOFC	No-CC: AD No-CC: AD no SOFC CCS: AD CCS: AD no SOFC CCU-market: AD CCU-market: AD no SOFC	No-CC: DF+AD No-CC: DF+AD no SOFC CCS: DF+AD CCS: DF+AD no SOFC CCU-market: DF+AD CCU-market: DF+AD no SOFC	CCU-market is captured CO ₂ compressed and assumed to enter the CO ₂ market			

Facility siting

Location will influence both feedstock availability and renewable energy supply options, it is an important factor in sustainable production of chemical compounds such as ammonia for maximizing both productivity and sustainability. As the inputs and outputs for this proposed ammonia production process are FW and BW, wastewater treatment and solid waste management facilities are the resources of interest. Based on the inputs and outputs of this proposed ammonia production process, a site suitability analysis is necessary in determining where the proposed facility should be located. Siting was based on analysis of FW and BW in central California and overlapped with solar energy availability. Among the three energy supply options (solar, wind, and grid) considered in this analysis, solar power was selected as the base case electricity supply option (based on location assessment method using RETScreen software) (Natural Resources Canada, 2019) and calculations were conducted based on National Renewable Energy Laboratory (NREL)'s PVWatts® Calculator (NREL, 2014). The geographic analysis of these led to the estimation of the distance from waste treatment and waste management facility to the ammonia plant at 24.9+/-10% (km) and

45.4 \pm 10% (km) respectively. \pm 10% distance from the waste treatment facility to the proposed ammonia plant has been selected to allow flexibility in placement.

Geographic location assessment of the proposed ammonia plant

It is assumed that the proposed ammonia plant is located in North America, specifically in California. The locations of all ammonia plants in North America are shown in Fig. 5.5.

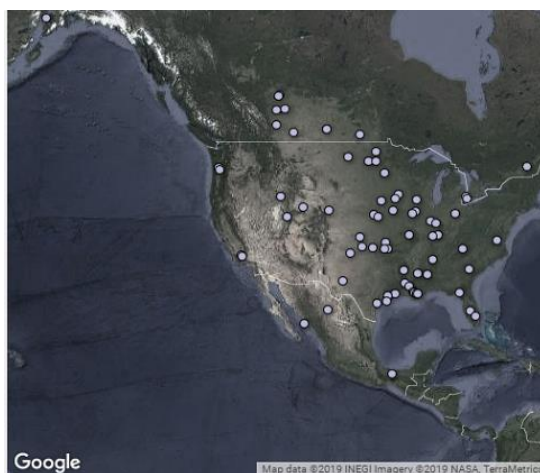


Fig. 5.5: Ammonia plants located in North America.

Based on Fig. 5.5, there are two ammonia plants located in Bakersfield, California. A location assessment was carried out on both ammonia plants and it was determined that one of the locations was more suitable for setting up a plant based on accessibility to feedstock (BW and FW). The first plant was located in Tupman, California, the closest waste management and Waste Water Treatment (WWT) facilities able to provide the selected feedstock to the plant include: Wasco Waste Water Treatment Plant (WWTP), 5410 7th St, Wasco, CA 93280 and 274 E Cedar St, Taft, CA 93268. This WWTP is in the vicinity (3.8 km) of Wasco city which has a population of 25,000, making it suitable to supply the ammonia plant with BW (human feces without urine). Fig. 5.6 shows the distance of the chosen WWTP to the Wasco city center.



Fig. 5.6: The distance between the Wasco wastewater treatment plant to Wasco city center.

The waste management facility is in the vicinity (56.6 km) of the Bakersfield metropolitan area which has a population of 839,631, making it suitable to supply the ammonia plant with FW. Fig 5.7 shows the distance of the chosen waste management facility from the Bakersfield metropolitan area.

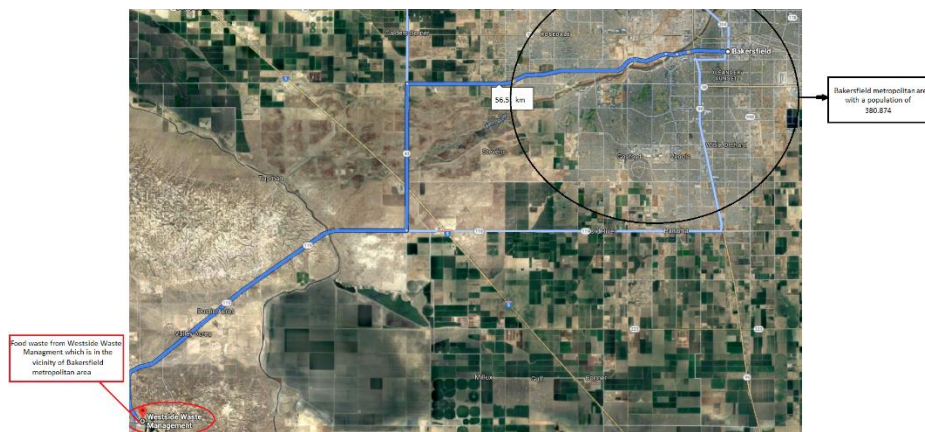


Fig. 5.7: The distance between the Westside waste management facility and the Bakersfield metropolitan area.

The Wasco wastewater treatment plant and Westside waste management facilities are geographically the closest to both ammonia facilities located in California. The distance between the Wasco WWTP and Westside waste management facility is shown in Fig. 5.8.

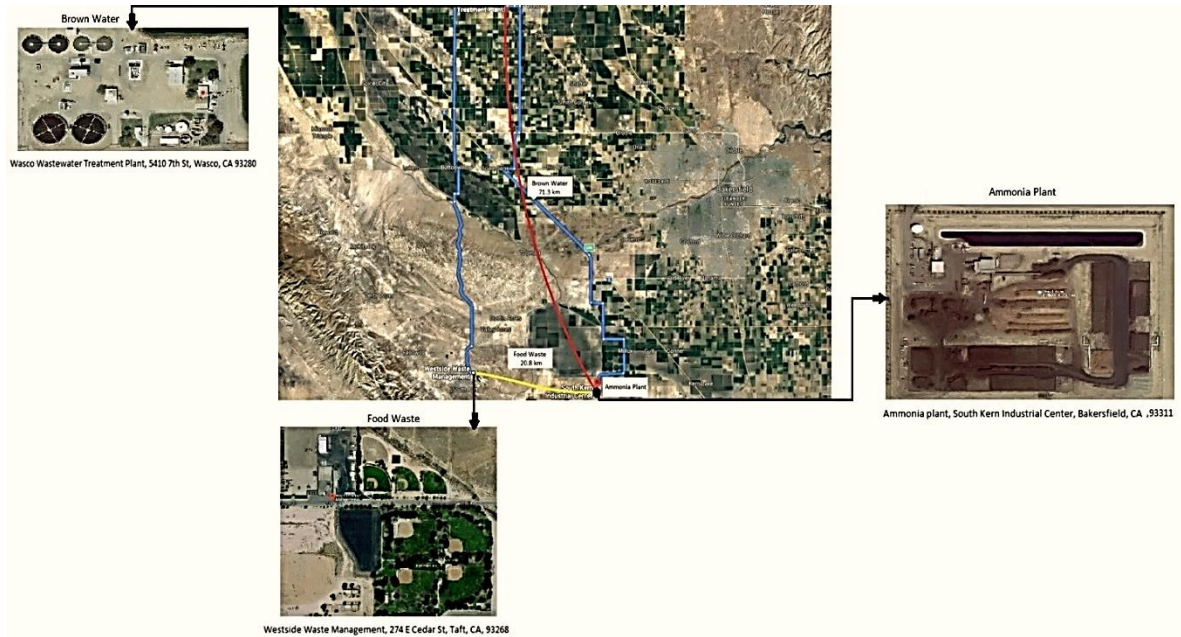


Fig. 5.8: The distance between the ammonia plant in Kern industrial center to both WWTP and waste management facility.

The following data (Fig. 5.9) was obtained from RETScreen software to study the feasibility of adding solar PV or wind power as either an alternative source of power for the proposed plant or to be integrated as a hybrid system. Fig. 5.10 shows the average solar radiation and wind speed for the proposed geographic location.

	Unit	Climate data location		Facility location	Source
Latitude		35.2		35.1	NASA
Longitude		-118.8		-119.2	
Climate zone		4B - Mixed - Dry			NASA - Map
Elevation	m	817		102	NASA
Heating design temperature	°C	-0.6			NASA
Cooling design temperature	°C	32.0			NASA
Earth temperature amplitude	°C	23.8			NASA

Month	Daily solar radiation - horizontal		Atmospheric pressure		Wind speed		Earth temperature		Heating degree-days	Cooling degree-days
	Air temperature °C	Relative humidity %	Precipitation mm	kWh/m ² /d	kPa	m/s	°C	18 °C °C-d	10 °C °C-d	
January	7.1	61.3%	48.67	2.65	92.5	3.0	5.8	338	0	
February	7.9	64.3%	52.92	3.67	92.4	3.1	7.2	283	0	
March	10.1	62.8%	40.30	5.15	92.3	3.1	9.9	245	3	
April	12.8	55.1%	17.70	6.54	92.2	3.4	13.3	156	84	
May	17.2	44.0%	8.37	7.53	92.1	3.4	18.5	25	223	
June	22.0	31.5%	2.40	8.05	92.0	3.2	23.8	0	360	
July	26.2	25.6%	1.86	7.76	92.1	2.7	28.1	0	502	
August	25.8	25.1%	1.24	6.96	92.1	2.5	27.2	0	490	
September	22.6	30.2%	3.60	5.90	92.1	2.5	23.2	0	378	
October	16.6	39.3%	12.40	4.47	92.2	2.6	16.3	43	205	
November	10.5	50.7%	22.50	3.15	92.4	2.9	9.4	225	15	
December	6.8	57.9%	39.99	2.53	92.5	3.0	5.4	347	0	
Annual	15.5	45.5%	251.95	5.37	92.2	3.0	15.7	1,662	2,260	
Source	NASA	NASA	NASA	NASA	NASA	NASA	NASA	NASA	NASA	
Measured at						m	10	0		

Fig. 5.9: Climate data obtained from RETScreen software for the Kern industrial center.

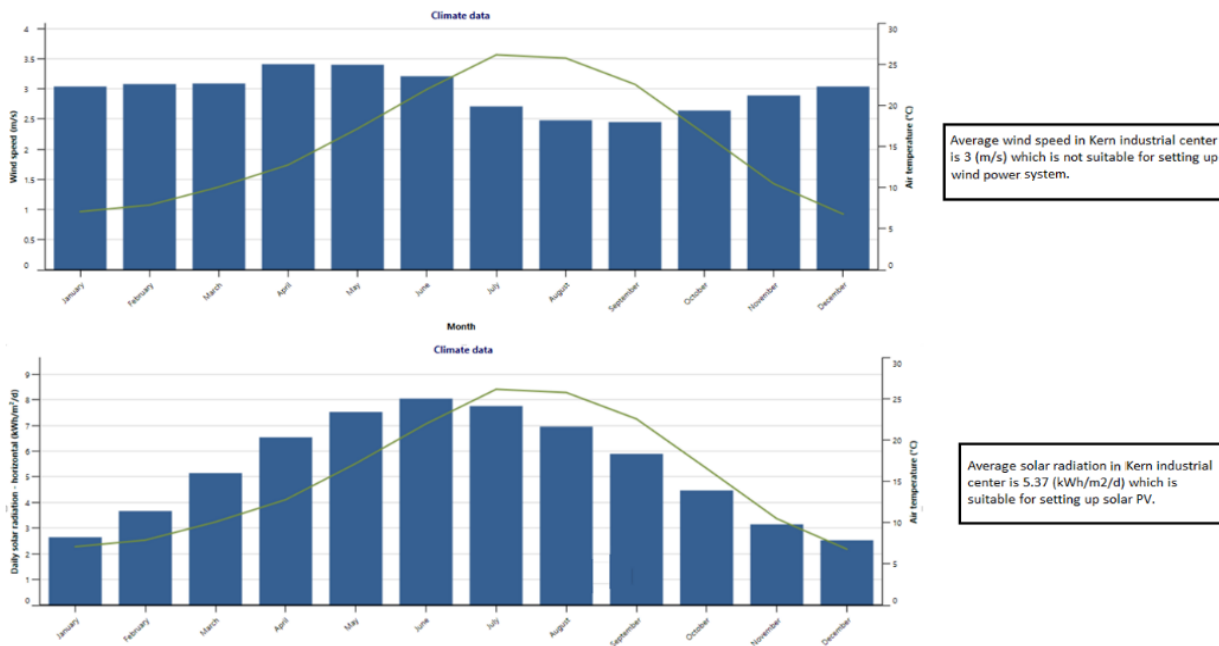


Fig. 5.10: Wind speed and solar radiation throughout a year for a given location (Kern industrial center).

Based on the data obtained from RETScreen software this location is not suitable for setting up wind power (3 m/s), but solar radiation (5.37 kWh/m²/d) is in the acceptable range to use in a hybrid power generation system.

The other ammonia plant located in Tupman is geographically closer to BW and FW suppliers when compared to the Kern industrial center location as shown in Fig. 5.11. Based on the climate data obtained from RETScreen for Tupman location, the solar radiation (5.21 kWh/m²/d) and wind speed (2.9 m/s) characteristics are almost the same as the Kern industrial center which is shown in the Fig. 5.12.

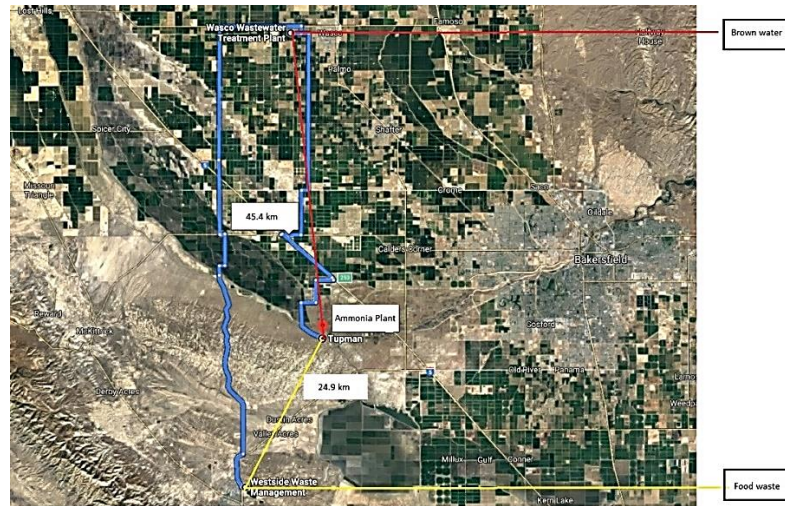


Fig. 5.11: The distance between the ammonia plant in Tupman, California from both WWTP and waste management facility.

	Unit	Climate data location	Facility location	Source
Latitude		35.4	35.3	
Longitude		-119.1	-119.4	
Climate zone		3B - Warm - Dry		
Elevation	m	150	135	Ground+NASA
Heating design temperature	°C	1.6		Ground - Map
Cooling design temperature	°C	38.1		Ground
Earth temperature amplitude	°C	20.9		NASA

Month	Air temperature	Relative humidity	Precipitation	Daily solar radiation - horizontal	Atmospheric pressure	Wind speed	Earth temperature	Heating degree-days 18 °C	Cooling degree-days 10 °C
	°C	%	mm	kWh/m ² /d	kPa	m/s	°C	°C-d	°C-d
January	8.6	79.8%	56.73	2.29	100.3	2.3	7.1	291	0
February	11.5	70.4%	61.32	3.34	100.2	2.7	8.6	182	42
March	14.1	65.3%	46.50	4.65	100.0	2.8	11.4	121	127
April	17.0	53.4%	20.40	6.16	99.8	3.2	14.8	30	210
May	21.5	45.0%	9.61	7.38	99.6	3.4	19.9	0	357
June	25.4	39.7%	2.70	8.05	99.5	3.5	25.2	0	462
July	28.7	38.3%	2.48	7.97	99.5	3.3	29.5	0	580
August	27.8	40.7%	1.55	7.21	99.5	3.1	28.6	0	552
September	24.8	43.5%	4.20	5.93	99.5	2.9	24.6	0	444
October	19.4	50.4%	14.57	4.42	99.8	2.6	17.8	0	291
November	12.5	67.6%	27.00	2.86	100.1	2.3	11.0	165	75
December	8.4	75.8%	47.43	2.11	100.3	2.3	6.8	298	0
Annual	18.3	55.8%	294.49	5.21	99.8	2.9	17.2	1,087	3,140
Source	Ground	Ground	NASA	Ground	Ground	Ground	NASA	Ground	Ground
Measured at					m	10	0		

Fig. 5.12: Climate data obtained from RETScreen software for the Tupman location.

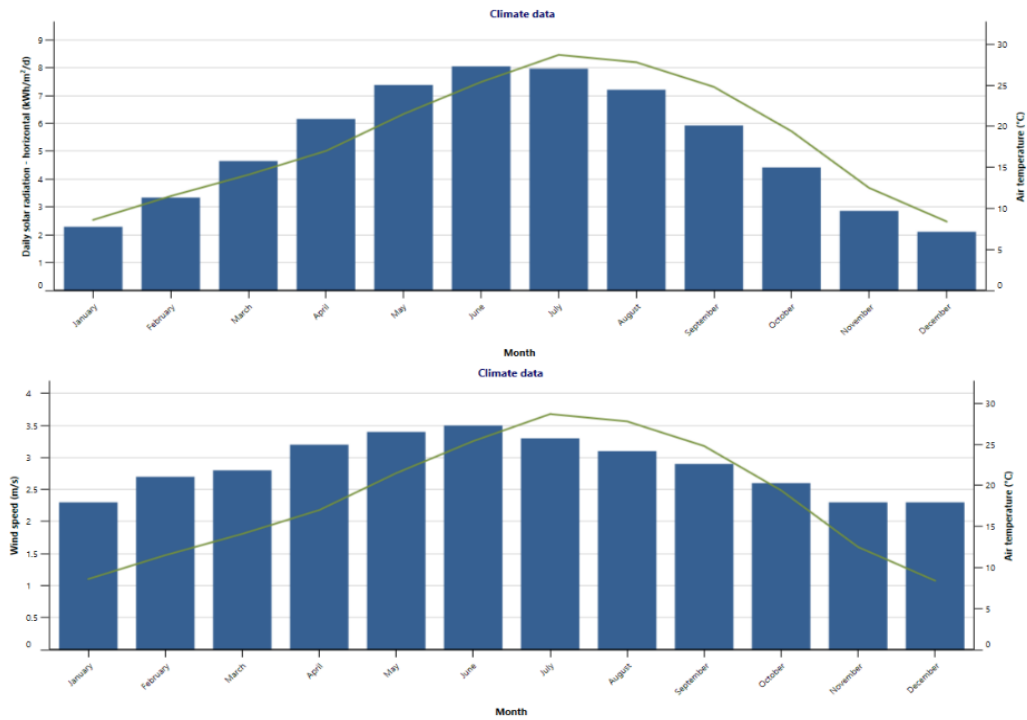


Fig. 5.13: Wind speed and solar radiation throughout a year for a given location (Tupman).

Calculations are based on the solar panel specifications (solar radiation, efficiency, and PV array size) for the process demand of 17 MW, located in the city of Bakersfield, California, with the latitude and longitude of 35.37, -119.02 respectively. Photovoltaic (PV) array sizes range from under 300 m² to over 800 m² based on efficiency and solar irradiance. The system is modelled with a PV array size of 4401.705 m² for a 570kW installed capacity using a modified library process for solar electricity. The impact of using wind as the primary electricity source was assessed, as was the impact of using grid electricity, to allow for consideration in situations where this plant is employed in other geographic locations where wind power works effectively (wind speed is in an acceptable range 30-55 mph) and solar radiation is not in an acceptable range (<6 kWh/m²/day) (NWW, 2005; U.S. Department of Energy's FEMP, 2017).

5.1.1.7 Library processes

Table 5.4 shows the list of library processes used from ecoinvent for conducting the LCA for this study. The last two items, for solar PV and SOFC were modified to fit this system. For solar, the PV mounting system and panel calculations and for the SOFC, composition materials using proxy background data based on monolayer calculations were modified (detailed calculations can be found in *Chapter 6*).

Table 5.4: Library processes used for ammonia production model.

Library process used (from ecoinvent 3.6)
Electricity, medium voltage {WECC, US only} electricity voltage transformation from high to medium voltage Cut-off, U
Electricity, low voltage {RoW} electricity production, photovoltaic, 3kWp flat-roof installation, single-Si Cut-off, U
Water, deionised, from tap water, at user {RoW} production Cut-off, U
Tap water {GLO} market group for Cut-off, U
Sodium hydroxide, without water, in 50% solution state {GLO} market for Cut-off, U
Transport, freight, lorry with refrigeration machine, 7.5-16 ton, EURO3, carbon dioxide, liquid refrigerant, cooling {GLO} Cut-off, U
Urea, as N {RoW} production Cut-off, U
Compost {RoW} treatment of biowaste, industrial composting Cut-off, U
Sulfur {GLO} market for Cut-off, U
Electricity, medium voltage {WECC, US only} market for Cut-off, U
Electricity, high voltage {WECC, US only} electricity production, wind, <1MW turbine, onshore Cut-off, U
Lanthanum oxide {GLO} market for Cut-off, U
Activated carbon, granular {RoW} activated carbon production, granular from hard coal Cut-off, U
Platinum {GLO} market for Cut-off, U
*Modified Solar Electricity, low voltage {WECC, US only} electricity production, photovoltaic, 570kWp open ground installation, multi-Si Cut-off, U
*New SOFC Modified Heat, future {GLO} Hydrogen, burned in solid oxide fuel cell, with micro gas turbine, 180kWe, future Cut-off, U

*Modified

5.1.1.8 Data quality and uncertainty

Table 5.5 shows the uncertainty characteristics used for various inventory components, based on data quality estimates. For the estimation of default uncertainty distributions and parameters of values from flow data and their related processes, pedigree matrices are used. In the pedigree matrix approach, expert judgement is used to determine the uncertainty factors rather than empirical variability data. For the developmental technologies created here, three different pedigree matrices were used depending on the degree of speculativeness (new, lab, and pre-pilot stage) and/or maturity (more established components). The values for material and energy inputs have a relatively narrow left skewed uncertainty, while output yields of mature technology (e.g., urea production) are less narrow because they reflect the uncertainty in the modelling. Finally, a broader distribution is applied for output yields for technologies under development (e.g., ammonia). Uncertainty for the nitrous oxide (N₂O) leakage rates is treated with a pedigree matrix rather than a uniform distribution like the other leakages because it is a value derived from the modelled quantity where it has a mechanistic process of conversion to N₂O prior to release. The background processes, taken from the ecoinvent library, also use the pedigree approach, with matrices assigned to parameters within each library process.

Table 5.5: Data quality characteristics of inventory parameters.

Uncertainty based on pedigree matrix				Uncertainty based on distribution
Pedigree matrix	(3,1,1,1,1)	(4,1,1,1,4)	(4,1,1,1,5)	Uniform
SD/2SD	1.11	1.56	2.05	N. A
Inventory components	-Material inputs (waste stream and water) - N ₂ O leakage rate	- Urea daily output flow rate -Electricity demand -CO ₂ emissions -Array incidence	- Daily output flow rate for ammonia and by-products -Number of membrane cells and tubes	-NH ₃ and CO ₂ leakage rates -CH ₄ leakage rate -Distance travelled from collection facility to the plant

Uncertainty analysis

An uncertainty analysis was carried out in order to identify the range of possible values of the impact categories evaluated in this study. Monte Carlo simulations with 3,000 steps were run for all of the technologies and scenarios, and their substituent parts, to assess distinguishability of technology scenarios and major contributors to uncertainty for the primary impact assessment methods. In order to confirm convergence, simulations were run with 1,000, 2,000, 4,000 and 5,000 steps for both two-stage and AD-only for the base case and urea production scenario sets without using SOFC.

After an initial series of uncertainty analyses, in which the extremely high responsiveness to leakage overwhelmed all other factors, leakage rates were treated as fixed values in the uncertainty analysis and assessed via sensitivity analysis.

5.1.1.9 Sensitivity analysis

Sensitivity analyses were performed to determine which input variables may substantially change the results of the analysis. As the proposed production processes in this study are comprised of different magnitudes of energy and material inputs, gas leakage, product yields, water use, and distance from waste hub to the facility, it is important to determine which of these variables have the most effect on the proposed processes and whether this could change the relative performance rankings. Parameters assessed in the sensitivity analyses include: leakages (CH₄, CO₂, N₂O, and NH₃), input feedstock, gross energy demand for ammonia and urea production, electricity supplied from SOFC, injection energy use, ammonia and urea production yields, distance of transportation for both FW and BW, dilution water and DI water for CH₄ assisted-SOFEC. Each parameter is varied independently by \mp 5% and 10% from the base case to see the effect in the results. Each parameter was changed independently in order to assess the magnitude of its effect on the base case. The sensitivity analyses were carried out using IPCC GWP 100a, ReCiPe 2016 endpoint (H), and AWARE impact assessment methods.

Conclusion

The ammonia production technologies are assessed for environmental performance from cradle-to-gate using two configurations, four CO₂ fates, including use for urea production, and several smaller variations, resulting in 72 assessed processes. Carbon dioxide capture and utilization provides a valuable route to additional valuable products while avoiding direct release of CO₂ emissions, where those products are able to displace their high impact, fossil derived analogues.

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Chapter 6

Results and Discussion

for

The Life Cycle Assessment

This chapter discusses the results obtained from the contribution, comparative, uncertainty, and sensitivity analyses. The results are based on solar as the main source of power with coproduct credits for sulfur and compost and using mass allocation, avoided product, and the unallocated process per tonne of processed input waste as indicated. The importance of electricity supply to the studied technologies and the effect of changing the source of electricity on the results were assessed in the contribution analysis. The effect of leakage was also assessed in the contribution and treated as fixed values in the uncertainty and assessed via sensitivity analysis.

This chapter was drafted based on the publication submitted to the journal of cleaner production:

Ghavam, S., Taylor, C.M. and Styring, P., (2021). The life cycle environmental impacts of a novel sustainable ammonia production process from food waste and brown water. *Journal of Cleaner Production* [online]. 320, 128776. [Viewed 22 September 2021]. Available from: <https://doi.org/10.1016/j.jclepro.2021.128776>.

6. Results and discussion

Results in the contribution, comparison, uncertainty, and sensitivity analyses presented below are based on the parameters in Table 5.3, with a combination of FW and BW, using solar power and SOFC, with coproduct credits for sulfur and compost and either mass allocation, avoided product for urea, and per tonne of processed waste (unallocated) as indicated. Unless otherwise stated, the results shown include leakage.

6.1 Comparative analysis

Figs 6.1, 6.2, and 6.3 show the impacts associated with ammonia produced through the waste-based process for different carbon fates. The fate of the waste CO₂ stream is the primary determinant in relative performance for all impact categories. The additional urea product carries a share of the impacts, reducing the burden associated with ammonia – (mass allocation) shown in Fig. 6.1 and 6.2. When system expansion is used and the green urea product displaces conventional urea, the decreased ammonia impacts are dramatic. All of the calculations are relative to the FU of the reference product, in this case 1 kg NH₃, therefore, the impact in resources has almost the same trend for CC(u) and base case except for CCS and the urea case. Amongst non-urea cases, CCS has a higher impact for the resources damage which reflects the energy use for injection into the ground (Fig. 6.2c). For this damage category the results for AD and DF+AD are relatively similar for each carbon fate case.

As can be seen in Fig. 6.1 and 6.2, ammonia produced using the AD-only process has higher GHG emissions and impact on ecosystems, human health, and resources compared to the two-stage (DF+AD). Leakage is the largest contributor to different life cycle impacts in the two core technologies (AD-only and DF+AD). This is more evident for GHG emissions compared to the three other damage categories, while the impacts from AD-only and DF+AD are non-negligible in ecosystem and human health impact categories. However, the aggregated damage values show very little difference between the two core technologies. The distinction between AD-only and DF+AD is more visible for GWP. Both the AD-only and the two-stage processes result in very similar GHG emissions, ecosystems, and human health impacts in almost all carbon fates, except for the resources damage in which the impact is higher in non-urea cases, specifically for the CCS.

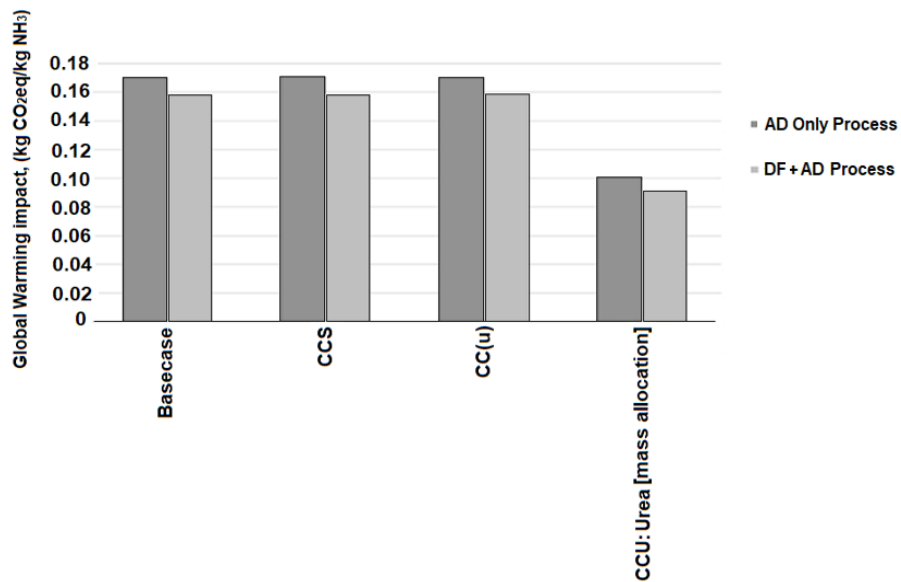


Fig. 6.1: GHG impacts of waste-to-ammonia and ammonia+urea processes for all CO₂ fates for both AD-only and two-stage (DF+AD technologies) via the default (with SOFC) configurations using mass allocation with leakage impacts included (Impact assessment method: IPCC 2013 GWP 100a).

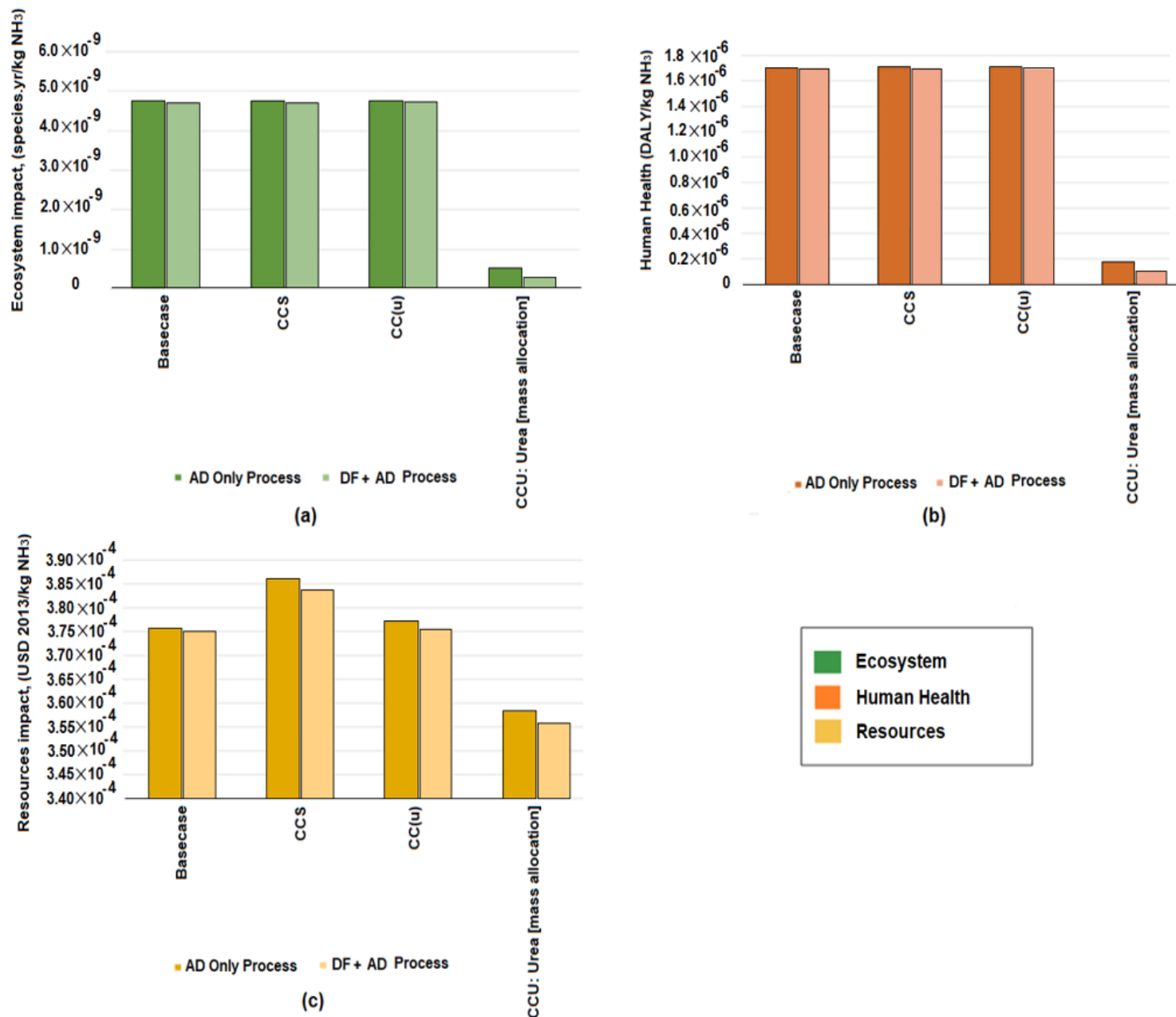


Fig. 6.2: Damage impacts of waste-to-ammonia and ammonia+urea processes for all CO₂ fates for both AD-only and two-stage (DF+AD technologies) via the default (with SOFC) configurations using mass allocation with leakage impacts included (a) Ecosystem, (b) Human Health, and (c) Resources (Impact assessment method: ReCiPe 2016 endpoint H/A).

As shown in Fig. 6.3, the impact of water consumption (dilution and DI water) is higher in AD-only process compared to the DF+AD, this is due to higher water consumption in AD-only compared to the two-stage. As urea is produced, its byproduct water which is reclaimed to be utilized for dilution, reduces the consumption of external sources of water. This will result in lower impact for the scenario set where urea is produced compared to non-urea cases.

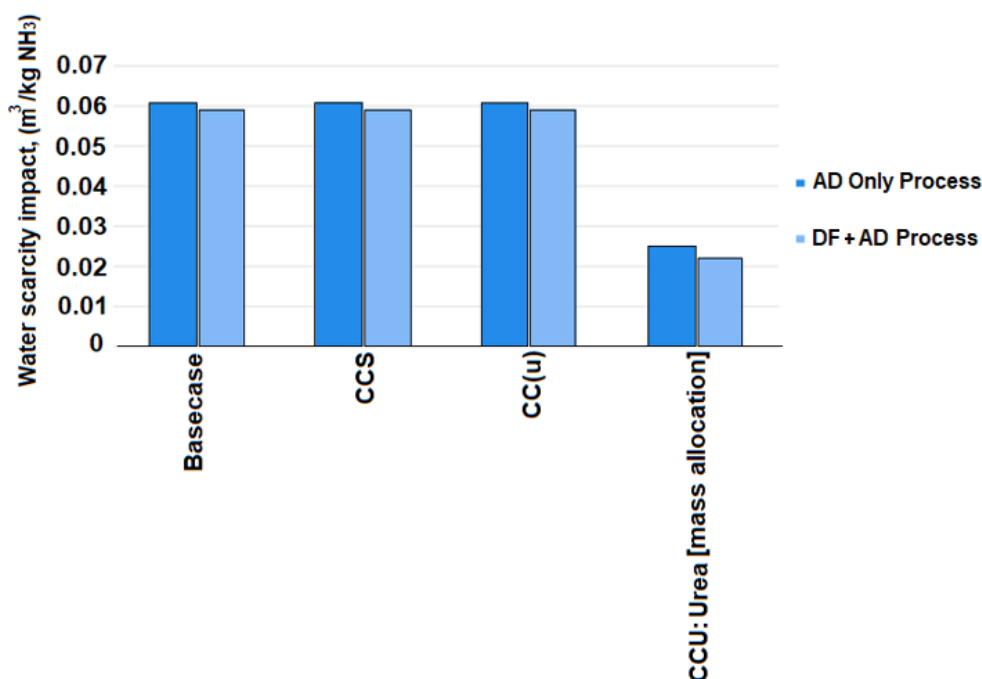


Fig. 6.3: Water scarcity impacts of waste-to-ammonia and ammonia+urea processes for all CO₂ fates for both AD-only and two-stage (DF+AD technologies) via the default (with SOFC) configurations using mass allocation with leakage impacts included (Impact assessment method: AWARE).

6.2 Contribution analysis

The contributions to the life cycle environmental impacts for the production of ammonia/ammonia+urea from the co-digestion of FW and BW for all CO₂ fates for both AD-only and two stage (DF+AD technologies) are shown in Figs 6.4 -6.17 and Table 6.1-6.5. The results include the life cycle GHG emissions, human health, ecosystem, resources damage, and water scarcity. The contribution analysis results using both IPCC 2013 GWP 100a and ReCiPe 2016 endpoint H/A impact assessment methods for all CO₂ fates for both technologies are provided in Appendix C.

The comparison of the results for all proposed green ammonia processes show that leakage is the highest contributor to all impact categories shown in Figs 6.4a, 6.8a, 6.9a, 6.14a, 6.15a, and 6.16a except for the resources damage.

6.2.1 Contribution results for the GHG impacts (GWP₁₀₀)

Leakage is overwhelmingly the largest contributor to GHG impacts (Fig.6.4, panel a), once the leakage is removed (Fig. 6.4, panel b), the second largest contributor to global warming is electricity consumption followed by transportation from waste hub to the ammonia plant. The impact drivers mentioned are assessed in the contribution analysis and tested in the sensitivity analysis. The results point to the significance of electricity in the proposed

processes, especially in cases where urea is produced, the electricity dominates the impact in the contribution analysis compared to the non-urea cases.

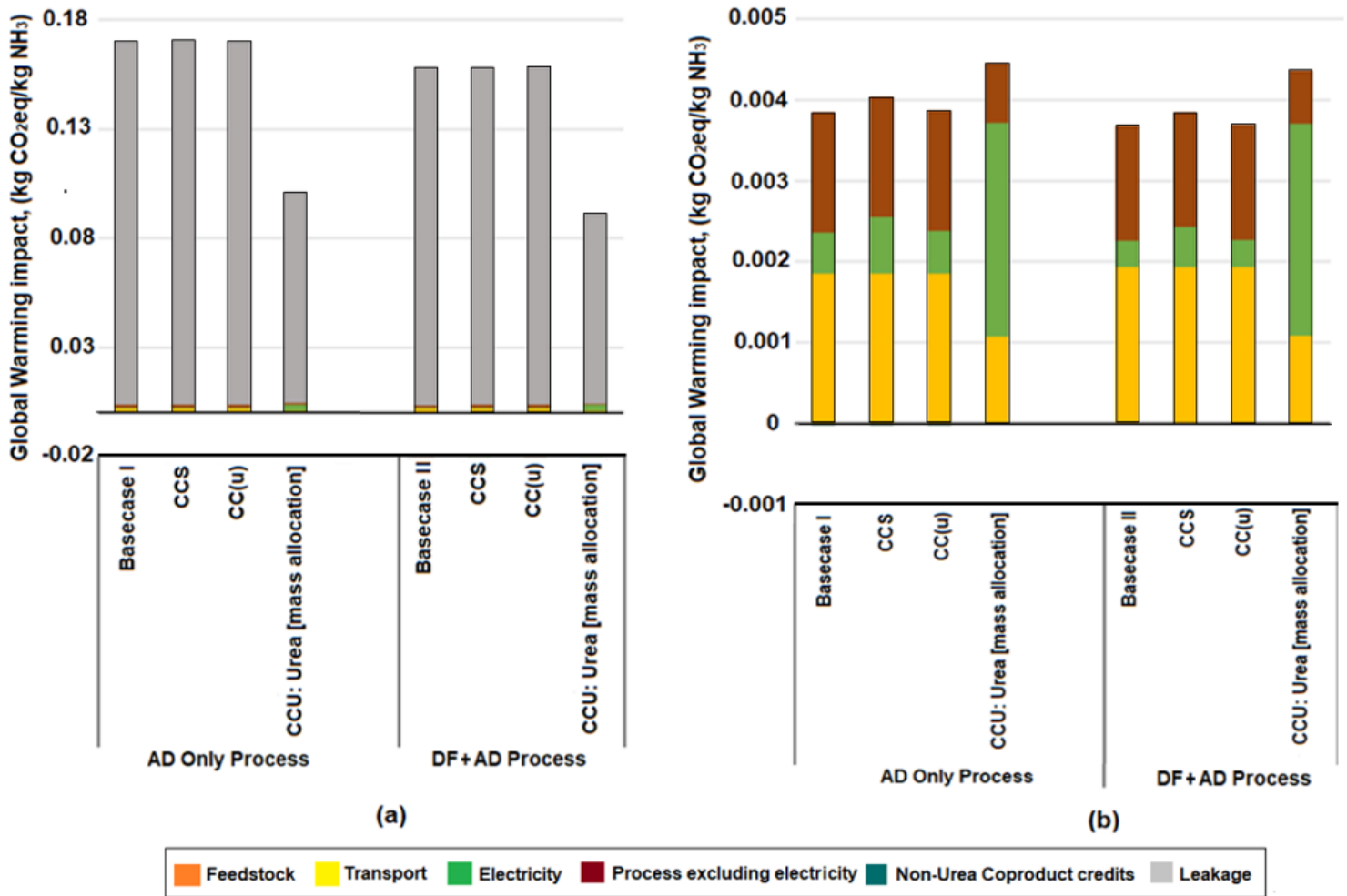


Fig. 6.4: GHG impacts of waste-to-ammonia and ammonia+urea processes for all CO₂ fates for both AD-only and two-stage (DF+AD technologies) via the default configurations (with solar energy and SOFC) using mass allocation (a) leakage impacts included (b) leakage impacts excluded (Impact assessment method: IPCC 2013 GWP 100a).

6.2.1.1 Impact of emerging membranes incorporated into the modelled process

Despite being a crucial component of the technology, the composition of the membranes has a negligible effect on the impact (Fig. 6.5). The results indicate that impacts for the modelled technologies are non-responsive to the production impacts of these membranes and their components (Fig. 6.5 inset), however, their performance with low energy draw directly contributes to the relative benefit of this technology over alternatives.

The membranes make a very small direct contribution to the system impacts, this has been clearly demonstrated in Table 6.1. The newness of the membranes utilized in the modelled technology contributes to a high level of speculativeness of the membranes utilized in the studied process. Lifetime, performance, and detailed composition of membranes all have significant uncertainty (section 6.5). The composition materials breakdown for each membrane, electrolyzer, and fuel cell incorporated into the modelled system along with their impacts using IPCC 2013 GWP 100a and the results of the calculations using proxy background data based on modified monolayer calculations are shown in Table 6.1. The materials in the cell/tube were used for the membrane calculations. Each membrane was treated as consisting entirely of the active materials and their quantities calculated based on membrane area and thickness. Global market processes from the ecoinvent library were used for each membrane material. Where possible, the exact material was used, and the most similar options based on chemistry and production routes were selected from the available library materials for those without an exact match. The membranes make a very small direct contribution to the system impacts. The main determinant of their contribution is their estimated lifetime of 10 years (based on this study's analogy to other similar materials and data) (Ramsden, 2013). The effect of time to replacement was assessed via sensitivity analysis. Even if replacement were to be required annually, the membrane production and disposal contribution to impact remains insignificant, even in the absence of leakage.

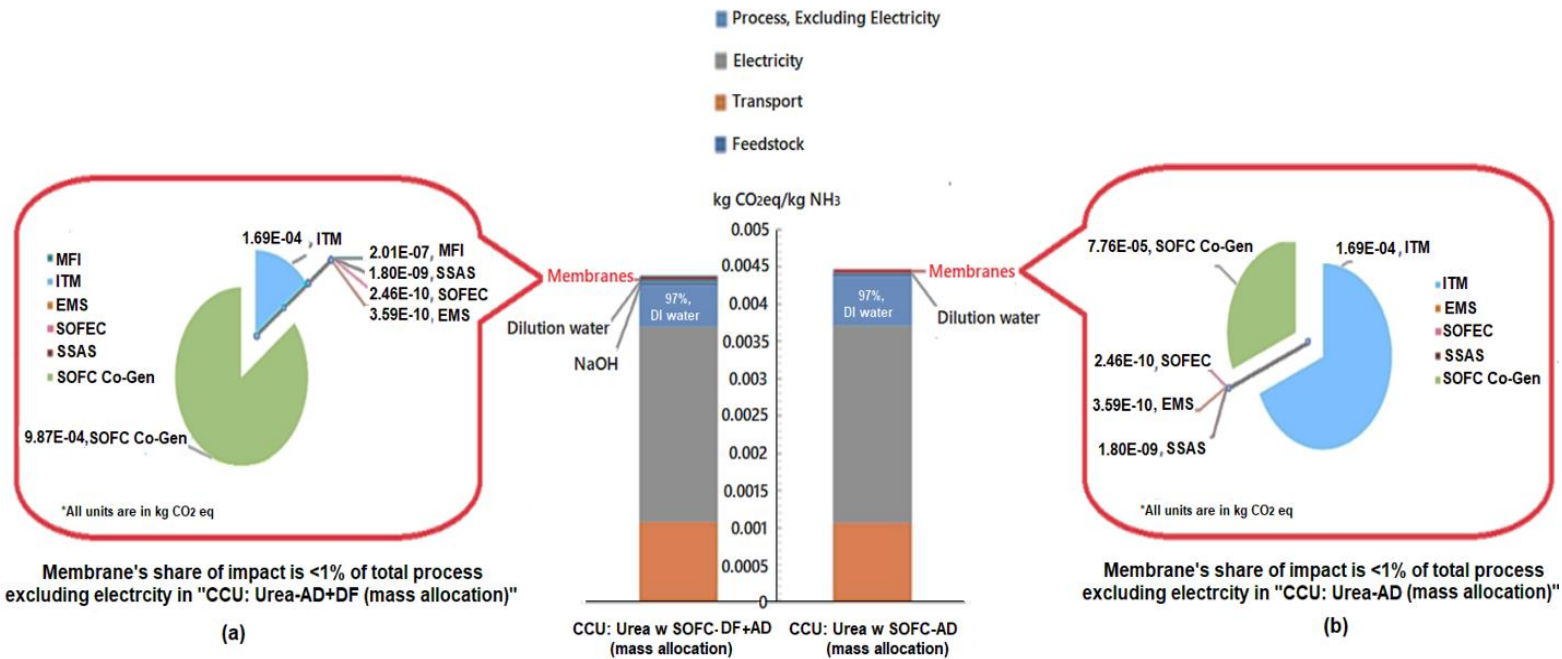


Fig. 6.5: Each membrane's share of impact for both AD-only and two-stage (DF+AD technologies) using mass allocation for urea case with SOFC and with leakage impacts excluded (a) DF+AD and (b) AD-only process (Impact assessment method: IPCC 2013 GWP 100a).

Table 6.1: The composition material and the results of the monolayer calculations used for different membranes, electrolyzer, and fuel cell incorporated into the modelled process (Impact assessment method: IPCC 2013 GWP 100a).

DF+AD process					
Impact category	Unit	Processing Unit	Membrane Composition	Value	Total
IPCC GWP 100a	kg CO ₂ eq/kg NH ₃	MFI_tube	Zeolite, powder {GLO} market for Cut-off, U	2.01E-07	2.01E-07
		ITM_Tube_Proxy	Lanthanum oxide {GLO} market for Cut-off, U	1.60E-07	
		EMS_Cell_Proxy	Platinum {GLO} market for Cut-off, U	1.69E-04	3.59E-10
			Activated carbon, granular [RoW] activated carbon production, granular from hard coal Cut-off, U	1.29E-10	
		SOFEC_Cell_Proxy	Lanthanum oxide {GLO} market for Cut-off, U	1.44E-10	2.46E-10
			Nickel, 99.5% {GLO} market for Cut-off, U	1.02E-10	
		SSAS_Cell_Proxy	Lanthanum oxide {GLO} market for Cut-off, U	1.12E-12	1.81E-09
			Rhodium {GLO} market for Cut-off, U	1.80E-09	
		SOFC Co-Gen, using new SOFC, electricity with heat	New SOFC Modified Electricity, low voltage {GLO} hydrogen, burned in solid oxide fuel cell, with micro gas turbine, 180kWe, future Cut-off, U	9.54E-04	9.87E-04
			New SOFC Modified Heat, future {GLO} hydrogen, burned in solid oxide fuel cell, with micro gas turbine, 180kWe, future Cut-off, U	3.26E-05	
AD-only process					
Impact category	Unit	Processing Unit	Membrane Composition	Value	Total
		ITM_Tube_Proxy	Lanthanum oxide {GLO} market for Cut-off, U	1.60E-07	0.000169
			Platinum {GLO} market for Cut-off, U	1.69E-04	
		EMS_Cell_Proxy	Lanthanum oxide {GLO} market for Cut-off, U	2.30E-10	3.59E-10
			Activated carbon, granular [RoW] activated carbon production, granular from hard coal Cut-off, U	1.29E-10	

IPCC GWP 100a	kg CO ₂ eq/kg NH ₃	SOFEC_Cell_Proxy	Lanthanum oxide {GLO} market for Cut-off, U	1.44E-10	2.46E-10
			Nickel, 99.5% {GLO} market for Cut-off, U	1.02E-10	
		SSAS_Cell_Proxy	Lanthanum oxide {GLO} market for Cut-off, U	1.12E-12	1.81E-09
			Rhodium {GLO} market for Cut-off, U	1.80E-09	
		SOFC Co-Gen, using new SOFC, electricity with heat	New SOFC Modified Electricity, low voltage {GLO} hydrogen, burned in solid oxide fuel cell, with micro gas turbine, 180kWe, future Cut-off, U	4.50E-05	7.75E-05
			New SOFC Modified Heat, future {GLO} hydrogen, burned in solid oxide fuel cell, with micro gas turbine, 180kWe, future Cut-off, U	3.26E-05	

6.2.1.2 Electricity supply scenarios

Fig. 6.6 demonstrates the importance of electricity supply to the studied technologies and the effect of changing the source of electricity on the results. This figure shows different configurations in which some of the energy is generated internally based on resource availability within the process, while prioritizing ammonia and urea. It clearly shows that the source of electricity does not have an effect on the non-urea cases compared to the urea production ones.

The effect of changing the primary source of energy for the studied processes from solar to wind on all impact categories (ecosystem, resources, human health, and GWP₁₀₀) is relatively similar, however, switching from renewable to fossil-based (grid) energy, leads to visible changes in the following impact categories. This especially applies to resources damage followed by GWP impacts for the CCU cases (Fig.6.6b). This is due to the fact that urea production processes are energy intensive, in addition, the impact of changing the source of energy, on both human health and ecosystem is relatively similar.

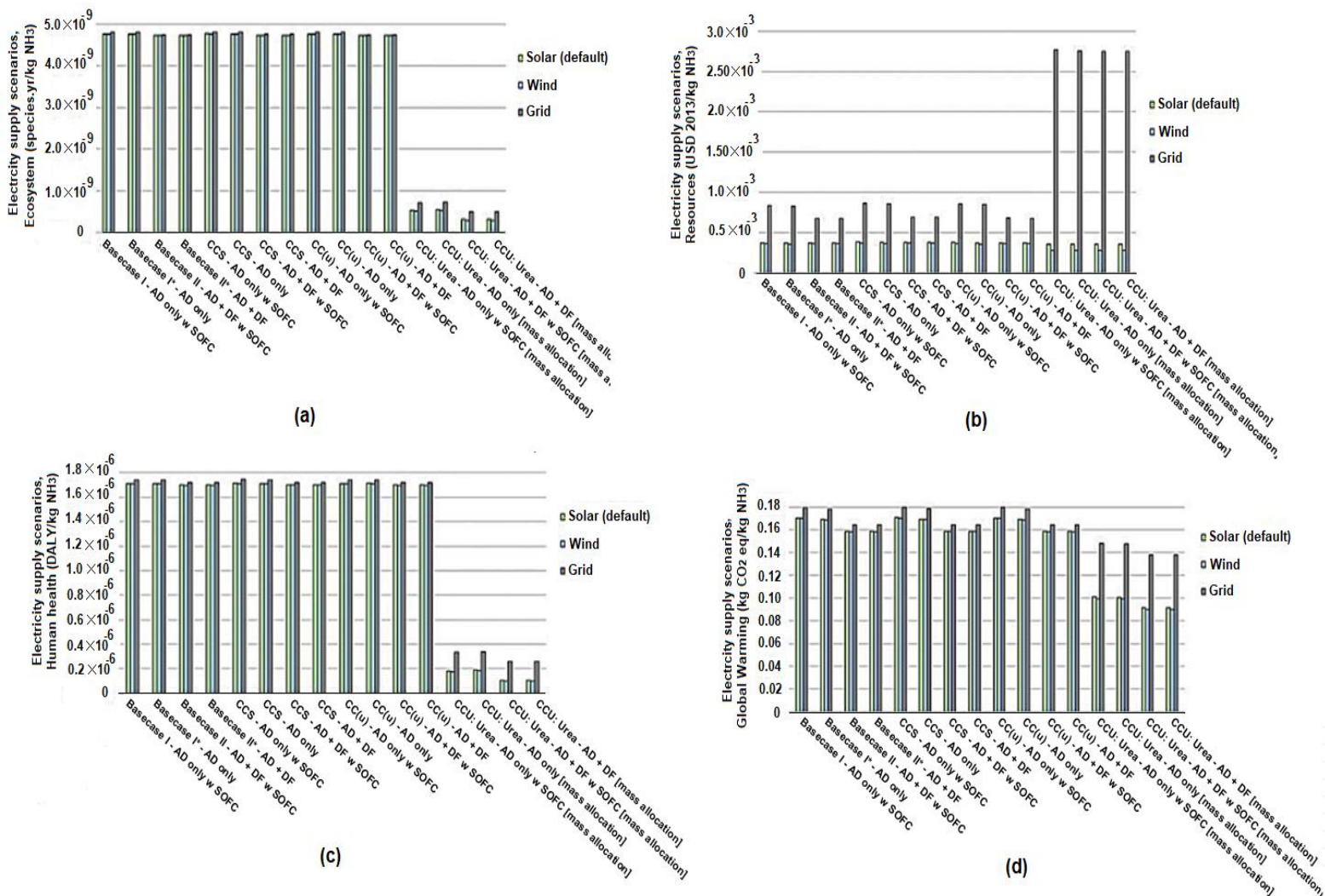
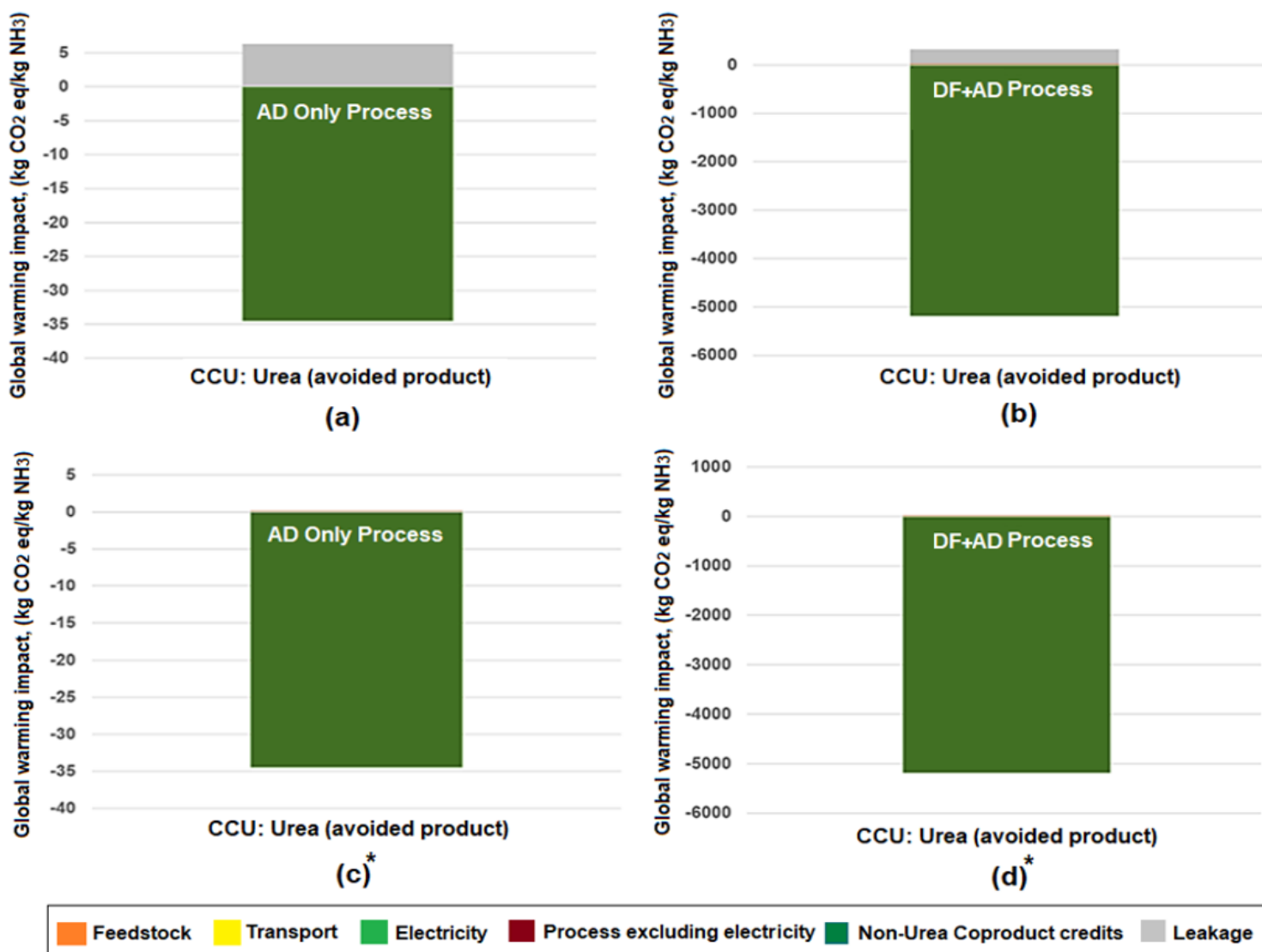


Fig. 6.6: Electricity supply scenarios of waste-to-ammonia and ammonia+urea processes for all CO₂ fates for both AD-only and two-stage (DF+AD technologies) using mass allocation with leakage impacts included (a) Ecosystem (b) Resources (c) Human health, using ReCiPe 2016 endpoint H/A and (d) GHG emissions, using IPCC 2013 GWP 100a.

6.2.1.3 Avoided product

The ammonia impacts with system expansion used to account for urea production is shown in Fig. 6.7. The magnitude of credit from the avoided production of conventional, fossil-based urea is almost three thousand-fold larger than the ammonia impacts using mass allocation, which emphasizes the importance of offsetting urea production in this system. This holds for both two-stage and AD-only processes and is independent of leakage inclusion. However, the higher urea yield for the two-stage technology results in a larger avoided product credit for that route. The benefit of shifting from conventional fossil-based urea production processes to biogenic routes such as the one presented in this study is dramatic. Since the urea credit overwhelms the contribution from all process categories (feedstock, transportation, electricity, process excluding electricity, leakage, and co-product credits) assessed in this study, the rest of the results are shown for mass allocation.



*Without leakage

Fig. 6.7: GHG impacts of waste-to-ammonia and ammonia+urea processes using system expansion and avoided products for urea and other coproducts (a) AD-only process including the impacts from leakage, (b) DF+AD process including the impacts from leakage, (c) AD-only process excluding the contribution from leakage, and (d) DF+AD process excluding the contribution from leakage (Impact assessment method: IPCC 2013 GWP 100a).

6.2.2 Contribution results for the non-GHG impacts (damage categories)

The largest contributors to ecosystem and human health for non-urea cases, after leakage (ammonia followed by methane leakage), are electricity and transportation, respectively. As transportation is the largest contributor to the impact from resources damage and due to urea being the avoided product (along with ammonia as the primary product) for this scenario set, the impact from transportation is smaller, resulting in a lower impact for the resources damage compared to non-urea cases. The two damage categories (ecosystem and human health) have almost the same contribution as the other categories (Fig. 6.8 and 6.9). Ammonia is the largest contributor to leakage in non-urea cases followed by methane leakage, while in urea cases, the highest impact comes from methane leakage.

However, in the resources damage category, the impact of transportation is the highest due to the use of petroleum followed by electricity in both urea and non-urea cases (Fig. 6.10).

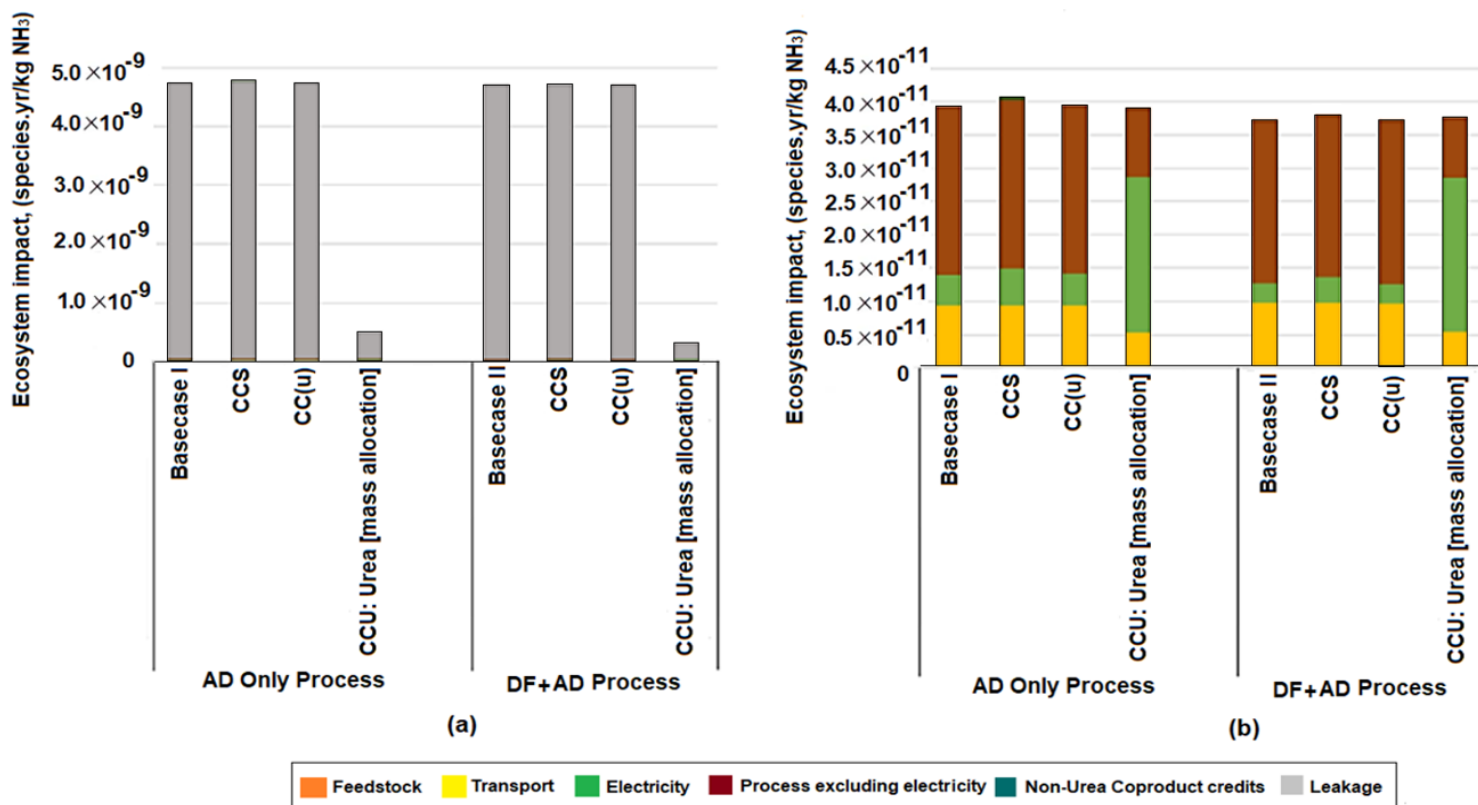


Fig. 6.8: Ecosystem impacts of waste-to-ammonia and ammonia+urea processes for all CO₂ fates for both AD-only and two-stage (DF+AD technologies) via the default (with SOFC) configurations using mass allocation (a) leakage impacts included (b) leakage impacts excluded (Impact assessment method: ReCiPe 2016 endpoint H/A).

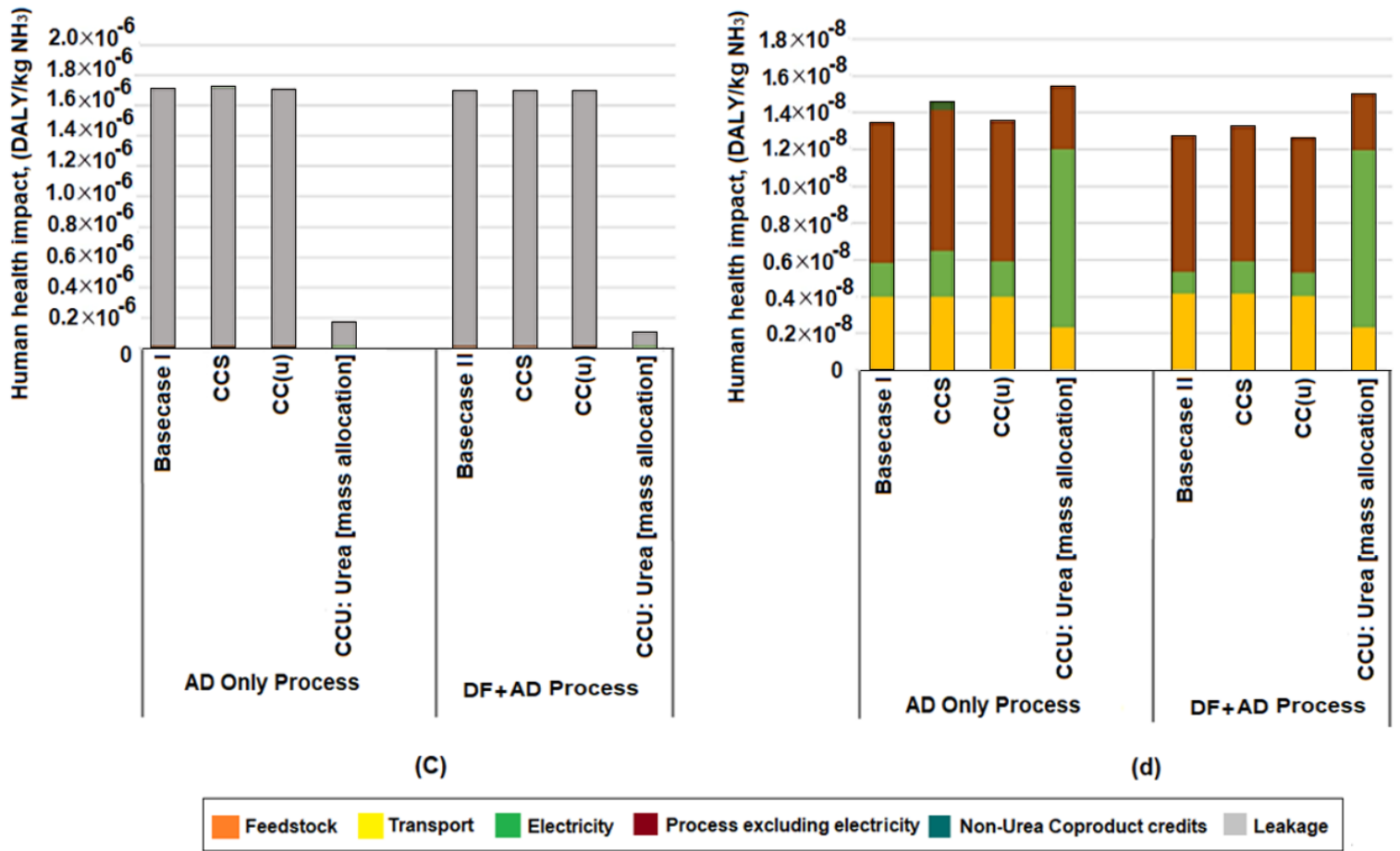


Fig. 6.9: Human health impacts of waste-to-ammonia and ammonia+urea processes for all CO₂ fates for both AD-only and two-stage (DF+AD technologies) via the default (with SOFC) configurations using mass allocation (c) leakage impacts included (d) leakage impacts excluded (Impact assessment method: ReCiPe 2016 endpoint H/A).

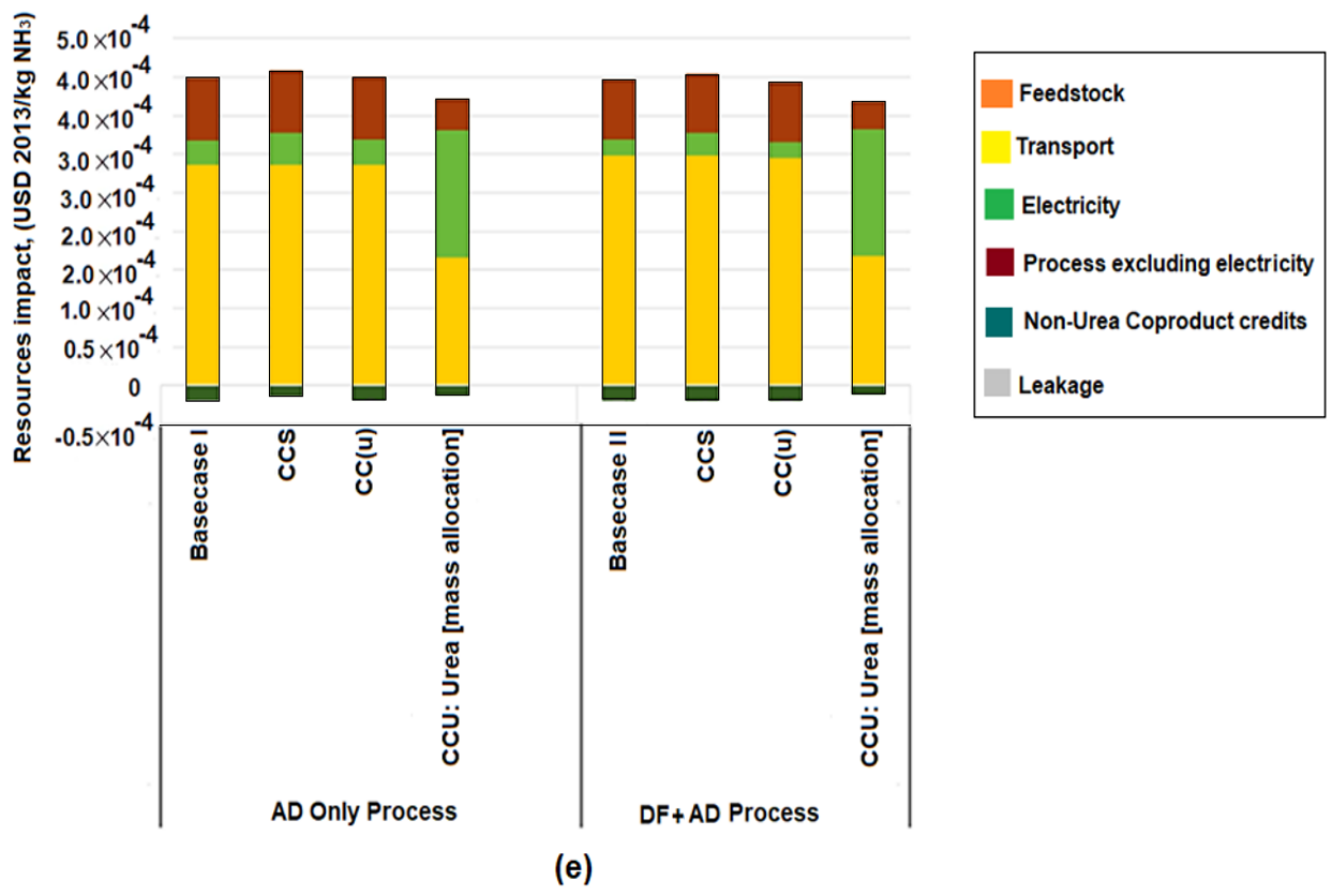
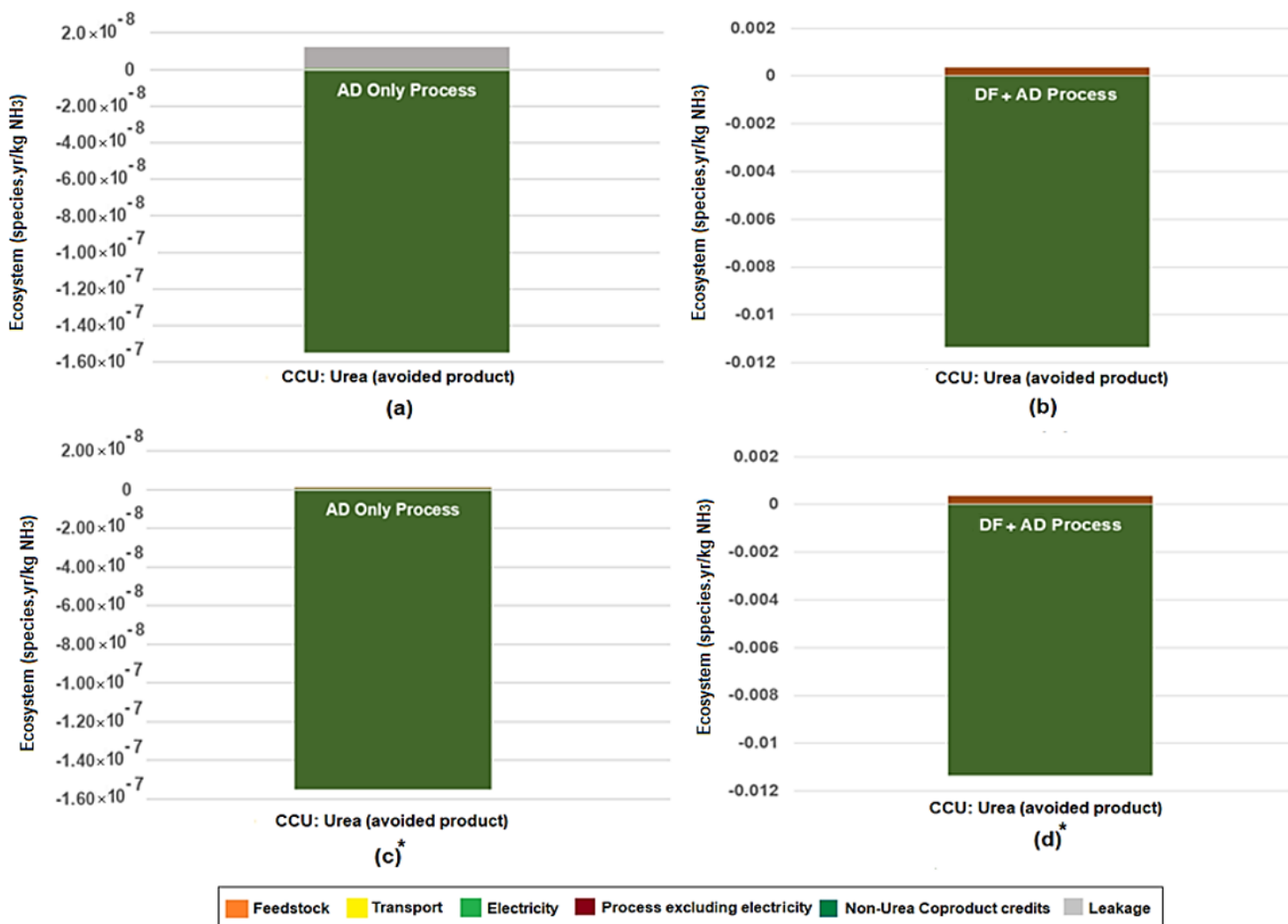


Fig. 6.10: Resources impacts of waste-to-ammonia and ammonia+urea processes for all CO₂ fates for both AD-only and two-stage (DF+AD technologies) via the default (with SOFC) configurations using mass allocation with leakage impacts included (Impact assessment method: ReCiPe 2016 endpoint H/A).

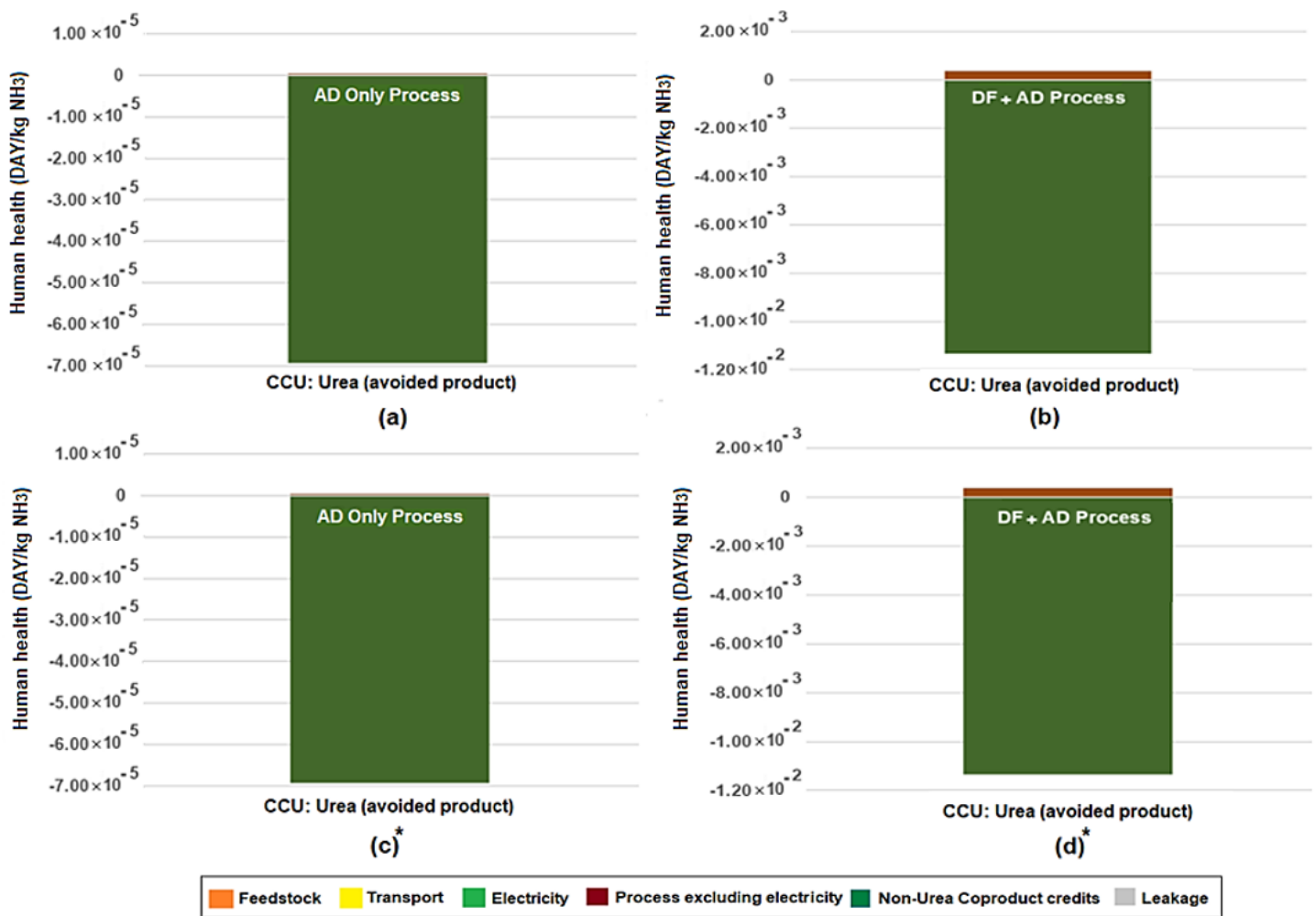
6.2.2.1 LCA results with system expansion for urea (conventional urea as avoided product) using ReCiPe 2016 endpoint H/A impact assessment method

The ammonia impacts with system expansion used to account for urea production in non GHG impact categories are the same as in GHG impact assessment method and are shown in Figs. 6.11- 6.13.



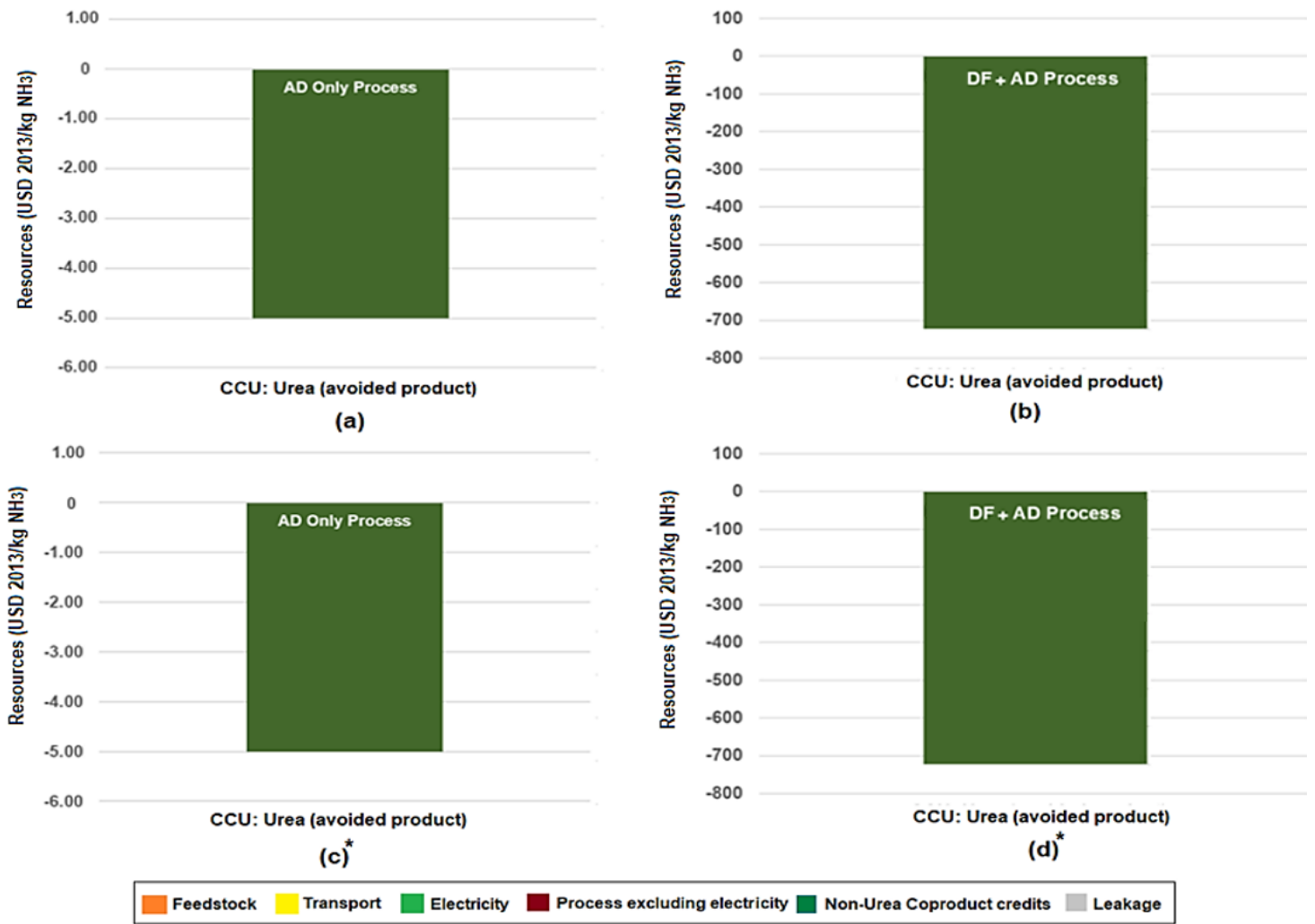
**Without leakage*

Fig. 6.11: Ecosystem impacts of waste-to-ammonia and ammonia+urea processes using system expansion and avoided products for urea and other coproducts (a) AD-only process including the impacts from leakage, (b) DF+DF process including the impacts from leakage, (c) AD-only process excluding the contribution from leakage, and (d) DF+AD process excluding the contribution from leakage (Impact assessment method: ReCiPe 2016 endpoint H/A).



*Without leakage

Fig. 6.12: Human health impacts of waste-to-ammonia and ammonia+urea processes using system expansion and avoided products for urea and other coproducts (a) AD-only process including the impacts from leakage, (b) DF+AD process including the impacts from leakage, (c) AD-only process excluding the contribution from leakage, and (d) DF+AD process excluding the contribution from leakage (Impact assessment method: ReCiPe 2016 endpoint H/A).



*Without leakage

Fig. 6.13: Resources impacts of waste-to-ammonia and ammonia+urea processes using system expansion and avoided products for urea and other coproducts (a) AD-only process including the impacts from leakage, (b) DF+AD process including the impacts from leakage, (c) AD-only process excluding the contribution from leakage, and (d) DF+AD process excluding the contribution from leakage (Impact assessment method: ReCiPe 2016 endpoint H/A).

6.2.3 Contribution results for GHG and non-GHG impacts per tonne of processed waste (unallocated)

Figs 6.14- 6.17 shows the results of the impact from processing one tonne of waste based on various CO₂ fates and whether there are any credits for green urea production to offset the conventional method.

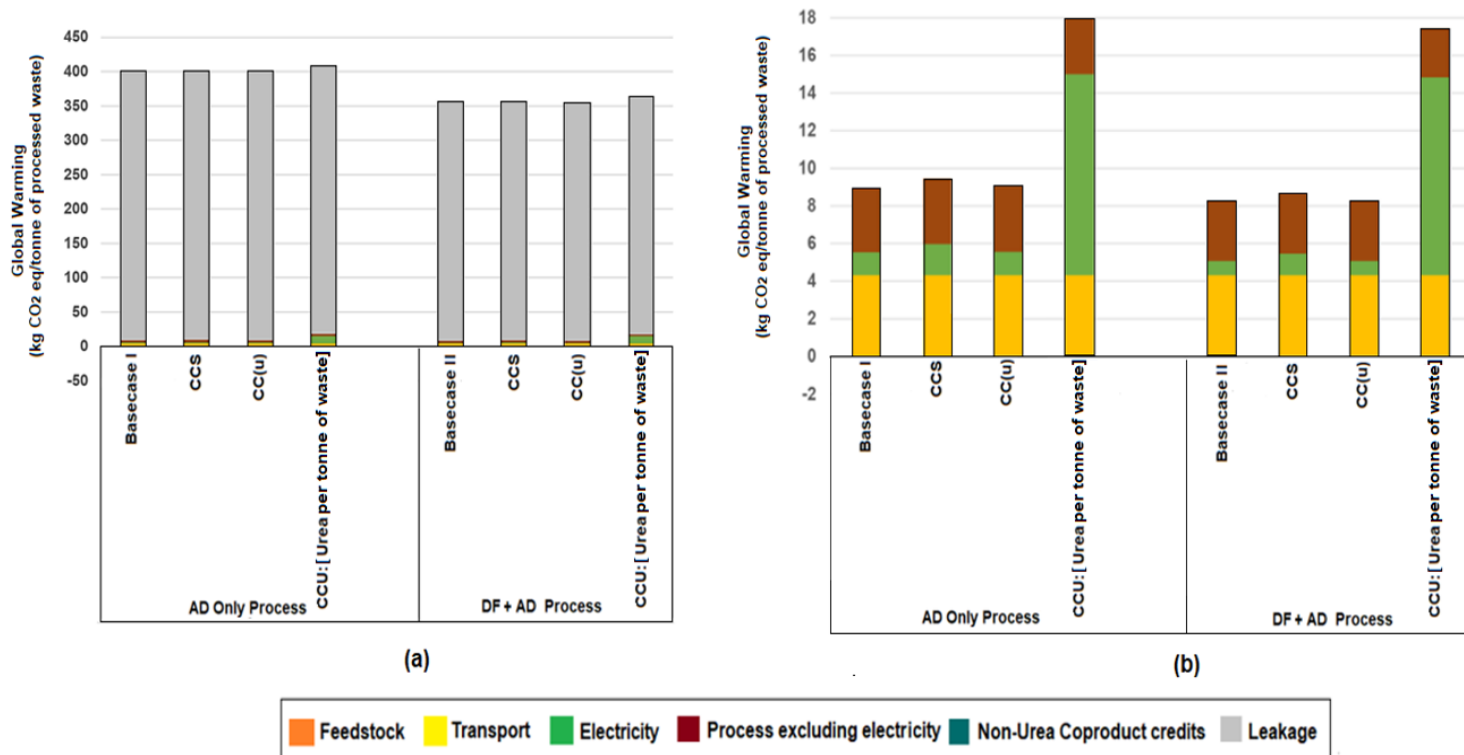


Fig. 6.14: GHG impacts of waste-to-ammonia and ammonia+urea processes for all CO₂ fates for both AD-only and two stage (DF+AD technologies) using per tonne of processed waste for the default (with SOFC) configurations (a) leakage impacts included (b) leakage impacts excluded (Impact assessment method: IPCC 2013 GWP 100a).

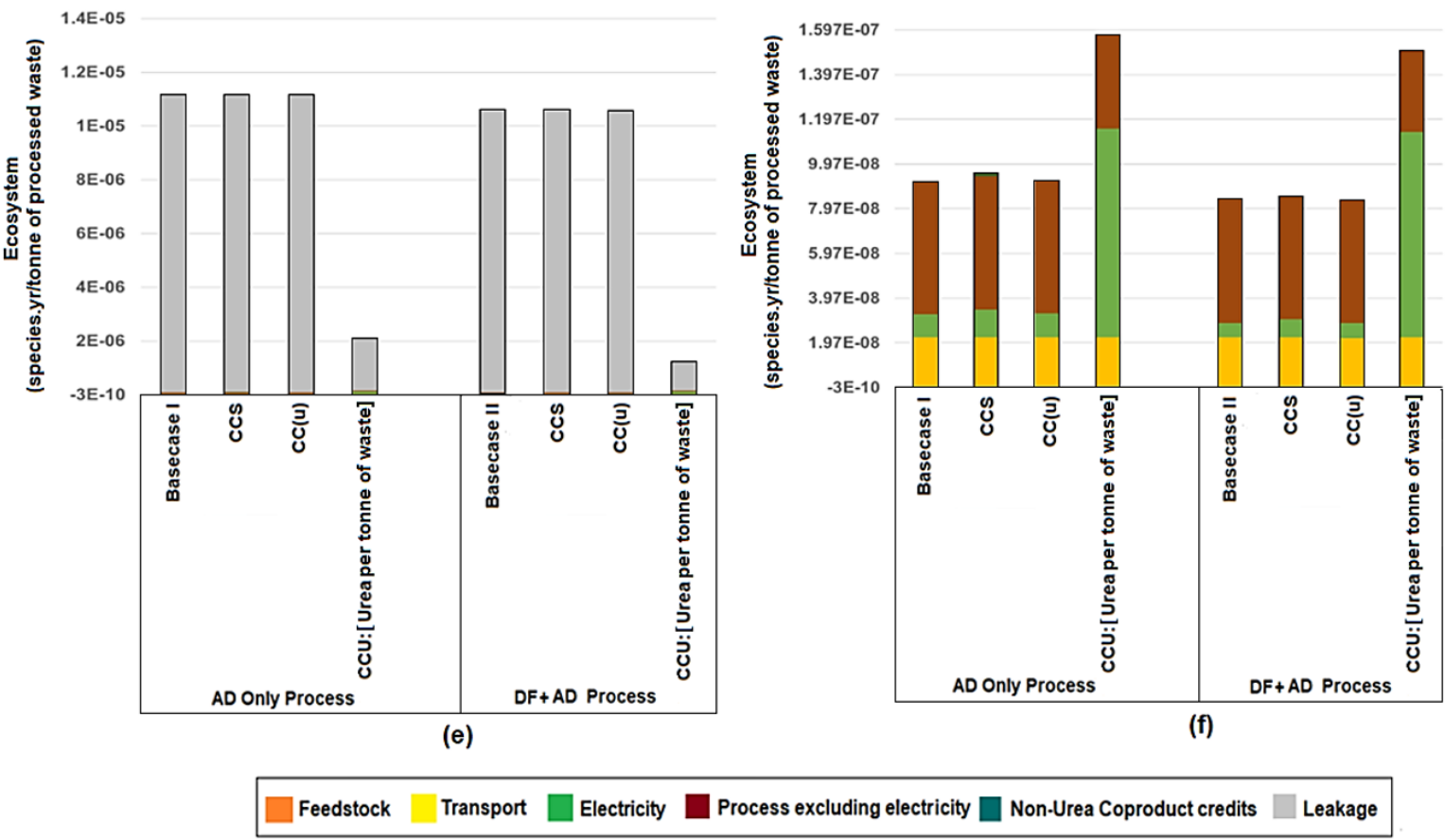


Fig. 6.15: Ecosystem impacts of waste-to-ammonia and ammonia+urea processes for all CO₂ fates for both AD-only and two stage (DF+AD technologies) using per tonne of processed waste for the default (with SOFC) configurations (e) leakage impacts included (f) leakage impacts excluded (Impact assessment method: ReCiPe 2016 endpoint H/A).

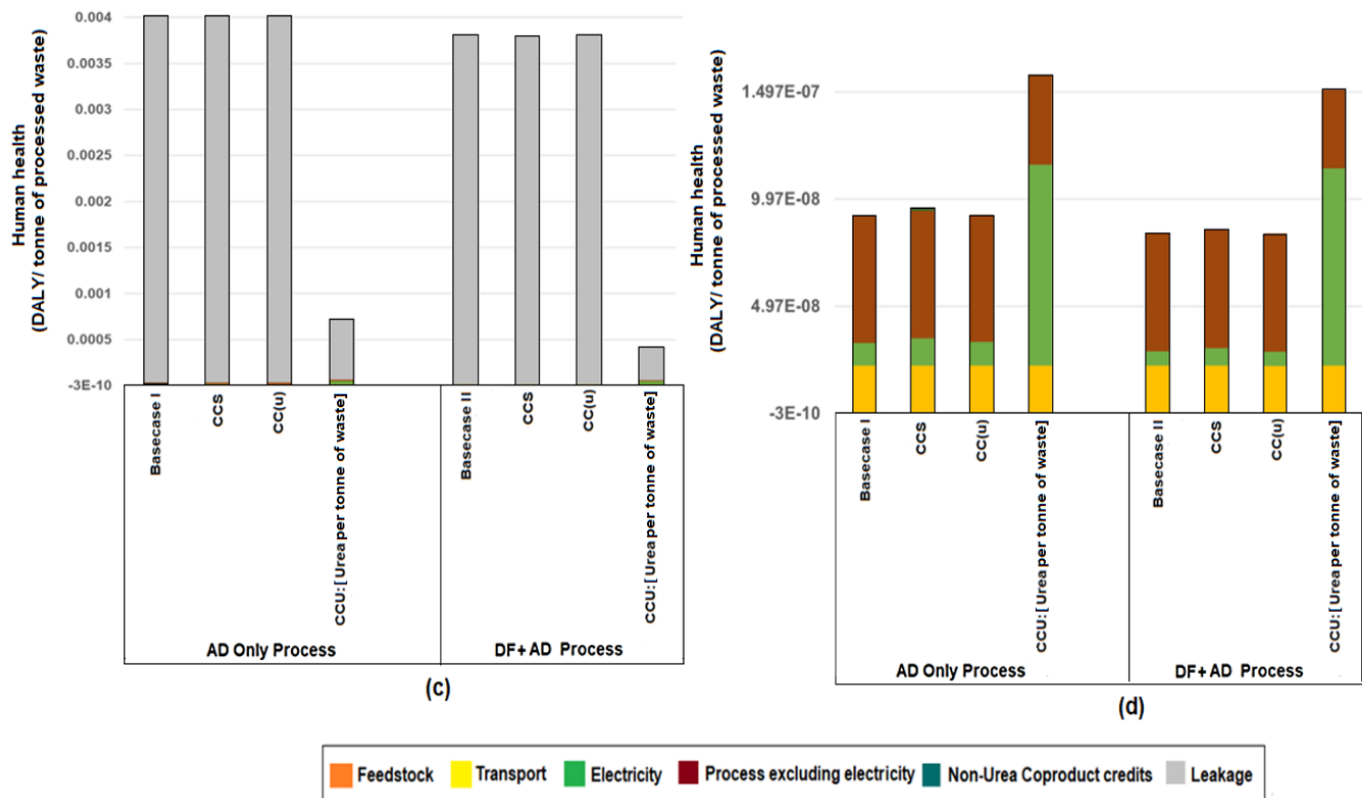


Fig. 6.16: Human health impacts of waste-to-ammonia and ammonia+urea processes for all CO₂ fates for both AD-only and two stage (DF+AD technologies) using per tonne of processed waste for the default (with SOFC) configurations (c) leakage impacts included (d) leakage impacts excluded (Impact assessment method: ReCiPe 2016 endpoint H/A).

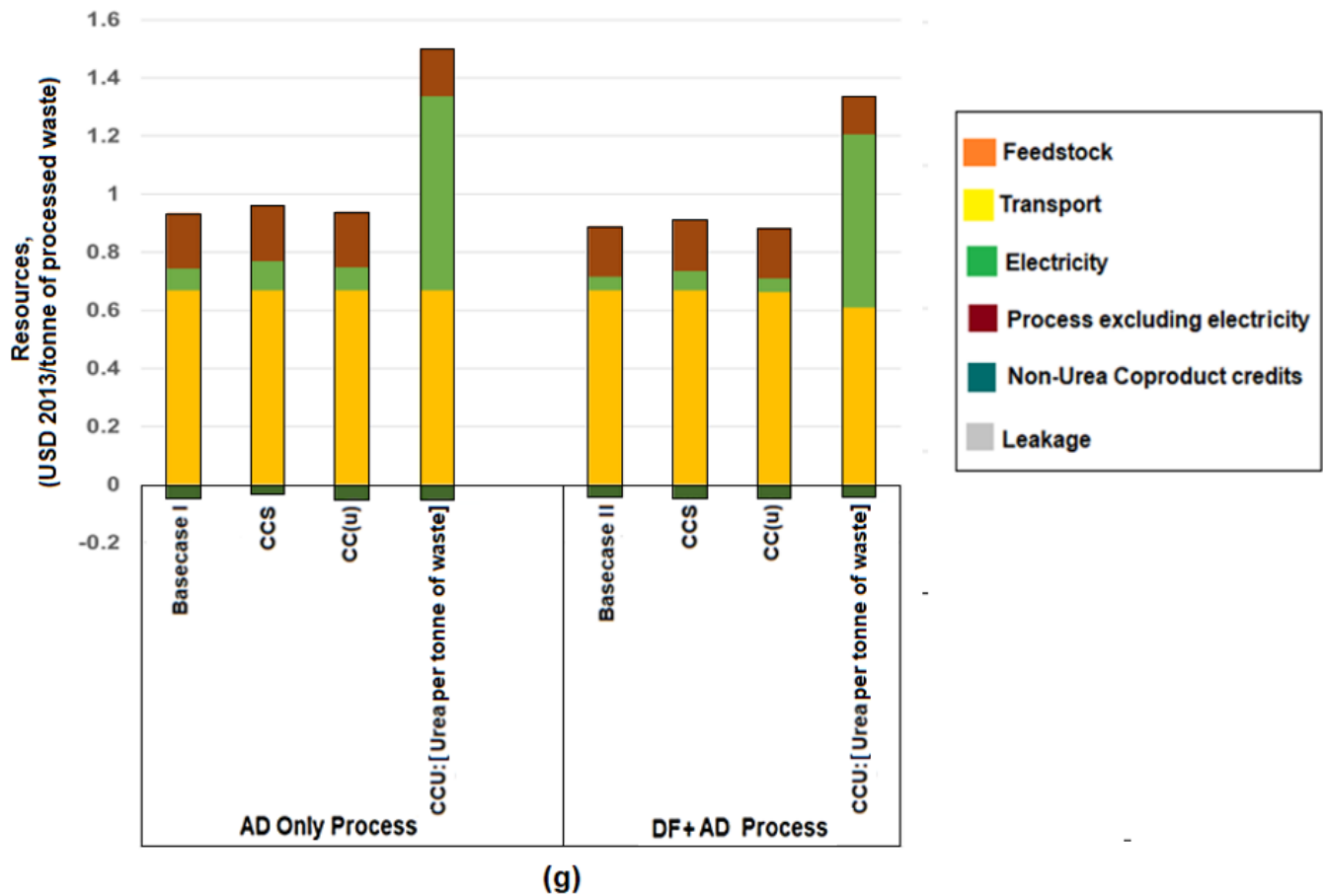


Fig. 6.17: Resources impacts of waste-to-ammonia and ammonia+urea processes for all CO₂ fates for both AD-only and two stage (DF+AD technologies) using per tonne of processed waste for the default (with SOFC) configurations (g) with leakage impacts included (Impact assessment method: ReCiPe 2016 endpoint H/A).

6.2.4 GHG impacts on the basis of total nutrient N (kg urea-N + kg NH₃-N)

Although the primary FU used in this analysis is 1 kg of NH₃, impacts were also assessed on a urea production basis, in which a FU of 1 kg urea is considered, as well as on the basis of total nutrient N (kg urea-N + kg NH₃-N). GHG impacts on the basis of total nutrient N (kg urea-N + kg NH₃-N) from the production of waste-to-ammonia and ammonia+urea processes for all CO₂ fates for the two stage (DF+AD) using unallocated and mass allocation, with and without SOFC, including the impacts from leakage are shown in Table 6.2 and 6.3.

Table 6.2: Impacts on the basis of total nutrient N (kg urea-N + kg NH₃-N) from the production of waste-to-ammonia and ammonia+urea processes for all CO₂ fates for the two stage (DF+AD) using unallocated and mass allocation, with and without SOFC, including the impacts from leakage.

Green Ammonia, 20 tonnes/day of waste, 50:50 Food Waste: Human Waste	Urea w SOFC (unallocated)	Urea (unallocated)	Urea w SOFC (mass allocation)	Urea (mass allocation)	Base case w SOFC	Base case	CCS	CCS w SOFC	CCU w SOFC	CCU SOFC
Unallocated, total (per kg NH ₃)	321.72154	292.47765	0.09131	0.09131	0.15845	0.15845	0.15876	0.15862	0.15846	0.15843
Total impact per day	7300.82687	7300.82715	7227.83980	7227.84214	7117.24266	7117.24289	7131.33340	7124.69015	7117.55464	7116.48692
Total, per kg fertilizer N	0.19759	0.19758	0.19562	0.19561	0.19241	0.19240	0.19278	0.19261	0.19242	0.19238
Impacts associated w Urea	0.19754	0.19752	0.29517	0.19555	N. A	N. A	N. A	N. A	N. A	N. A
Impacts associated w NH ₃	0.00006	0.00006	0.00008	0.19561	0.19241	0.19240	0.19278	0.19261	0.19242	0.19238

Table 6.3: Impacts on the basis of total nutrient N (kg urea-N + kg NH₃-N) from the production of waste-to-ammonia and ammonia+urea processes for all CO₂ fates for the AD-only using unallocated and mass allocation, with and without SOFC, including the impacts from leakage.

Green Ammonia, 20 tonnes/day of waste, 50:50 Food Waste: Human Waste	Urea w SOFC (unallocated)	Urea (unallocated)	Urea w SOFC (mass allocation)	Urea (mass allocation)	Base case w SOFC	Base case	CCS	CCS w SOFC	CCU w SOFC	CCU SOFC
Unallocated, total (per kg NH ₃)	2.35	2.13	0.15	0.10	0.17	0.17	0.17	0.17	0.17	0.17
Total impact per day	8177.31850	8152.97757	11993.05200	8030.16590	7966.730	8025.886	8025.886	7966.73210	7966.73210	8025.88649
Total, per kg fertilizer N	0.21210	0.20991	0.31108	0.20675	0.20643	0.20643	0.20643	0.20643	0.20643	0.20643
Impacts associated w Urea	0.20287	0.19991	0.29754	0.19689	N. A	N. A	N. A	N. A	N. A	N. A
Impacts associated w NH ₃	0.00923	0.01001	0.01354	0.00986	0.20643	0.20643	0.20643	0.20643	0.20643	0.20643

6.2.5 Biogenic emissions

As the process feedstocks are derived from plant and animal matter, emissions are biogenic. The GHG emissions also calculated using the GHG Protocol method, which augments the IPCC values with non-zero characterization factors for biogenic carbon, from the production of waste-to-ammonia and ammonia+urea processes for all CO₂ fates. This is for both AD-only and two-stage using mass allocation with and without the contribution from leakage via the default (with SOFC) configuration. Biogenic emissions for non-urea cases under GWP_{biogenic} are significantly higher compared to GWP_{100} , due to increased CO₂ leakage rates. Most importantly, however, CO₂ uptake is not included for the waste feedstock, which is an organic material. Including CO₂ uptake would decrease emissions close to the IPCC values. Since impacts for the modelled systems are almost entirely from leakage, when this factor is removed, the GHG impacts using GWP_{biogenic} are equivalent to GWP_{100} , highlighting the significance of controlling leakage in this study. Life cycle impacts using GWP_{biogenic} impact assessment method is shown in Table 6.4 and 6.5.

Table 6.4: Life cycle impacts using the GHG Protocol impact assessment method from the production of waste-to-ammonia and ammonia+urea processes for all CO₂ fates for the two stage (DF+AD) using mass allocation and avoided product with and without SOFC, including the impacts from leakage.

DF+AD process							
CCU							
	Unit	feedstock	Transport	Electricity	Leakage	Process, Excluding Electricity	Co-Product Credits
Fossil CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	0.001907	0.000335	0	1.42E-03	-1.88E-05
Biogenic CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	7.85E-06	1.04E-05	1.26571	1.91E-04	-9.34E-08
CO ₂ eq from land transformation	Kg CO ₂ eq/kg NH ₃	0	5.16E-07	7.05E-07	0	2.04E-06	-4.89E-09
CO ₂ uptake	Kg CO ₂ eq/kg NH ₃	0	7.28E-06	1.03E-05	0	2.16E-05	-6.78E-08
CCU w SOFC							
	Unit	feedstock	Transport	Electricity	Leakage	Process, Excluding Electricity	Co-Product Credits
Fossil CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	1.93E-03	3.35E-04	0	1.42E-03	-1.88E-05
Biogenic CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	7.90E-06	1.04E-05	1.26576	1.91E-04	-9.34E-08
CO ₂ eq from land transformation	Kg CO ₂ eq/kg NH ₃	0	5.20E-07	7.05E-07	0	2.04E-06	-4.89E-09
CO ₂ uptake	Kg CO ₂ eq/kg NH ₃	0	7.31E-06	1.03E-05	0	2.16E-05	-6.78E-08
CCS							
	Unit	feedstock	Transport	Electricity	Leakage	Process, Excluding Electricity	Co-Product Credits
Fossil CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	0.001931	0.000334	0	1.42E-03	-1.88E-05
Biogenic CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	7.89E-06	1.04E-05	1.26577	1.91E-04	-9.34E-08
CO ₂ eq from land transformation	Kg CO ₂ eq/kg NH ₃	0	5.2E-07	7.04E-07	0	2.04E-06	-4.89E-09
CO ₂ uptake	Kg CO ₂ eq/kg NH ₃	0	7.31E-06	1.02E-05	0	2.16E-05	-6.78E-08
CCS w SOFC							
	Unit	feedstock	Transport	Electricity	Leakage	Process, Excluding Electricity	Co-Product Credits
Fossil CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	0.001931	1.59E-04	0	1.42E-03	-1.88E-05
Biogenic CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	7.9E-06	4.16E-06	1.26581	1.91E-04	-9.34E-08
CO ₂ eq from land transformation	Kg CO ₂ eq/kg NH ₃	0	5.2E-07	8.87E-09	0	2.04E-06	-4.89E-09
CO ₂ uptake	Kg CO ₂ eq/kg NH ₃	0	7.31E-06	3.13E-06	0	2.16E-05	-6.78E-08
Base case I							
	Unit	feedstock	Transport	Electricity	Leakage	Process, Excluding Electricity	Co-Product Credits
Fossil CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	0.001931	0.000328	0	1.42E-03	-1.88E-05
Biogenic CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	7.89E-06	1.02E-05	2.38800	1.91E-04	-9.34E-08
CO ₂ eq from land transformation	Kg CO ₂ eq/kg NH ₃	0	5.2E-07	6.91E-07	0	2.04E-06	-4.89E-09
CO ₂ uptake	Kg CO ₂ eq/kg NH ₃	0	7.31E-06	1E-05	0	2.16E-05	-6.78E-08
Base case w SOFC							
	Unit	feedstock	Transport	Electricity	Leakage	Process, Excluding Electricity	Co-Product Credits
Fossil CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	0.001931	0.000328	0	1.42E-03	-1.88E-05
Biogenic CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	7.9E-06	1.02E-05	2.38803	1.91E-04	-9.34E-08
CO ₂ eq from land transformation	Kg CO ₂ eq/kg NH ₃	0	5.2E-07	6.91E-07	0	2.04E-06	-4.89E-09
CO ₂ uptake	Kg CO ₂ eq/kg NH ₃	0	7.31E-06	1E-05	0	2.16E-05	-6.78E-08
CCU (Urea)/mass allocation							
	Unit	feedstock	Transport	Electricity	Leakage	Process, Excluding Electricity	Co-Product Credits
Fossil CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	0.001085	0.002611	0	6.60E-04	-1.06E-05
Biogenic CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	4.43E-06	8.09E-05	0.086939	1.05E-04	-5.25E-08

CO ₂ eq from land transformation	Kg CO ₂ eq/kg NH ₃	0	2.92E-07	5.51E-06	0	9.44E-07	-2.75E-09
CO ₂ uptake	Kg CO ₂ eq/kg NH ₃	0	4.11E-06	8.01E-05	0	9.80E-06	-3.81E-08
CCU (Urea) w SOFC/mass allocation							
	Unit	feedstock	Transport	Electricity	Leakage	Process, Excluding Electricity	Co-Product Credits
Fossil CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	0.001085	2.61E-03	0	6.60E-04	-1.06E-05
Biogenic CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	4.44E-06	8.09E-05	0.093224	1.05E-04	-5.25E-08
CO ₂ eq from land transformation	Kg CO ₂ eq/kg NH ₃	0	2.92E-07	5.51E-06	0	9.44E-07	-2.75E-09
CO ₂ uptake	Kg CO ₂ eq/kg NH ₃	0	4.11E-06	8.01E-05	0	9.80E-06	-3.81E-08
CCU (Urea)/avoided product							
	Unit	feedstock	Transport	Electricity	Leakage	Process, Excluding Electricity	Co-Product Credits
Fossil CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	3.474951	8.364349	0	2.11E+00	-4713.12
Biogenic CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	0.014207	0.259165	278.4906	3.37E-01	-13.1385
CO ₂ eq from land transformation	Kg CO ₂ eq/kg NH ₃	0	0.000935	0.017635	0	3.02E-03	-1.15374
CO ₂ uptake	Kg CO ₂ eq/kg NH ₃	0	0.013159	0.256431	0	3.14E-02	-12.7391
CCU (Urea) w SOFC/avoided product							
	Unit	feedstock	Transport	Electricity	Leakage	Process, Excluding Electricity	Co-Product Credits
Fossil CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	3.8224	9.20E+00	0	2.32E+00	-5184.37
Biogenic CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	0.015627	2.85E-01	328.5495	3.70E-01	-14.4522
CO ₂ eq from land transformation	Kg CO ₂ eq/kg NH ₃	0	0.001029	1.94E-02	0	3.32E-03	-1.26909
CO ₂ uptake	Kg CO ₂ eq/kg NH ₃	0	0.014475	2.82E-01	0	3.45E-02	-14.0128

Table 6.5: Life cycle impacts using the GHG Protocol impact assessment method from the production of waste-to-ammonia and ammonia+urea processes for all CO₂ fates for the AD-only using mass allocation and avoided product, with and without SOFC, including the impacts from leakage.

AD-only process							
CCU							
	Unit	feedstock	Transport	Electricity	Leakage	Process, Excluding Electricity	Co-Product Credits
Fossil CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	0.001837	0.000521	0	1.48E-03	-2.01E-05
Biogenic CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	7.51E-06	1.61E-05	1.35453	2.04E-04	-1.00E-07
CO ₂ eq from land transformation	Kg CO ₂ eq/kg NH ₃	0	4.94E-07	1.1E-06	0	2.12E-06	-5.23E-09
CO ₂ uptake	Kg CO ₂ eq/kg NH ₃	0	6.96E-06	1.6E-05	0	2.23E-05	-7.26E-08
CCU w SOFC							
	Unit	feedstock	Transport	Electricity	Leakage	Process, Excluding Electricity	Co-Product Credits
Fossil CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	0.001851	5.25E-04	0	1.49E-03	-2.03E-05
Biogenic CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	7.57E-06	1.63E-05	1.36460	2.05E-04	-1.01E-07
CO ₂ eq from land transformation	Kg CO ₂ eq/kg NH ₃	0	4.98E-07	1.11E-06	0	2.13E-06	-5.27E-09
CO ₂ uptake	Kg CO ₂ eq/kg NH ₃	0	7.01E-06	1.61E-05	0	2.25E-05	-7.32E-08
CCS							
	Unit	feedstock	Transport	Electricity	Leakage	Process, Excluding Electricity	Co-Product Credits
Fossil CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	0.001837	0.00052	0	1.48E-03	-2.01E-05
Biogenic CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	7.51E-06	1.61E-05	1.35454	2.04E-04	-1.00E-07
CO ₂ eq from land transformation	Kg CO ₂ eq/kg NH ₃	0	4.94E-07	1.1E-06	0	2.12E-06	-5.23E-09

CO ₂ uptake	Kg CO ₂ eq/kg NH ₃	0	6.96E-06	1.6E-05	0	2.23E-05	-7.26E-08
CCS w SOFC							
	Unit	feedstock	Transport	Electricity	Leakage	Process, Excluding Electricity	Co-Product Credits
Fossil CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	0.001851	5.24E-04	0	1.49E-03	-2.03E-05
Biogenic CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	7.57E-06	1.62E-05	1.364596	2.05E-04	-1.01E-07
CO ₂ eq from land transformation	Kg CO ₂ eq/kg NH ₃	0	4.98E-07	1.11E-06	0	2.13E-06	-5.27E-09
CO ₂ uptake	Kg CO ₂ eq/kg NH ₃	0	7.01E-06	1.61E-05	0	2.25E-05	-7.32E-08
Base case II							
	Unit	feedstock	Transport	Electricity	Leakage	Process, Excluding Electricity	Co-Product Credits
Fossil CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	0.001837	0.000498	0	1.48E-03	-2.01E-05
Biogenic CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	7.51E-06	1.54E-05	2.55575	2.04E-04	-1.00E-07
CO ₂ eq from land transformation	Kg CO ₂ eq/kg NH ₃	0	4.94E-07	1.05E-06	0	2.12E-06	-5.23E-09
CO ₂ uptake	Kg CO ₂ eq/kg NH ₃	0	6.96E-06	1.53E-05	0	2.23E-05	-7.26E-08
Base case w SOFC							
	Unit	feedstock	Transport	Electricity	Leakage	Process, Excluding Electricity	Co-Product Credits
Fossil CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	0.001851	5.01E-04	0	1.49E-03	-2.03E-05
Biogenic CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	7.57E-06	1.55E-05	2.57472	2.05E-04	-1.01E-07
CO ₂ eq from land transformation	Kg CO ₂ eq/kg NH ₃	0	4.98E-07	1.06E-06	0	2.13E-06	-5.27E-09
CO ₂ uptake	Kg CO ₂ eq/kg NH ₃	0	7.01E-06	1.53E-05	0	2.25E-05	-7.32E-08
CCU (Urea)/mass allocation							
	Unit	feedstock	Transport	Electricity	Leakage	Process, Excluding Electricity	Co-Product Credits
Fossil CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	0.00107	0.002622	0	7.33E-04	-1.17E-05
Biogenic CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	4.37E-06	8.12E-05	0.103281	1.17E-04	-5.82E-08
CO ₂ eq from land transformation	Kg CO ₂ eq/kg NH ₃	0	2.88E-07	5.53E-06	0	1.05E-06	-3.05E-09
CO ₂ uptake	Kg CO ₂ eq/kg NH ₃	0	4.05E-06	8.04E-05	0	1.08E-05	-4.23E-08
CCU (Urea) w SOFC /mass allocation							
	Unit	feedstock	Transport	Electricity	Leakage	Process, Excluding Electricity	Co-Product Credits
Fossil CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	0.001075	2.63E-03	0	7.36E-04	-1.18E-05
Biogenic CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	4.39E-06	8.16E-05	0.103726	1.17E-04	-5.85E-08
CO ₂ eq from land transformation	Kg CO ₂ eq/kg NH ₃	0	2.89E-07	5.55E-06	0	1.05E-06	-3.06E-09
CO ₂ uptake	Kg CO ₂ eq/kg NH ₃	0	4.07E-06	8.07E-05	0	1.09E-05	-4.25E-08
CCU (Urea)/avoided product							
	Unit	feedstock	Transport	Electricity	Leakage	Process, Excluding Electricity	Co-Product Credits
Fossil CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	0.022662	0.055527	0	1.55E-02	-27.5224
Biogenic CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	9.26E-05	0.00172	2.187584	2.47E-03	-0.0828
CO ₂ eq from land transformation	Kg CO ₂ eq/kg NH ₃	0	6.1E-06	0.000117	0	2.22E-05	-0.00727
CO ₂ uptake	Kg CO ₂ eq/kg NH ₃	0	8.58E-05	0.001702	0	2.30E-04	-0.08028
CCU (Urea) w SOFC/avoided product							
	Unit	feedstock	Transport	Electricity	Leakage	Process, Excluding Electricity	Co-Product Credits
Fossil CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	0.024928	6.11E-02	0	1.71E-02	-30.2746
Biogenic CO ₂ eq	Kg CO ₂ eq/kg NH ₃	0	0.000102	1.89E-03	2.406343	2.72E-03	-0.09108
CO ₂ eq from land transformation	Kg CO ₂ eq/kg NH ₃	0	6.71E-06	1.29E-04	0	2.44E-05	-0.008

CO ₂ uptake	Kg CO ₂ eq/kg NH ₃	0	9.44E-05	1.87E-03	0	2.53E-04	-0.08831
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6.3 A comparison of this study with existing ammonia production technologies

6.3.1 CML 2001 impact assessment method

The proposed ammonia production processes are intended to be a more environmentally-benign option to conventional technologies. The potential impacts for the proposed processes are thus compared with other renewable options (electrolysis) and to conventional ammonia production routes. This comparison is based on the literature obtained from Bicer et al. (2016) and conventional ammonia production methods using library processes from the ecoinvent 3.6 database, which reflect global averages for those routes. The CML 2001 impact assessment method was used to allow comparison with the literature values, and with other impact assessment methods. The GWP, human toxicities, and abiotic depletions are shown in Fig. 6.18 (log scale) for the comparison of ammonia production processes. A similar comparison using Eco-indicator 99 impact assessment method (Goedkoop and Spriensma, 2000) can be found in section 6.3.2 and for urea production using IPCC 2013 GWP 100a is detailed in section 6.4. As Fig. 6.18 shows, abiotic depletion, human toxicity, and global warming impacts for both conventional and electrolysis routes are much higher than for the proposed modelled processes.

The Cocamide diethanolamine route has the highest impact on human toxicity, about 12.65 kg 1,4-DB eq/kg NH₃, due to the dehusking process for coconut and the production process for diethanolamine. This is followed by partial oxidation (due to the use of fossil fuels) and the nuclear power-based high temperature electrolysis method (drivers unspecified in Bicer et al. (2016)). Conversely, for the proposed waste-based processes, human toxicity, and abiotic depletion are driven by solar PV cells, while methane leakage dominates contributions to the GWP. The decreased solar energy consumption and corresponding decrease in impact from construction of solar PV (Fig. 6.18a) means that the base case for AD-only process (using SOFC) has the lowest human toxicity impact of 0.0027 kg 1,4-DB eq/kg NH₃.

Amongst the proposed technology configurations, abiotic depletion impacts (Fig. 6.18a) are lowest for the base case (AD using SOFC) at 2.68E-05 kg Sb eq/ kg NH₃, due to low power consumption. The CCU* market case is the next lowest. As can be seen from Fig. 6.18 a, the abiotic depletion impact is the highest for partial oxidation with 0.021 kg Sb eq/kg NH₃, followed by natural gas steam reforming, and nuclear high temperature-based ammonia production processes resulting from petroleum and gas production.

As shown in Fig. 6.18 b, the highest GWP under GWP₁₀₀ is partial oxidation at 2.79 kg CO₂eq /kg NH₃, due to the high impact operation of refining petroleum followed by natural gas reforming (SMR) at 1.74 kg CO₂eq /kg NH₃. In contrast, the CCU for urea production described in this study has a GWP of 0.024 kg CO₂eq /kg NH₃ which is the lowest among all three categories. The dramatic decrease in impact is due to the fact that offsetting high-impact conventional urea production significantly lowers the life cycle GHGs.

The absence of burden on the feedstocks means that the waste-based processes have the lowest GWP impacts: electrolysis with power from municipal solid waste is the lowest impact among the electrolysis routes, and CCU with urea production is the lowest among the low impact waste-to-ammonia technologies modelled here. The lowest GWP

amongst the conventional ammonia production process categories is from the bio-based feedstock production process, cocamide diethanolamine, this impact is the result of coconut production.

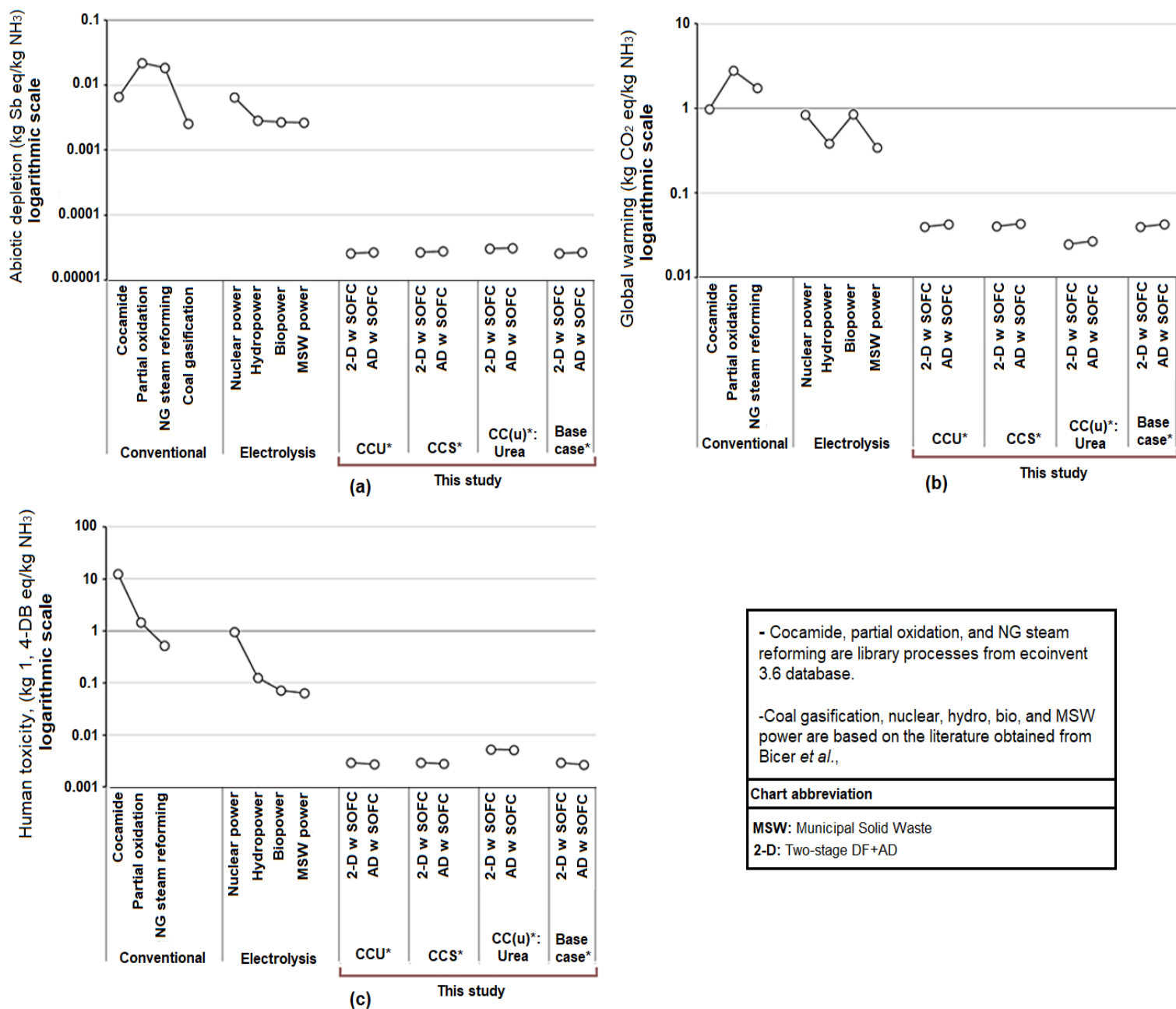


Fig. 6.18: A comparison of impacts for waste-to-ammonia and ammonia+urea processes (using mass allocation with leakage impacts included) along with conventional, and electrolysis technologies for (a) Abiotic depletion, (b) GHG emissions (GWP₁₀₀), and (c) Human toxicity, values are shown on a log scale (base case, CCU and CCS routes: this study; electrolysis routes and coal gasification (abiotic depletion only): from Bicer *et al.* (2016); conventional routes except coal gasification: ecoinvent 3.6 library processes) (Impact assessment method: CML 2001).

6.3.2 Eco-indicator 99 impact assessment method

A comparison of the proposed study with existing ammonia production technologies using Eco-indicator 99 impact assessment method is shown in Fig. 6.19. The trends in human health and ecosystem impacts for conventional, electrolysis, and this study are similar. The impact of the modelled systems is the lowest when compared to electrolysis and conventional technologies in terms of resources.

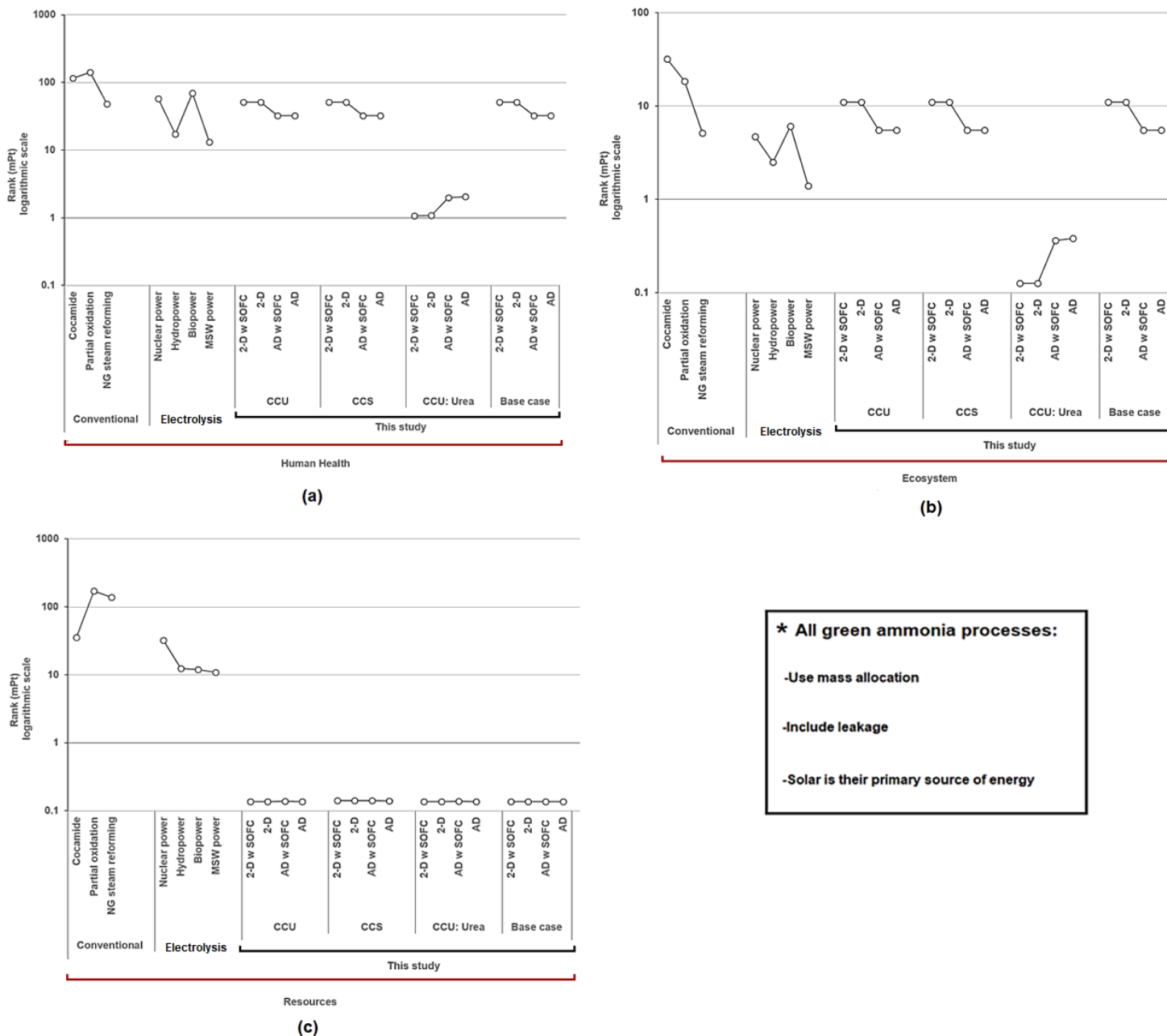


Fig. 6.19: A comparison of impacts for this waste-to-ammonia and ammonia+urea processes (using mass allocation with leakage impacts included) along with conventional, and electrolysis technologies for (a) Human health, (b) Ecosystem, and (c) Resources impacts, values are shown on a log scale (base case, CCU and CCS routes: this study; electrolysis routes: from Bicer et al. (2016); conventional routes: ecoinvent 3.6 library processes) (Impact assessment method: Eco-indicator 99).

6.4 A comparison of this study with library urea production processes

The GWI from Rest-of-the-World (RoW) and Global (GLO) shortcuts are higher for urea production compared to European (RER) ones (Fig. 6.20). Fig. 6.20 shows that the library urea production process has a higher GWI compared to the urea processes presented in this study. This shows the significance of displacing conventional fossil-based urea production processes (library) with the biogenic based ones (this study).

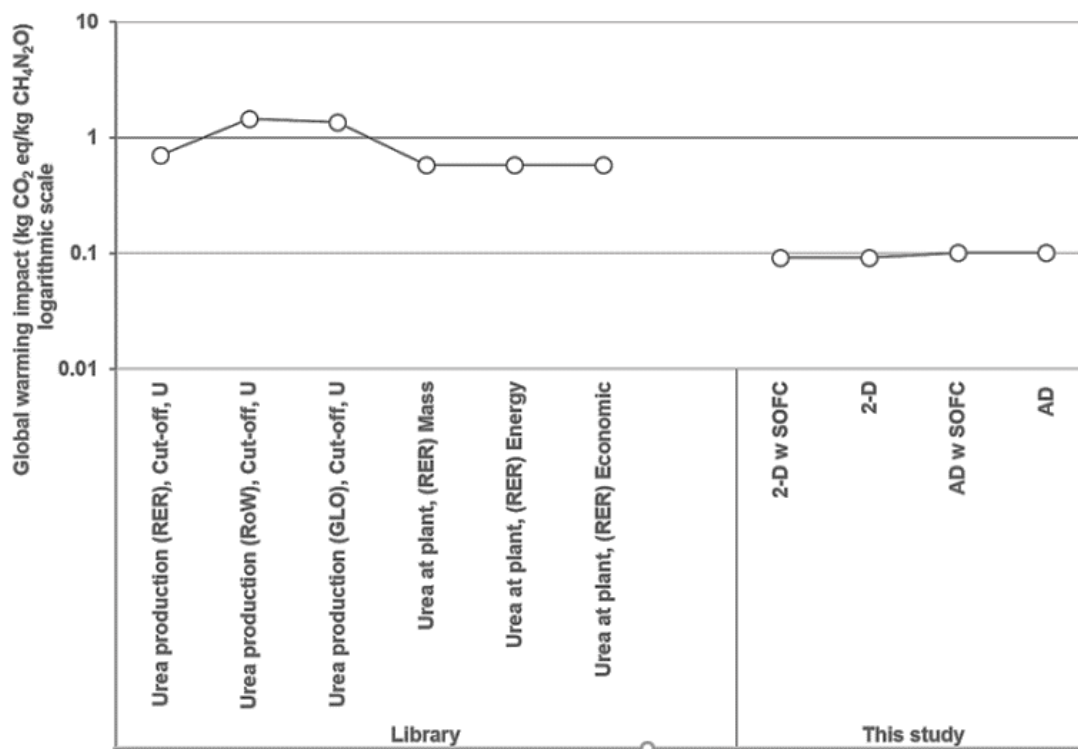


Fig. 6.20: A comparison of GHG impacts for this waste-to-ammonia+urea processes (using mass allocation with leakage impacts included) along with library processes for urea, values are shown on a log scale (Impact assessment method: IPCC 2013 GWP 100a).

A comparison of the proposed urea production processes (two stage and AD-only with and without SOFC) including leakage rates with library processes using ReCiPe 2016 impact assessment method is shown in Fig. 6.21. The benefit of the waste-based process is so large that these are shown on a log scale. The figure shows that the modelled process has a lower human health, resources, and ecosystem impact compared to the library processes (Agri footprint) for urea production. The difference between the impacts of library processes and the proposed process is more evident in resources, this is due to the library processes being fossil-based, whereas, the modelled process is biogenic. The library results show that the impacts are dominated by the feedstock for urea production.

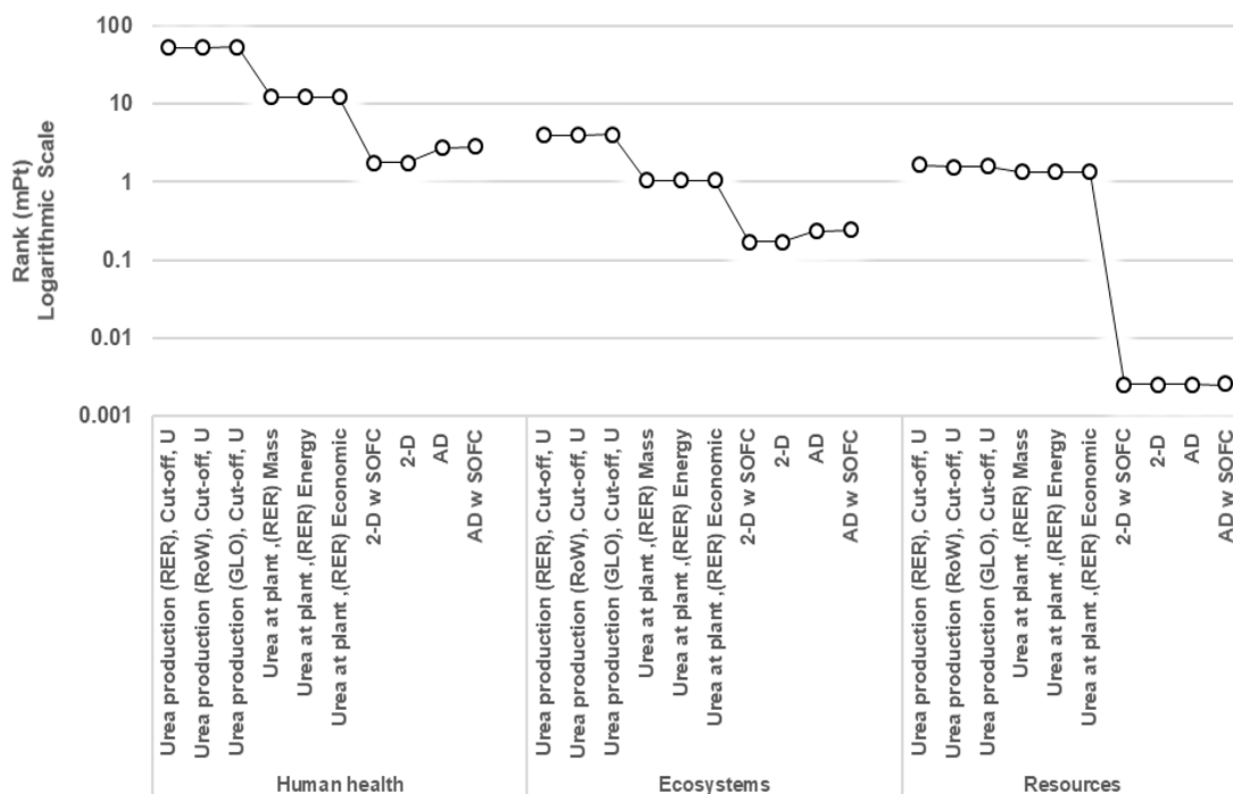


Fig. 6.21: A comparison of damage (human health, ecosystem, and resources) impacts for this waste-to-ammonia and ammonia+urea processes (using mass allocation with leakage impacts included) along with library processes for urea, values are shown on a log scale (Impact assessment method: ReCiPe 2016 endpoint H/A).

6.5 Uncertainty analysis

The results of the uncertainty analysis are shown in Fig. 6.22 (error bars show the 95% confidence interval). Methane leakage is by far the strongest factor which drives the uncertainty analysis, it overwhelms any other contributions to the uncertainty, as the contribution results imply. In order to interrogate the importance of uncertainty for comparing alternatives, leakages have been treated separately via sensitivity analyses. Comparison of the results indicates that, when leakage rates are held fixed, electricity is contributing the most uncertainty to both AD-only and two-stage. The magnitude of uncertainty is consistent across all process types except for urea cases (see Fig. 6.23 for per tonne of processed waste). In cases where urea is produced, allocation of impacts between ammonia and the dominant urea co-product results in an apparently smaller uncertainty. This is also illustrated in Fig. 6.22c and 6.22d, which shows the results of uncertainty analysis using system expansion for the urea coproduct: the uncertainty on the avoided product basis dwarfs that of the non-urea cases. In the urea-production scenario sets, the amount of ammonia produced is small while large amounts of urea are produced. Thus, variation in the urea, results in large changes (e.g., the avoided product credit for urea is magnifying the uncertainty). Uncertainty analysis for green ammonia through AD-only process using IPCC 2013 GWP 100a impact assessment method for mass allocations, avoided product, and

per tonne of processed waste (including leakage with fixed rates as mentioned in *Chapter 5*, section 5.1.1.8) are shown in Fig.6.22 and 6.23. The significant increase of impact in response to switching the primary source of power from renewable (solar) to fossil-based (grid) is shown in the contribution analysis section. However, changing the source of energy from solar to grid (shown in red) does not have a significant effect on the uncertainty analysis, since the uncertainty (in the absence of uncertainty on leakage rates) comes from the speculativeness of the process and not from the energy source (Fig.6.22a and 6.22b).

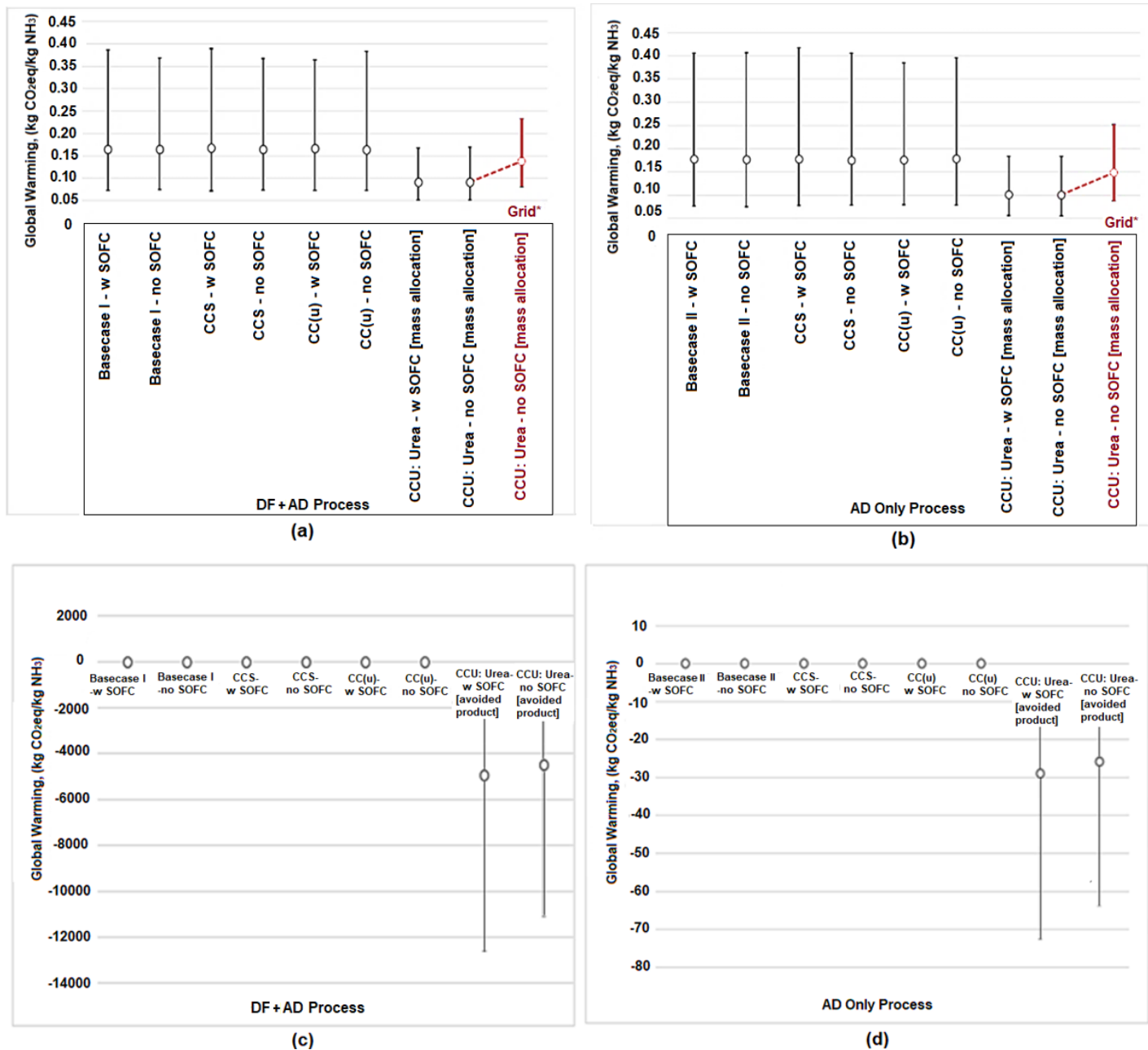


Fig. 6.22: Uncertainty analysis of waste-to-ammonia and ammonia+urea processes for all CO₂ fates for (a), (c) DF+AD process and (b), (d) AD-only process, with and without SOFC using mass allocation (a, b) and avoided product (c,d) for urea production, leakage impacts included (Impact assessment method: IPCC 2013 GWP 100a).

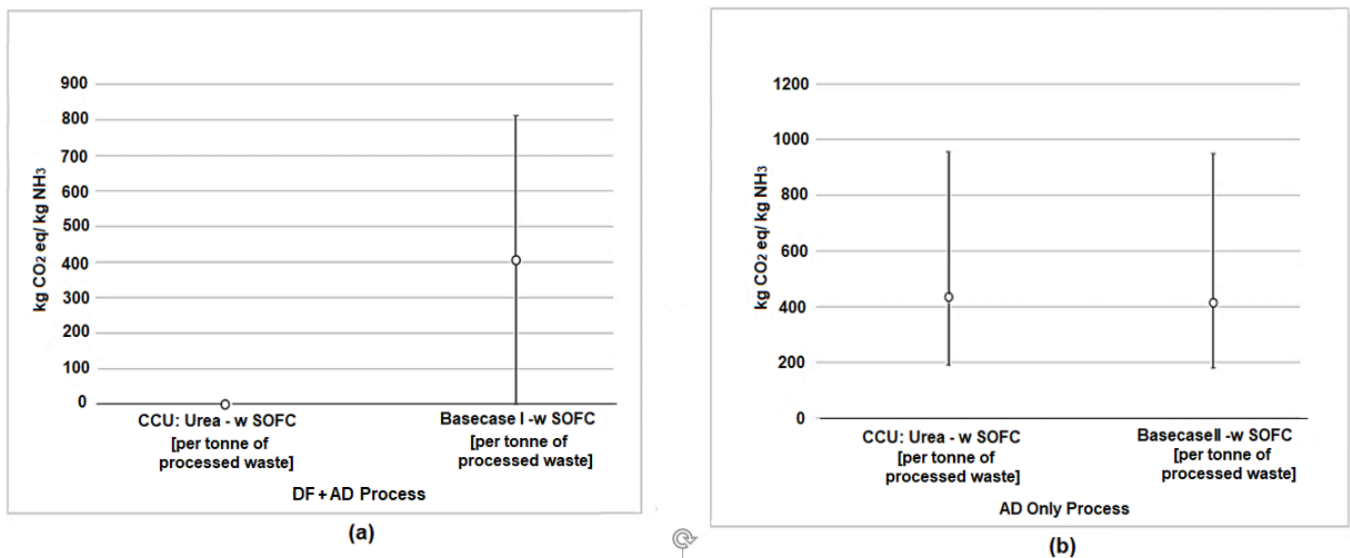


Fig. 6.23: Uncertainty analysis of waste-to-ammonia and ammonia+urea processes for urea and base case (a) DF+AD process and (b) AD-only process, using per tonne of processed waste (unallocated) for the default (with SOFC), leakage impacts included (Impact assessment method: IPCC 2013 GWP 100a).

The most significant contributors to uncertainty in the tests run for the processes that produce urea are urea product mass, followed by methane leakage, ammonia product yield, electricity, and small amounts from the remainder of the parameters in the entire process. For the scenario where urea is not produced, the most significant contributors to uncertainty in the tests run for the ammonia processes are the methane leakage followed by ammonia and small amounts from the rest of the parameters in the entire process. This was consistent for each of the technologies. Because of the extremely high responsiveness to leakage, these factors were assessed via sensitivity analysis and were treated as fixed values in the uncertainty analysis. This has the effect of magnifying the apparent uncertainty disproportionately, as no other factor in this study contributes to the impact as much as leakage.

6.6 Sensitivity analysis

Results of the sensitivity analyses for each impact category indicate that the potential impacts are relatively insensitive to changes in everything except product yields and leakage rates. Potential impacts respond strongly to changes in leakage assumptions, supporting the significance of these two factors visible in the contribution analysis. Figs 6.24-6.28 show the results of sensitivity analysis on key parameters and the factors driving the responses are discussed below.

6.6.1 Sensitivity analysis of GWP results to changes in feedstock parameters, primary product yields, leakage rates, and electricity demand

Fig. 6.24 shows the results of sensitivity analysis for GWP₁₀₀. The results for water scarcity using AWARE and for damage categories using ReCiPe2016 on key parameters and the factors driving the responses are assessed in section 6.6.2 and 6.6.3 respectively. Based on the sensitivity analysis results (Fig.6.24), the GWP is relatively insensitive to most input parameters. It is, however, strongly sensitive to the methane leakage, which can significantly change the

results of GHG emissions. The sensitivity analysis was carried out for both SOFC and non-SOFC cases and the results show that the two configurations are almost indistinguishable.

- **Waste flow rate:** The proposed process is sensitive to flow rate especially for the two-stage, this is followed by BW distance, FW distance, and the fraction of FW/BW as shown in Fig.6.24a. Increasing the flow rate leads to a small increase in the impact.
- **Transportation distance of FW and BW to the plant:** Varying the transportation distance of BW to the plant has a stronger impact than for FW. As the ratio of FW to BW decreases, more BW is moved over long distances which is inversely proportional to the mass of BW.
- **FW/BW ratio:** When the amount of FW goes up relative to the amount of BW, more water is consumed which in turn increases the electricity usage for generating water in the system, resulting in a slightly higher impact. Availability of the particular feedstock will vary seasonally, regionally, and can even vary on a day-to-day basis, factors which need to be considered in deployment and siting decisions and in technology selection based on impact.
- **Product yield:** In cases where urea is not produced, sensitivity to ammonia product yields increases, while in the cases where urea is produced, the sensitivity to urea product yields increases. Despite the CCU cases where the process is sensitive to urea product yields, especially in the two-stage process. Primary product yields (ammonia/ammonia+urea) are inversely proportional to the environmental impact, as the product yield goes down, the impact goes up (higher yields will result in a lower impact).
- **Leakage rates:** Methane leakage is the most significant factor in this sensitivity analysis, showing a nearly linear response for GWP results. In cases where urea is not produced, sensitivity to ammonia leakage rates are higher compared to where there is urea production, this is due to the consumption of ammonia in urea production cases, as urea carries a share of the burden. On the other hand, the two-stage is more sensitive to N₂O leakage rates despite the AD-only processes. In the assessed model, the only factor that significantly affects climate change is methane leakage.
- **Electricity demand:** Electricity demand has a higher impact compared to the use of injection energy followed by energy derived from the SOFC. Incorporating SOFC increases the CapEx and added process complexity with no tangible environmental benefit, based on the results obtained, making it an unattractive option. In cases where urea is produced sensitivity to electricity demand is higher especially for the two-stage, as urea is carrying a share of the impact. Fig.6.24d shows that this process is not sensitive to energy derived from the SOFC. The same applies to the injection energy use except for the CCS cases where CO₂ for the CCS cases is injected into the ground. The sensitivity would be far more pronounced if grid electricity was required.

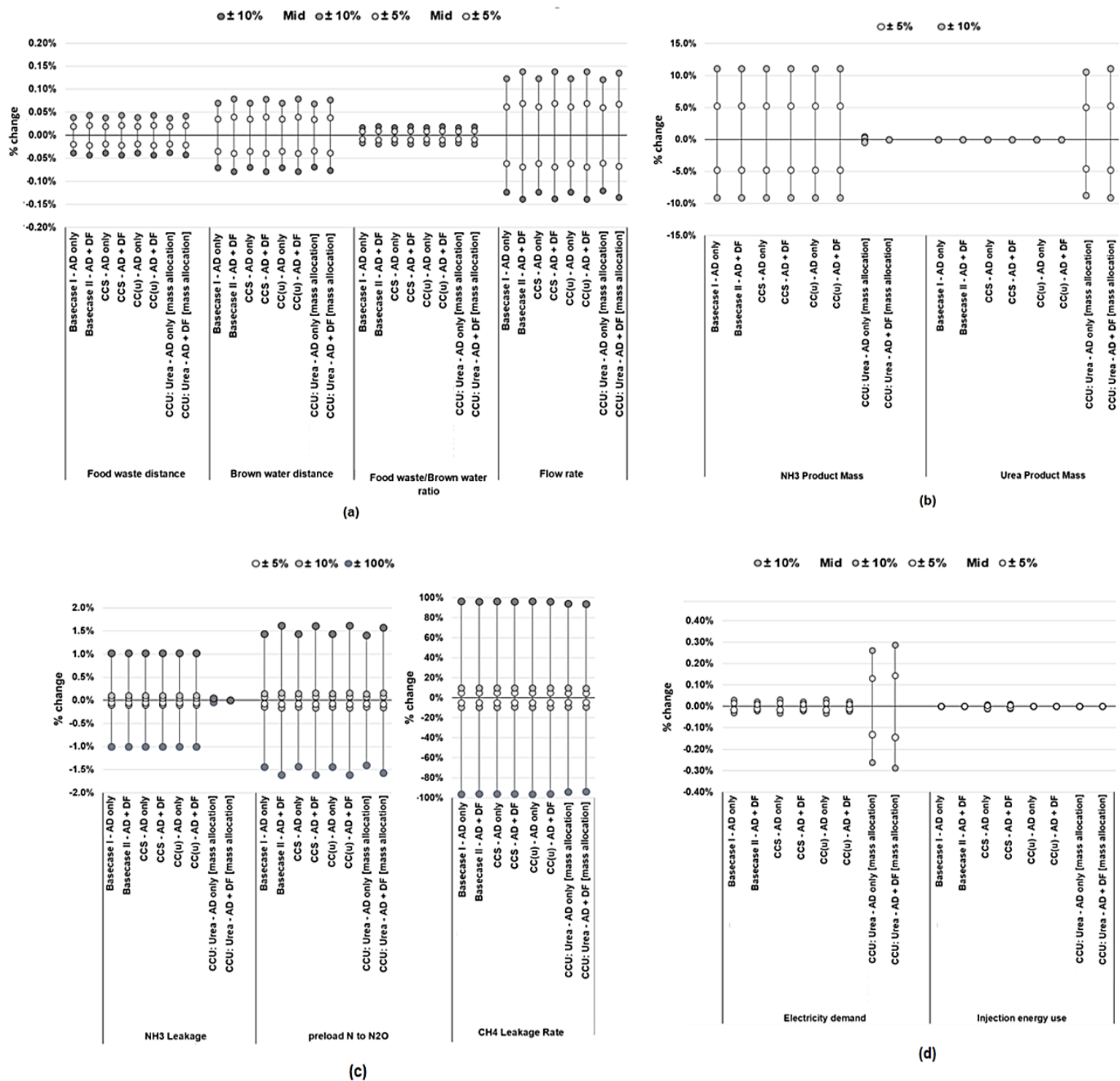


Fig. 6.24: Sensitivity of GWP results for the production of waste-to-ammonia and ammonia+urea processes for all CO₂ fates for both AD-only and two-stage (DF+AD technologies) via the default (with SOFC) configurations using mass allocation to changes in (a) feedstock parameters, (b) primary product yields, (c) leakage rates, and (d) electricity demand (Impact assessment method: IPCC 2013 GWP 100a).

6.6.2 Sensitivity analysis of resources, human health, and ecosystem damage to changes in feedstock parameters, primary product yields, leakage rates, and electricity demand (ReCiPe2016)

The resources damage category results show that the proposed process is sensitive to waste flow rate, especially in the non-urea cases for the AD-only process. This is followed by BW distance, FW distance, and the fraction of FW/BW, as shown in Fig. 6.25a. Sensitivity to feedstock parameters, primary product yields, and electricity demand for GHG emissions and resources damage is similar, except for the leakage rates, as this process is more sensitive to ammonia leakage rates than methane leakage. However, the effect of the changes in the aforementioned variables on the results of the sensitivity analysis, show that both human health and ecosystem damage categories are responding similarly to the model. The impact of these processes with SOFC is negligible for all three impact categories.

Ammonia product yield for the AD-only-CCU (mass allocation) is more sensitive to changes in both ecosystem and human health, this is due to the fact that the amount of produced ammonia is lower and the urea product yield is higher in the two-stage compared to AD-only.

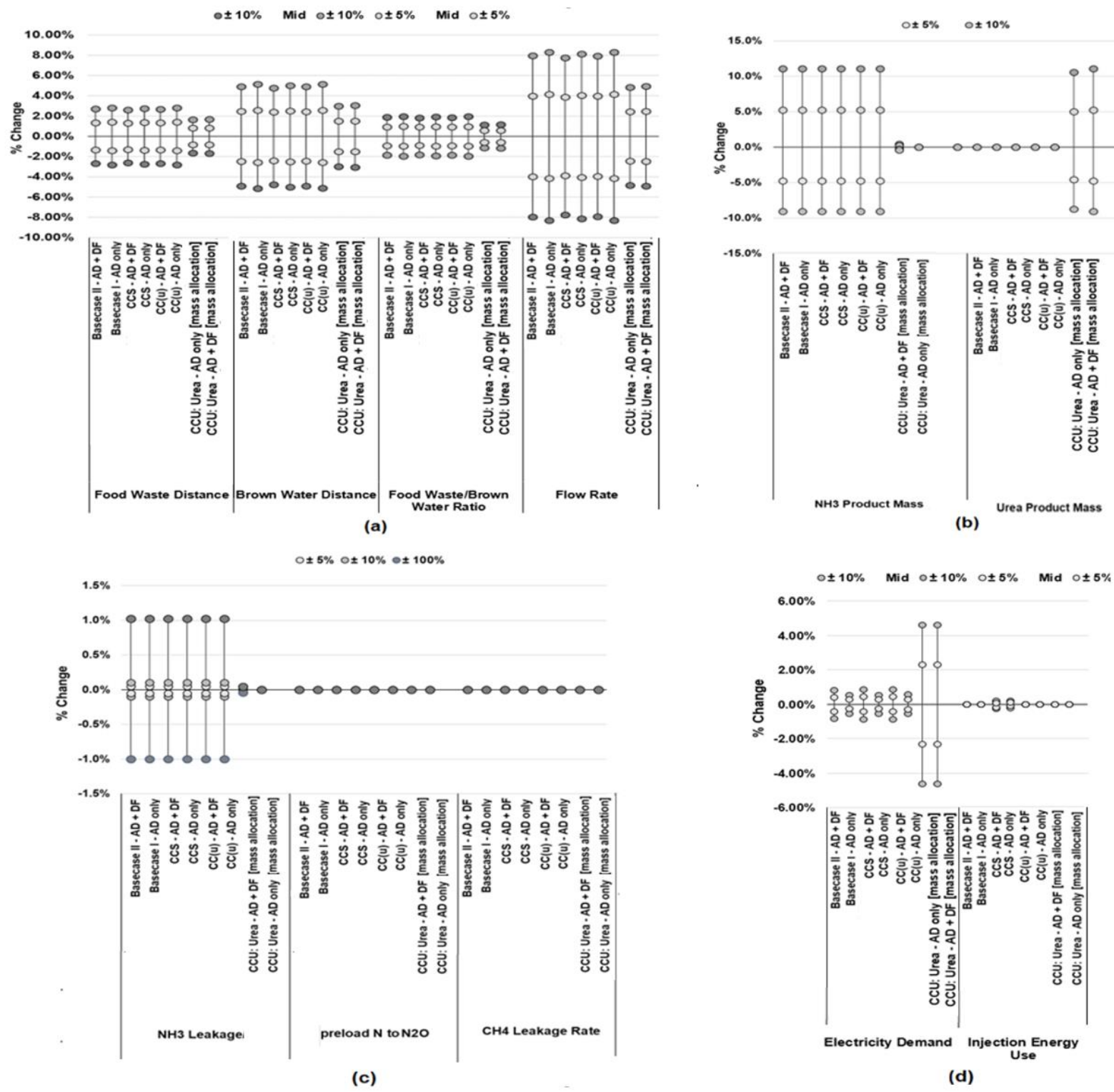


Fig. 6.25: Sensitivity of resources damage results for the production of waste-to-ammonia and ammonia+urea processes for all CO₂ fates for both AD-only and two stage (DF+AD technologies) via the default (with SOFC) configurations using mass allocation to changes in (a) feedstock parameters, (b) primary product yields, (c) leakage rates, and (d) electricity demand (Impact assessment method: ReCiPe2016 endpoint H/A).

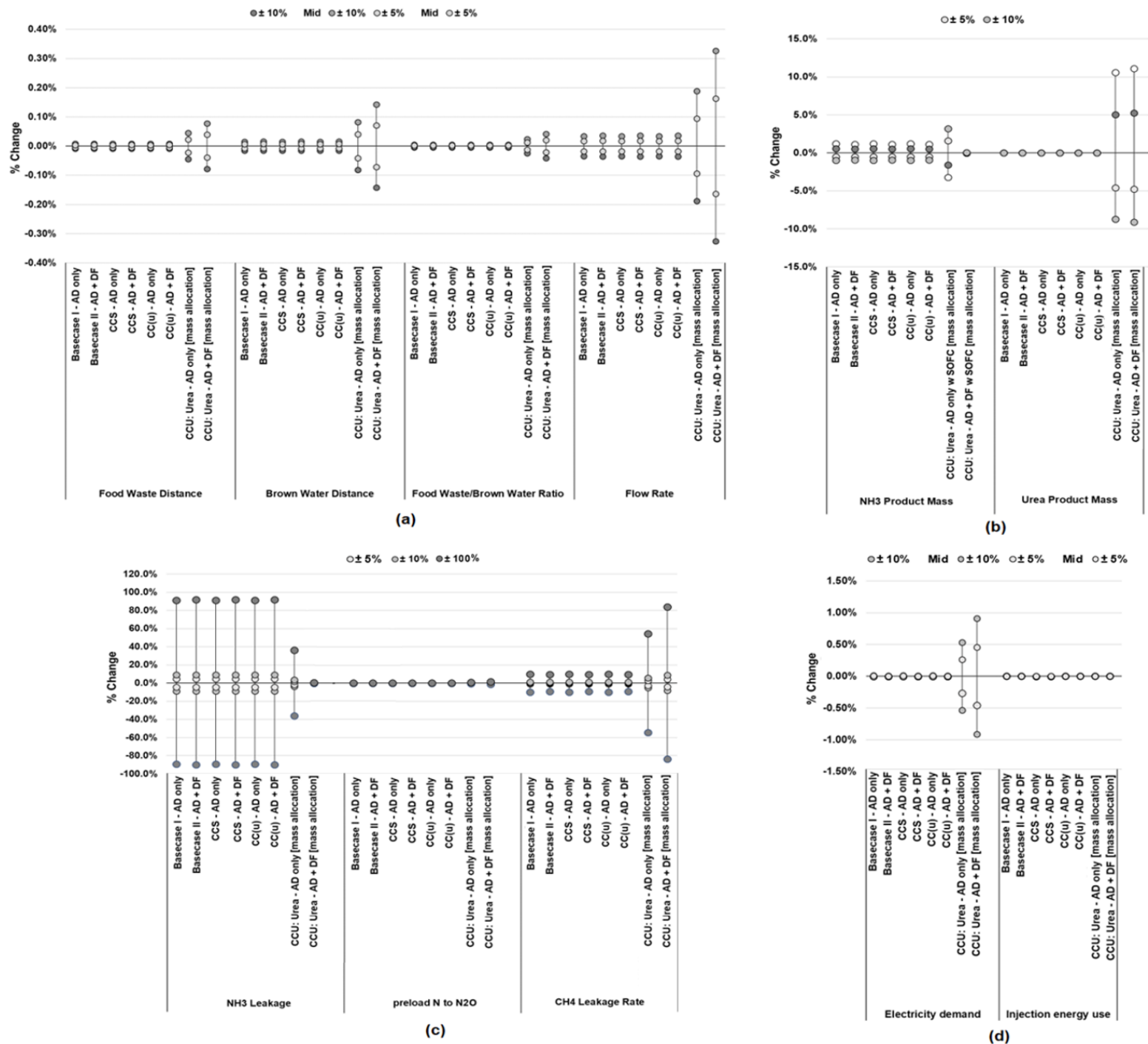
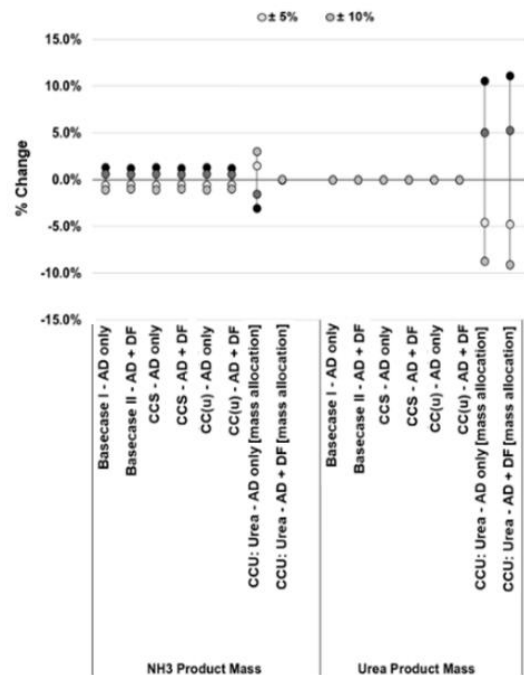
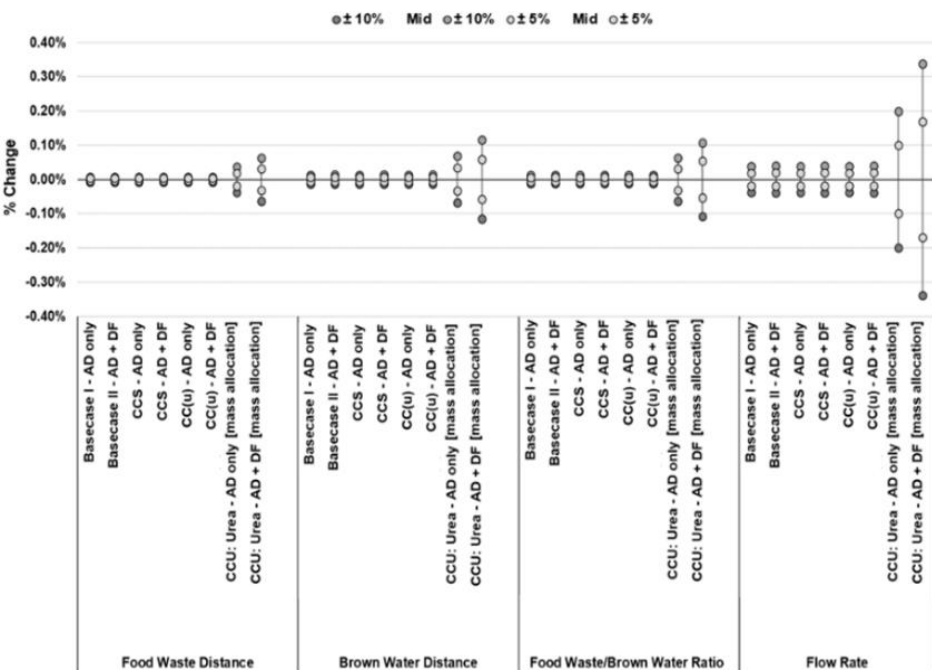
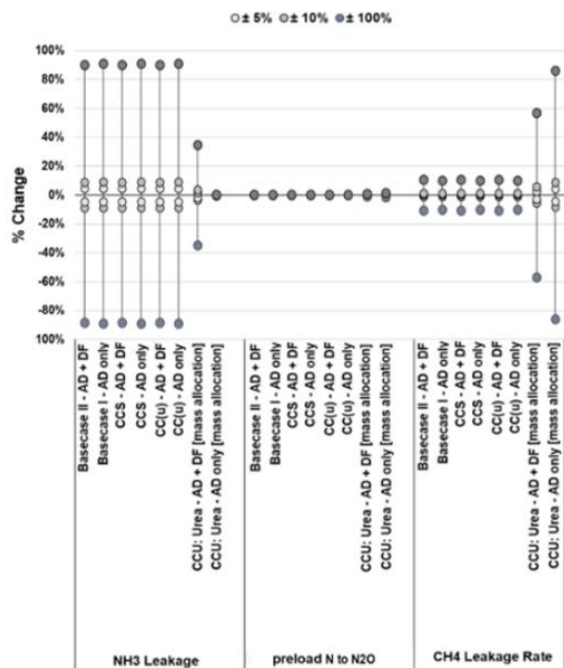


Fig. 6.26: Sensitivity of human health damage results for the production of waste-to-ammonia and ammonia+urea processes for all CO₂ fates for both AD-only and two-stage (DF+AD technologies) via the default (with SOFC) configurations using mass allocation to changes in (a) feedstock parameters, (b) primary product yields, (c) leakage rates, and (d) electricity demand (Impact assessment method: ReCiPe2016 endpoint H/A).

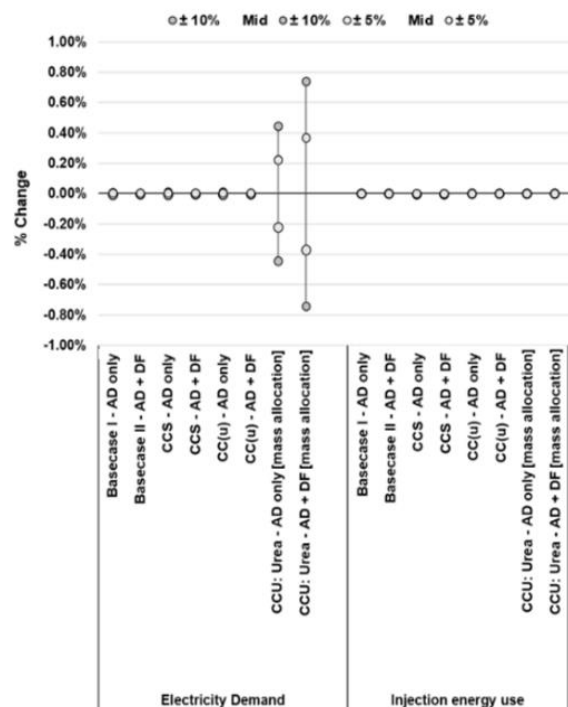


(a)

(b)



(c)



(d)

Fig. 6.27: Sensitivity of ecosystem damage results for the production of waste-to-ammonia and ammonia+urea processes for all CO₂ fates for both AD-only and two-stage (DF+AD technologies) via the default (with SOFC) configurations using mass allocation to changes in (a) feedstock parameters, (b) primary product yields, (c) leakage rates, and (d) electricity demand (Impact assessment method: ReCiPe2016 endpoint H/A).

6.6.3 Sensitivity analysis of water scarcity impacts to changes in water use (WSI, AWARE)

The results of the sensitivity analyses indicate that the water scarcity impacts, assessed with AWARE water use, are somewhat sensitive to the amount of water used for dilution and more so to DI water use. The much lower sensitivity to changes in external water added for dilution in scenarios where urea is produced is a result of the recirculation of the water byproduct. Since the water produced is utilized in the proposed process, the need for external sources of water is reduced (Fig. 6.28). The effect of varying the DI water volume for urea cases is higher compared to non-urea ones due to higher amount of DI water usage for the SOFEC with urea production. As all of the results in these figures use ammonia as the reference product, the impact in water scarcity is almost the same in all scenarios except for the urea cases, as urea is carrying a part of the environmental burden. The amount of that burden carried is determined by mass allocation. Therefore, the impact from DI water is higher, resulting in a large impact for the water scarcity compared to non-urea cases.

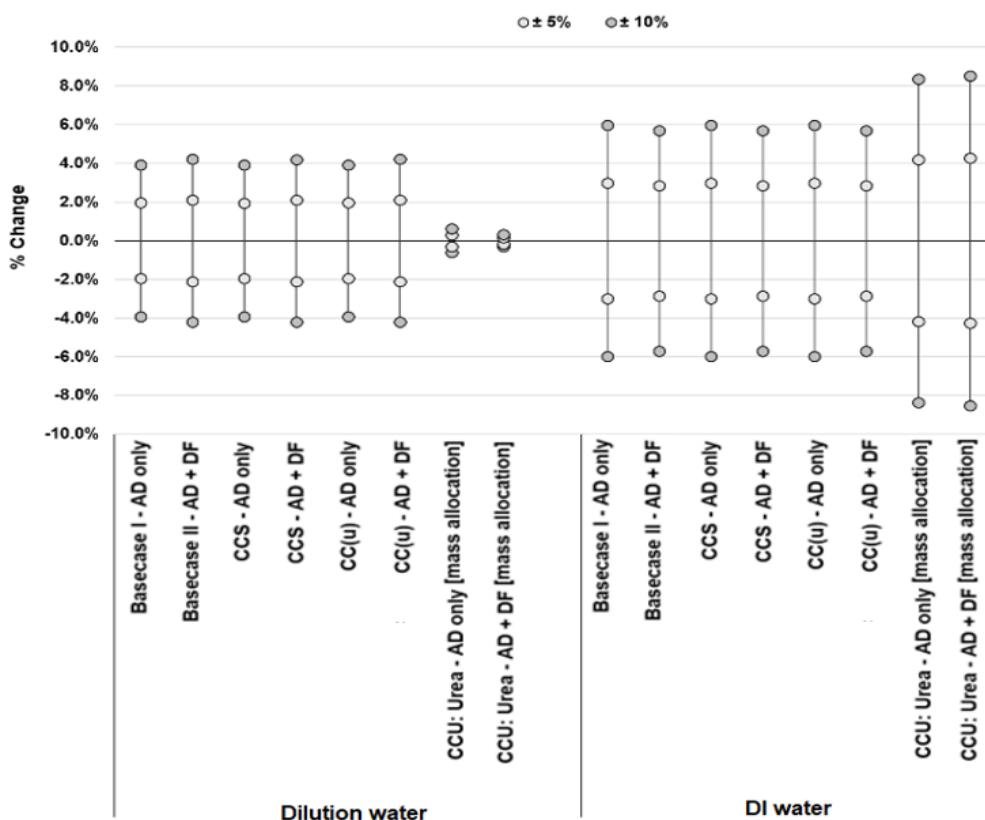


Fig. 6.28: Sensitivity of water scarcity results for the production of waste-to-ammonia and ammonia+urea processes for all CO₂ fates for both AD-only and two stage (DF+AD technologies) via the default (with SOFC) configurations using mass allocation to changes in (a) feedstock parameters, (b) primary product yields, (c) leakage rates, and (d) electricity demand (Impact assessment method: AWARE).

Conclusion

In this work, technologies developed based on SDP were assessed to emphasize GHG mitigation (CO₂ utilization) and waste utilization. The goal has been to determine whether a waste-based process designed first around CO₂ capture can compete with other available ammonia technologies on an environmental impact basis, with or without urea production. The ammonia production technologies are assessed for environmental performance from cradle-to-gate using two configurations, four CO₂ fates, including use for urea production, and several smaller variations, resulting in 72 assessed processes. Much of the success for reducing potential impacts in this study arises from the integration of novel and emerging membranes. This is a direct result of the design principles used where the LCA results validate this.

The results show that the emissions from leakage completely dominate the climate impacts of the studied process in every configuration even by using conventional (U.S.EPA) assumptions for emissions from methane, natural gas, and waste. Failing to prevent leakage undermines the effectiveness of new technologies such as the one presented in this study.

References

Bicer Y., Dincer, I., Zamfirescu, C., Vezina, G. and Raso, F., (2016). Comparative life cycle assessment of various ammonia production methods. *Journal of Cleaner Production* [online]. 135, 1379-1395. [Viewed 13 June 2021]. Available from: doi: 10.1016/j.jclepro.2016.07.023.

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Ramsden, T., (2013). *An Evaluation of the Total Cost of Ownership of Fuel Cell Powered Material Handling Equipment* No. HT12.8610 [online]. Colorado: NREL. [Viewed 13 October 2020]. Available from: <https://www.nrel.gov/docs/fy13osti/56408.pdf>.

Chapter 7

Conclusions and Future Work

This chapter brings together the main conclusions, contributions of the study, and the associated challenges along with future work.

This chapter was drafted based on the publications submitted to the International journal of hydrogen energy and Frontiers in energy research:

Ghavam, S., Taylor, C.M. and Styring, P., (2021). The life cycle environmental impacts of a novel sustainable ammonia production process from food waste and brown water. *Journal of Cleaner Production* [online]. 320, 128776. [Viewed 22 September 2021]. Available from: <https://doi.org/10.1016/j.jclepro.2021.128776>.

Ghavam, S., Taylor, C.M. and Styring, P., (2021). Modelling and Simulation of a Novel Sustainable Ammonia Production Process from Food Waste and Brown Water. *Frontiers in Energy Research* [online]. 9, 42. [Viewed 22 July 2021]. Available from: <https://doi.org/10.3389/fenrg.2021.600071>.

7. Conclusions

The aims of this research were to design a technology using SDPs and LCT and to carry out a techno-environmental assessment by producing an integrated modelling platform of multiple configurations of the core waste-based processes integrating several carbon capture/utilization options in order to determine whether they can compete with other existing ammonia production technologies in terms of energy and water consumption and environmentally on a full life cycle impact basis. All of these aims have been met.

A number of tasks were carried out in this study to devise a technology based on multiple configurations of core waste-based processes: Integrating several carbon capture/utilization options, produce a modelling platform for the family of technologies, determine optimal yields and operating parameters, and assess the potential life cycle environmental impacts. Through this process, the core technologies, DF+AD/AD-only were linked to nascent technology (emerging membranes) components into a previously non-existent process for optimization and assessment of the technological performance. These were implemented in a VBA modelling platform that was then used for generating inventory data for an LCA model utilized to assess the potential environmental impacts of all 72 potential configurations. The process and its model designed here provide a new technology for the utilization of mixed waste for the production of ammonia+urea, demonstrating the potential for variable waste stream mixes to support flexibility in deployment. The model can be tuned to reflect various operating conditions and wastes type ratios. This model also assesses whether the incorporation of internal energy generation or external renewable energy sources would be more appropriate for a given scenario. A detailed listing of the objectives associated with this body of work is presented in Table 1.4. All the objectives of the research were accomplished and the outcomes are presented below.

7.1 General achievements

The significant demand for ammonia and other hydrogen and nitrogen carriers will continue to drive innovation in sustainable ammonia technologies. Growth in global demand for clean energy carriers and agricultural nutrients pairs with growing global waste volumes. Together with the growth of global population and, consequently, N-rich waste streams, a clear opportunity arises. A novel process for ammonia production from Food Waste (FW) and Brown Water (BW) is proposed in this study. Since the inputs and outputs of this proposed ammonia production process are FW and BW, wastewater treatment and solid waste management facilities are resources of interest.

To assess this process, a mass and energy balance model has been developed using VBA software. The results of the model for each component in the proposed ammonia production process are based on 20 TPD of input waste. Modelled yields range from 47 TPD of NH₃ when the resultant CO₂ is released or captured, or 3.8 TPD of NH₃ and 76.5 TPD of urea when the system is designed to produce no unutilized CO₂. The modelling results indicate that yields can be comparable to other industrial processes, with significant environmental benefits when the fate of CO₂ is managed. When comparing the proposed ammonia processes to the literature data, water electrolysis powered by renewable technologies is the best of all processes in terms of GHG emissions while SMR coupled with Haber-Bosch (H-B) has the lowest water consumption of all the processes mentioned.

Insights from the technology integrations show that the inclusion of SOFC has a negligible effect on electricity consumption. The negligible reduction in electricity consumption means that including SOFC provides no benefit and including it would serve only to increase complexity and add an additional potential point of failure. While inclusion of SOFC was ultimately not useful in displacing energy use, selection of renewable electricity options, such as on-site solar production, can counterbalance this in those scenarios where SOFC is not utilized. The LCA results indicate that the two-stage process using SOFC is the most efficient for GHG emissions, abiotic depletion, and human toxicity compared to the AD-only process. However, the comprehensive modelling of configurations demonstrated that AD alone is sufficient, and, indeed, more productive, indicating that the inclusion of DF reactors, while interesting, isn't the most optimal option for product yields.

All process configurations assessed here would result in lower GHG emissions per kg NH₃ and kg urea compared to conventional and renewable technologies. The non-urea processes generate approximately 90% lower GHG impact for GWP₁₀₀. In comparison to water electrolysis, a rapidly emerging and potentially sustainable technology, the GHG impact for urea cases under both GWP₁₀₀ and GWP_{biogenic} impact assessment methods are approximately 90% lower. The integration of novel and emerging membrane technologies is a crucial component of the waste-to-ammonia and urea processes. Their optimal performance with low energy draw directly contributes to the relative benefit of this technology over alternatives and the results indicate that the production impacts of these membranes and their components are insignificant to the total life cycle impacts. The LCT and SDP focus, validated by the LCA analyses of 72 configurations, resulted in a unique and flexible process. A major factor enabling this is the integration of these emerging membranes.

Acidification and eco-toxicity in the proposed processes are higher compared to the library processes for conventional ammonia production and the values in the literature. The relatively high leakage assumptions used here for the new technologies result in higher acidification impacts than that found with conventional processes, which may reflect either an underestimate in general leakage (as has been recently suggested in Bicer et al. (2016) and Wernet et al. (2016)) or an over-estimate of potential leakage in the proposed processes based on conservative values. The higher ecotoxicity impacts result from the construction of solar cells. However, shifting the energy source for the proposed process from solar to grid will result in a significant increase in GWI and all three damage categories. This is a classic example of trade-off and potential burden shifting.

An important implication of the proposed analysis is that controlling/avoiding leakage is an essential element of sustainable, climate safe design. For both two-stage and AD-only cases, impacts are driven primarily by N efficiency (primary product yields) and by leakage of methane (potential GHG emissions) and ammonia (potential human health and ecosystem damages). Emissions from leakage completely dominate the climate impacts of the studied process in every configuration even with conventional (U.S.EPA) assumptions for emissions from methane, natural gas, and waste. Failing to prevent leakage undermines the effectiveness of new technologies such as the one presented in this study, and the fact that highly toxic gases can be contained at scale, suggests that this is not an insurmountable issue.

The impact from abiotic depletion, GHG emissions, and human toxicity shows that this process is environmentally viable compared to fossil-based and renewable technologies.

7.2 Challenges associated with this study and future work

In some instances, the studied green-ammonia technology may not be the optimal technology option because it is based on urban and semi-urban waste and has some constraints on where it can be sited economically, whereas the conventional technologies generally based on natural gas do not have this limitation and are flexible in where they can be deployed. However, the novel set of technologies assessed in this study competes very well on a life cycle environmental basis and has significant potential for benefits, including avoided emissions. In order to clearly address the problem associated with the reduction of water in ammonia production processes, meta-analysis of various technologies and stages for ammonia production is required. These factors need to be addressed in future studies.

Additional research is needed in a few key areas of research on the production of ammonia/ammonia+urea through waste utilization, environmental impact of water usage for ammonia production and where an ammonia production plant needs to be located, in terms of both availability of feedstock and sustainability (accessibility to renewable energy sources such as solar PV and wind power, distance from the waste hub to the production plant, etc.). Location is an important factor in the development of sustainable production methods, for maximizing productivity and sustainability in the production of chemical compounds such as ammonia. Future work may also involve looking at linking recovery of other nutrients from BW which is rich in phosphorous (P) and potassium (K) that can be used for fertilizer production, as has begun being explored elsewhere. In addition, more detailed modelling of biological aspects/microbial behavior in the digester and fermenter and/or a full waste treatment model integrated with this system may be of use.

The process designed here and components utilized in it are in many cases at earlier stages of development (low TRL), so that the system and consequently, calculated impacts with fixed leakage show relatively high LCA uncertainty due to the speculative nature and the few contributors to impact. Higher resolution analysis of the various membranes incorporated in this study and their fabrication are important next steps in exploring this technology, as is narrowing practical leakage constraints. The ~99.9% recovery/FE considered in membranes were models carried out as a screening analysis with coarse grain data to establish the model and the suitable boundaries. Therefore, it is recommended that a multicriteria approach is adopted where a number of scenarios are run with increasingly fine inputs. In real world operation for the separation of high gas volumes it would be useful to incorporate a unit operation along with a membrane to achieve higher gas separation efficiency.

Appendix A: VBA Code

A.1 DF+AD+UREA Codes

```
1. Sub Sheet3_Button1_Click()
2.
3. '=====
4. '=====
5. '                DARK-BIO
6. Dim NUMTANKD As Integer, NUMTANKAB As Integer
7. '..... FOOD .....
8. '                Main DATA INPUT
9. '                Main DATA INPUT
10. H2OTEMPXX = ActiveWorkbook.Worksheets("SOFC").Cells(31, 4)
11. FLAG = 0
12. Pi = 3.14
13. TAMB = 25
14. TAMBK = TAMB + 273
15. MF1 = Cells(4, 4) 'Mass of Food (Kg /Day)
16. FWR = Cells(5, 4) 'Water Dilution Ratio for Feed
17. WD = MF1 * FWR 'H2O Mass (Kg/day)
18. Cells(6, 4) = WD 'H2O Mass (Kg/day)
19. MF = MF1 + WD + VRRKG 'Mass of Food after dilution (Kg/day)
20. FTOFC = Cells(7, 4) 'Ratio Food to Faeces
21. MFC = MF1 / FTOFC 'Mass of Faeces (Kg/Day)
22. Cells(8, 4) = MFC 'Mass of Faeces (Kg/Day)
23. RPVTS = Cells(32, 4) 'Ratio of VS/TS
24. PDFB = Cells(40, 4) 'Pressure Bio Reactor IN (atm.)
25. HRTD = Cells(43, 4)
26. TEMPD = Cells(42, 4) 'Dark Reactor Temperature oC
27. TEMPA = Cells(55, 4) 'Anaerobic Reactor Temperature oC
28. ADBP = Cells(56, 4) 'anaerobic Reactor Pressure (atm.)
29. HRTB = Cells(50, 4) 'Hydraulic Residence Time (day)
30. 'Densities
31. RHOFW = Cells(36, 4) 'Density of FW (KG/M^3)
32. RHOFW = Cells(37, 4) 'Density of FCW (KG/M^3)
33. GH56 = (WD + MF1) / ((WD / 1000) + (MF1 / RHOFW))
34. RHOMIX = (WD + MF1 + MFC) / (((WD + MF1) / (GH56)) + (MFC / RHOFW))
35. Cells(38, 4) = RHOMIX 'Density of Mixture (KG/M^3)
36. RHOMIXBNM = RHOMIX
37. Cells(61, 4) = RHOMIXBNM
38.
39. 'Food Input
40. MFV = MF / RHOFW 'Volume of Food (m^3/day)
41. Cells(10, 4) = MFV 'Volume of Food (m^3/day)
42. PTSF = Cells(11, 4) '% TS FOOD
43. PVSF = Cells(12, 4) '% VS FOOD
44. TCODF1 = Cells(13, 4) '% TCOD FOOD
45. SCODF1 = Cells(14, 4) '% SCOD FOOD
46. TKNF1 = Cells(15, 4) '% TKN FOOD
47. CHF1 = Cells(16, 4) '% of Carbohydrate content in food
48. PHF = Cells(17, 4) '% pH of food
49. '..... Food Output
50. TSF = MF * PTSF / 100 'TS Food (Kg/day)
51. VSF = MF * PVSF / 100 'VS Food (Kg/day)
52. TCODF = MF * TCODF1 / 100 'TCOD Food (Kg/day)
53. SCODF = MF * SCODF1 / 100 'SCOD Food (Kg/day)
54. TKNF = MF * TKNF1 / 100 'TKN Food (Kg/day)
55. CHF = MF * CHF1 / 100 'Carbohydrate content (Kg/day)
56. NH3F = MF * NH3F1 / 100 'TKN Food (Kg/day)
```

```

57. H2SF = MF * H2SF1 / 100 'H2S Food (Kg/day)
58. ' Cells
59. Cells(5, 9) = WD 'H2O Mass (Kg/day)
60. Cells(6, 9) = MF 'Mass of Food after dilution (Kg/day)
61. Cells(6, 10) = TSF 'TS Food (Kg/day)
62. Cells(6, 11) = VSF 'VS Food (Kg/day)
63. Cells(6, 12) = TCODF 'TCOD Food (Kg/day)
64. Cells(6, 13) = SCODF 'SCOD Food (Kg/day)
65. Cells(6, 14) = TKNF 'TKN Food (Kg/day)
66. Cells(6, 15) = CHF 'CHF Food (Kg/day)
67. '..... Faeces Input
68. MFCV = MFC / RHOFWC 'Volume of Faeces (m^3/day)
69. Cells(19, 4) = MFCV 'Volume of Faeces (m^3/day)
70. PTSFC = Cells(20, 4) '% TS Faeces
71. PVSFC = Cells(21, 4) '% VS Faeces
72. TCODFC1 = Cells(22, 4) '% TCOD Faeces
73. SCODFC1 = Cells(23, 4) '% SCOD Faeces
74. TKNFC1 = Cells(24, 4) '% TKN Faeces
75. CHFC1 = Cells(25, 4) '% of Carbohydrate content in Faeces
76. PHFC = Cells(26, 4) '% pH of Faeces
77. '..... Faeces Output
78. TSFC = MFC * PTSFC / 100 'TS Faeces (Kg/day)
79. VSFC = MFC * PVSFC / 100 'VS Faeces (Kg/day)
80. TCODFC = MFC * TCODFC1 / 100 'TCOD Faeces (Kg/day)
81. SCODFC = MFC * SCODFC1 / 100 'SCOD Faeces (Kg/day)
82. TKNFC = MFC * TKNFC1 / 100 'TKN Faeces (Kg/day)
83. CHFC = MFC * CHFC1 / 100 'Faeces Carbohydrate content (Kg/day)
84. ' Cells
85. Cells(7, 9) = MFC 'Mass of Faeces Kg/day)
86. Cells(7, 10) = TSFC 'TS Faeces(Kg/day)
87. Cells(7, 11) = VSFC 'VS Faeces (Kg/day)
88. Cells(7, 12) = TCODFC 'TCOD Faeces (Kg/day)
89. Cells(7, 13) = SCODFC 'SCOD Faeces (Kg/day)
90. Cells(7, 14) = TKNFC 'TKN Faeces (Kg/day)
91. Cells(7, 15) = CHFC 'CHF Faeces (Kg/day)
92. '..... MIXTURE .....
93. '.....Mixed IN
94. TCODMIX = Cells(33, 4)
95. BODMIX = 0.6 * TCODMIX
96. Cells(48, 4) = BODMIX
97. SCODMIX = Cells(34, 4)
98. TFVA = Cells(35, 4)
99. '===== Mixed OUT =====
100. MMIX = MF + MFC + VRRKG 'Mass of Mixture (kg/day)
101. If FLAG = 0 Then
102. VOLMIX = MMIX / RHOMIX 'Volume of Mixture (m^3/day)
103. GoTo 12
104. Else
105. VOLMIX = VOLMIX + VRR
106. 12 End If
107. 'TS (FOOD WASTE) AFTER DILUTION
108. TSA = PTSF * 0.346 'TS AFTER DILUTION
109. PTSMIX = (((MF * TSA / 100) + (MFC * PTSFC / 100) + VRRKG * TSREC / 100) / MMIX) * 100 '% TS MIXED (Kg/day)
110. PVSMIX = PTSMIX * RPVTS '% VS MIXED (Kg/day)
111. 'Mixed (Kg/day)
112. MTSMIX = MMIX * PTSMIX / 100 'TS MIXED (Kg/day)
113. MVSMIX = MMIX * PVSMIX / 100 'VS MIXED (Kg/day)
114. MTCODMIX = MMIX * TCODMIX / 100 'TCOD MIXED (Kg/day)
115. MSCODMIX = MMIX * SCODMIX / 100 'SCOD MIXED (Kg/day)
116. 'Cells
117. Cells(28, 4) = MMIX 'Mass of Mixture (kg/day)
118. Cells(29, 4) = VOLMIX 'Volume of Mixture (m^3/day)
119. Cells(30, 4) = PTSMIX '% TS MIXED
120. Cells(31, 4) = PVSMIX '% VS MIXED
121. Cells(32, 4) = RPVTS 'Ratio of VS/TS

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122. Cells(8, 9) = MMIX      'Flow Rate of Mixed Waste (kg/day)
123. Cells(8, 10) = MTSMIX  'TS MIXED (Kg/day)
124. Cells(8, 11) = MVSMIX  'MTCODMIX (Kg/day)
125. Cells(8, 12) = MTCODMIX 'MTCODMIX (Kg/day)
126. Cells(8, 13) = MSCODMIX 'MTCODMIX (Kg/day)
127. '=====
128. '..... ACIDOGENIC REACTOR .....
129. GTSMIX = MTSMIX * 1000 / MMIX      'TS MIX (g/L)
130. GVSMIX = MVSMIX * 1000 / MMIX      'VS MIX (g/L)
131. GTCODMIX = MTCODMIX * 1000 / MMIX  'TCOD MIX (g/L)
132. GSCODMIX = MSCODMIX * 1000 / MMIX  'TCOD MIX (g/L)
133. GTVFAMIX = (TFVA * 10)              'TFVA MIX (g/L)
134. 'Cells
135. Cells(11, 9) = GTSMIX
136. Cells(12, 9) = GVSMIX
137. Cells(13, 9) = GTCODMIX
138. Cells(14, 9) = GSCODMIX
139. Cells(15, 9) = GTVFAMIX
140. 'OUTPUT of INPUT as %
141. Cells(11, 10) = GTSMIX / 10
142. Cells(12, 10) = GVSMIX / 10
143. Cells(13, 10) = GTCODMIX / 10
144. Cells(14, 10) = GSCODMIX / 10
145. Cells(15, 10) = GTVFAMIX / 10
146. 'Cells Input
147. PHM = Cells(41, 4)
148. 'TD = Cells(43, 4)
149. RMIC = Cells(47, 4)  'Ratio of Micro
150. H2DARK = Cells(58, 4) 'Ratio of H2 from Dark to Anaerobic
151. CH4BIORAC = Cells(59, 4)
152. 'Calculations
153. 'Effluent (E)
154. TSE = (PTSMIX * 0.479) * 10
155. VSE = (0.5) * GVSMIX
156. KH = -((1 / HRTD) * Logn(VSE / GVSMIX))
157. SRT = 1 / KH
158. Cells(44, 4) = KH      'First Order Constant for H2 (1/day)
159. Cells(11, 16) = SRT   'SRT Effluent (g/L)
160. TCODE = GTCODMIX * 0.36
161. SCODEF = TCODE * 0.413
162. TVFAE = (TCODMIX * 0.07) * 10
163. OLR = (GVSMIX * KH * VSE) / (GVSMIX - VSE) 'Organic Loading Rate (gVS/L.day)
164. 'Cells Out
165. Cells(44, 4) = KH      'First Order Constant for H2 (1/day)
166. Cells(46, 4) = OLR     'Organic Loading Rate (gVS/L.day)
167. Cells(11, 12) = TSE    'TSE Effluent (g/L)
168. Cells(12, 12) = VSE    'VSE Effluent (g/L)
169. Cells(13, 12) = TCODE  'TCODE Effluent (g/L)
170. Cells(14, 12) = SCODEF 'SCODE Effluent (g/L)
171. Cells(15, 12) = TVFAE  'TVFAE Effluent (g/L)
172. 'Effluent (%)
173. TSEP = TSE / 10
174. VSEP = VSE / 10
175. TCODEP = TCODE / 10
176. SCODEP = SCODEF / 10
177. TVFAEP = TVFAE / 10
178. 'Cells out
179. Cells(11, 13) = TSEP   'TSE Effluent (%)
180. Cells(12, 13) = VSEP   'VSE Effluent (%)
181. Cells(13, 13) = TCODEP 'TCODE Effluent (%)
182. Cells(14, 13) = SCODEP 'SCODE Effluent (%)
183. Cells(15, 13) = TVFAEP 'TVFAE Effluent (%)
184. 'Reactor
185. 'Substrate
186. H2PERD = H2DARK

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187. Cells(17, 16) = H2PERD
188. VW = VOLMIX * HRTD 'Useful Volume (m^3)
189. SOBSRT = OLR * HRTD 'Amount of Substrate [Yield of Biogas] (kgCs/m^3) ...[S]
190. MU = 0.83 - (0.028 * VSEP) 'Theoretical Biogas Yield (m^3/kgVS)
191. YGPR = (MU * KH * VSE) / SOBSRT 'Biogas Yield = Specific Gas Production Rate (m^3/kgVS)
192. QBIOGAS = MMIX * YGPR
193. GASPR = YGPR * OLR 'Gas Production Rate (1/day)
194. Cells(17, 10) = GASPR
195. Cells(18, 10) = QBIOGAS 'Biogas Production Rate (m^3/day)
196. Cells(19, 10) = YGPR 'Biogas Yield (m^3/kgVS)
197. Cells(17, 16) = H2PERD
198. 'Useful Volume of Dark Bioreactor
199. VOLREACTOR = VW + 0.15 * VW 'Volume of Dark Bioreactor (m^3)
200. 'YIELD
201. YEXP = (H2PERD / 100) * YGPR
202. TOTBIOR = 100
203. CO2PER = TOTBIOR - H2PERD 'H2Yield (m^3/kgVS)
204. CO2YIELD = YGPR - YEXP 'CO2 Yield (m^3/kgVS)
205. BIOYIELD = YGPR
206. 'Cells Output-1
207. Cells(18, 16) = CO2PER
208. Cells(19, 16) = TOTBIOR
209. Cells(10, 16) = VOLREACTOR 'Working Volume (m^3)
210. Cells(12, 16) = OLR 'OLR Effluent (g/L)
211. Cells(13, 16) = MU 'Theoretical Biogas Yield (m^3/kgVS)
212. 'Cells Output-2
213. Cells(17, 13) = YEXP 'H2 Yield (m^3/kgVS)
214. Cells(18, 13) = CO2YIELD 'CO2 Yield (m^3/kgVS)
215. Cells(19, 13) = BIOYIELD 'BIOGAS Yield (m^3/kgVS)
216. H2VAR = QBIOGAS * H2PERD / 100
217. CO2VAR = QBIOGAS * CO2PER / 100
218. TOTVAR = QBIOGAS
219. TOTVARGT = H2VAR + CO2VAR
220. Cells(17, 20) = H2VAR
221. Cells(18, 20) = CO2VAR
222. Cells(19, 20) = TOTVARGT
223. '*****
224. ' OUTPUT FOR MFI (% H2, %CO2)'
225. '*****
226. T = TEMPD
227. RHOH2 = H2DENSITY(T) 'T=°C,Kg/m^3
228. RHOCO2 = CO2DENSITY(T) 'T=°C,Kg/m^3
229. RHOCH4 = CH4DENSITY(T) 'T=°C,Kg/m^3
230. 'Mass
231. H2MASSOUT = H2VAR * RHOH2 'H2 OUT (kg/day)
232. CO2MASSOUT = CO2VAR * RHOCO2 'CO2 OUT (kg/day)
233. TOTALGDK = H2MASSOUT + CO2MASSOUT 'Total Mass OUT
234. TOTALVOL = H2VAR + CO2VAR 'Total Volume Out (Kg/m^3)
235. RREEWW = TOTALVOL / (H2VAR + CO2VAR) 'Density of biogas from DF'
236. TOTALGDKF = RREEWW * TOTALVOL
237. 'Cells OUT
238. RTFDDEH2 = (H2PERD / 100) * 2
239. RTFDDECO2DF = (CO2PER / 100) * 44
240. TREETREER = RTFDDEH2 + RTFDDECO2DF
241. FTUUO0IDFH2 = RTFDDEH2 / TREETREER
242. FTUUO0IDFCO2 = RTFDDECO2DF / TREETREER
243. H2MASSOUT = TOTALGDKF * FTUUO0IDFH2
244. CO2MASSOUT = TOTALGDKF * FTUUO0IDFCO2
245. Cells(10, 20) = H2MASSOUT 'H2 OUT (kg/day)
246. Cells(11, 20) = CO2MASSOUT 'CO2 OUT (kg/day)
247. Cells(12, 20) = TOTALGDKF 'Total OUT (kg/day)
248. Cells(13, 20) = TEMPD 'REACTOR Temperature (°C)
249. Cells(14, 20) = PDFB 'REACTOR Pressure (atm)
250. Cells(15, 20) = TOTALVOL 'Total Volume (m^3/day)
251. '=====

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252. '..... CSTR'DF' .....
253. '=====
254. 'CSTRT = HRTD ' <<<===== Digested Time
255. CSTRDARKV = VOLREACTOR 'VOLUME of CSTR (m3)
256. CSTRDARKD = (CSTRDARKV * 2 / 3.14) ^ (1 / 3) 'Diameter of CSTR (m)
257. CSTRDARKH = CSTRDARKD * 2 'Height of CSTR (m)
258. CSTR = (2 * 3.14 * (CSTRDARKD / 2) * CSTRDARKH) + (2 * 3.14 * ((CSTRDARKD / 2) ^ 2)) 'Area of CSTR (m2)'To be print'
259. CSTRDARKV1 = VW 'VOLUME of CSTR (m3)
260. CSTRDARKD1 = (CSTRDARKV1 * 2 / 3.14) ^ (1 / 3) 'Diameter of CSTR (m)
261. CSTRDARKH1 = CSTRDARKD1 * 2 'Height of CSTR (m)
262. 'Cells..... CSTR
263. Cells(14, 16) = CSTRDARKD 'Diameter of CSTR (m)
264. Cells(15, 16) = CSTRDARKH 'Height of CSTR (m)
265. '=====
266. ' TANK DESIGN (DARK MIXER)
267. '=====
268. RHOACETACID = 1037.38 'DENSITY OF ACETIC ACID 'Density of Acetic Acid (kg/m3)
269. MMIXG = MMIX * 1000
270. FAO = MMIXG / RHOACETACID
271. TANKV9 = VW
272. MAXVOL = 50
273. NUMTANKD = VW / MAXVOL
274. If NUMTANKD < 1 Then
275. NUMTANKD = 1
276. Else
277. End If
278. '...RATE
279. 'Input Feed of Mixture (mol/g)
280. X1 = (1 - (VSE / GVSMIX)) 'Conversion Rate of Dark Fermentation'
281. 'AGITATOR DIMENSIONS FOR Dark fermentation'
282. IMPDAD = (CSTRDARKD / 3) 'Impeller diameter (m)
283. EMDAD = IMPDAD 'Impeller height above bottom of vessel(m)
284. LMPDAD = (IMPDAD / 4) 'Length of Impeller blade (m)
285. WMPDAD = (IMPDAD / 5) 'Width of Impeller blade(m)
286. WBAFD = (CSTRDARKD / 10) 'Width of baffle(m)
287. NOIMPD = 2 'Number of impellers
288. NOIMBPLD = 6 'Number of impeller blades
289. 'SHAPE FACTORS OF BLADES AS FOLLOWS 6BLADE'
290. DISTBD = IMPDAD 'Distance between two consecutive impellers (m)
291. S1BIOD = IMPDAD / CSTRDARKD 'Shape Factor(m)
292. S2BIOD = EMDAD / CSTRDARKD 'Shape Factor(m)
293. S3BIOD = LMPDAD / IMPDAD 'Shape Factor(m)
294. S4BIOD = WMPDAD / IMPDAD 'Shape Factor(m)
295. S5BIOD = WBAFD / CSTRDARKD 'Shape Factor(m)
296. S6BIOD = CSTRDARKH1 / CSTRDARKD 'Shape Factor(m)
297. 'Velocity of agitation
298. TVELAGD = 2 'Velocity of agitation
299. 'Speed of impellers'
300. SPEIMPD = ((TVELAGD) / (3.14 * IMPDAD)) * 60 '(RPM)
301. FT5 = (RHOMIX * (0.99))
302. DENDARK7 = (MMIX + KGOUTR) / ((KGOUTR / FT5) + (MMIX / RHOMIX)) 'DENSITY'
303. 'Energy impellers HORSEPOWER'
304. IMPHPD = (((NOIMBPLD) * (((SPEIMPD) * (0.016)) ^ (3)) * ((IMPDAD) ^ (5)) * (DENDARK7)) / (2447.578)) * NUMTANKD '(HP)'
305. RTEEQWSTDARK = (KGINADBR / FT5) - (KGINDARK / RHOMIX) 'Volume of solid in the DF'
306. POWBIO5 = IMPHPD * NUMTANKD 'Total Power for Total number of Vessels
307. 'IMPELLER EFFICIENCY'
308. EFF1G = Cells(47, 12) 'Efficiency of impellers(%)<=====
309. 'Power by considering the efficiency of impeller'
310. POWBIO5G = IMPHPD * ((EFF1G / 100))
311. 'Baffle design'
312. NOBAFD = 4 'Number of Baffles
313. WBAFD = ((CSTRDARKD) / (10)) 'Width of baffle (m)
314. HBAFLD = CSTRDARKH1 'HEIGHT of baffle (m)
315. 'corrosion allowance'
316. CORAL4 = ((2) * (10) ^ (-3)) 'Corrosion allowance (m)

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317. 'Wall thickness'
318. PSBIORACF = (RHOFW * (9.81) * CSTRDARKH) * 0.0000986 'Static pressure (atm)
319. POP1T = 0.0144 'OPERATIONAL PRESSURE (atm)
320. PTOTH5 = POP1T + PSBIORACF 'Maximum allowance pressure(atm)
321. 'Cells
322. Cells(35, 12) = NUMTANKD
323. Cells(36, 12) = FAO 'INPUT FLOW OF WASTE in (g/day)
324. Cells(37, 12) = X1 'Conversion Rate %
325. Cells(38, 12) = IMPDAD 'Impeller diameter (m)
326. Cells(39, 12) = EMDAD 'Impeller height above bottom of vessel(m)
327. Cells(40, 12) = LMPDAD 'Length of Impeller blade (m)
328. Cells(41, 12) = WMPDAD 'Width of Impeller blade(m)
329. Cells(42, 12) = NOIMPD 'Number of Propellers
330. Cells(43, 12) = NOIMBPLD 'Number of impeller blades
331. Cells(44, 12) = TVELAGD 'Velocity of agitation
332. Cells(45, 12) = SPEIMPD 'Rotation per minute (RPM)
333. Cells(46, 12) = IMPHPD 'Impeller Horse Power (HP)
334. Cells(48, 12) = POWBIO5G 'Impeller Horse Power at EFFICIENCY (HP)
335. Cells(49, 12) = NOBAFD 'Number of Baffles
336. Cells(50, 12) = WBAFLD 'Width of baffle (m)
337. Cells(51, 12) = HBAFLD 'HEIGHT of baffle (m)
338. Cells(52, 12) = CORAL4 'Corrosion allowance (m)
339. Cells(53, 12) = PSBIORACF 'Static pressure (atm)
340. Cells(54, 12) = POP1T 'OPERATIONAL PRESSURE (atm)
341. Cells(55, 12) = PTOTH5 'Maximum allowance pressure(atm)
342. 'Shape Factor
343. Cells(57, 12) = S1BIOD 'Shape Factor(m)
344. Cells(58, 12) = S2BIOD 'Shape Factor(m)
345. Cells(59, 12) = S3BIOD 'Shape Factor(m)
346. Cells(60, 12) = S4BIOD 'Shape Factor(m)
347. Cells(61, 12) = S5BIOD 'Shape Factor(m)
348. Cells(62, 12) = S6BIOD 'Shape Factor(m)
349. '=====
350. ' ANAEROBIC DIGESTER
351. '=====
352. H2SP = Cells(53, 4) 'H2S Percent %
353. NH3P = Cells(54, 4) 'NH3 Percent %
354. '.....EFFLUENT
355. VSREM1 = Cells(22, 13) 'Volatile Fatty Acids Removed (%)
356. CODREM1 = Cells(23, 13) 'COD Removed (%)
357. TSEBP = TSEP * 2.4 / 4.3 'TS OUT as (%)
358. VSREM = 100 - VSREM1 'VS removed as (%)
359. VSEPB = (VSE / 10) * VSREM / 100 'VS OUT as (%)
360. CODREM = 100 - CODREM1 'COD Removed (%)
361. CODEP = TCODEP * CODREM / 100 'Chemical Oxygen Demand (%)
362. VFAEP = TCDOMIX * 0.035 'Volatile Fatty Acid (%)
363. 'Cells Kg/m^3 OUT
364. TSEBG = TSEBP * 10 'TS effluent (g/L) or (Kg/m3)
365. VSEGB = VSEPB * 10 'VS effluent (g/L) or (Kg/m3)
366. CODEG = CODEP * 10 'COD effluent (g/L) or (Kg/m3)
367. VFAEG = VFAEP * 10 'Volatile Fatty Acids (g/L) or (Kg/m3)
368. 'Cells
369. Cells(23, 9) = TSEBG 'TS effluent (g/L) or (Kg/m3)
370. Cells(24, 9) = VSEGB 'VS effluent (g/L) or (Kg/m3)
371. Cells(25, 9) = CODEG 'COD effluent (g/L) or (Kg/m3)
372. Cells(26, 9) = VFAEG 'Volatile Fatty Acids (g/L) or (Kg/m3)
373. 'Cells % OUT
374. Cells(23, 10) = TSEBP 'TS effluent(%)
375. Cells(24, 10) = VSEPB 'VS effluent(%)
376. Cells(25, 10) = CODEP 'COD effluent(%)
377. Cells(26, 10) = VFAEP 'Volatile Fatty Acids Produced (%)
378. 'Sludge
379. TSOUT = TSEBP * 1.1 / 2.7 'TS rejected (%)
380. TSREC = TSEBP - TSOUT 'TS recycled (%)
381. Cells(27, 9) = TSREC * 10 '<=====

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382. 'Cells OUT
383. Cells(25, 13) = TSREC 'TS RECYCLED (%)
384. Cells(26, 13) = TSOUT 'TS rejected (%)
385. 'Recycle,Rates and Volume
386. MAXPRO = 2 'Recirculation rate (m^3/day)
387. VRR = VOLMIX * MAXPRO 'Recycled Volume (m^3/day)
388. VRRKG = MMIX * TSREC / PTSMIX 'Recycled Volume (kg/day) Ratio of Mixed to recycling
389. RB1 = (MMIX * TSREC) / (PTSMIX) 'To be print''flow rate of recycled(kg/day)'
390. QBIOL = MMIX + RB1 - TOTALGDK
391. VOLRBIOREA = 4 * VOLREACTOR 'Bioreactor Volume (m^3)
392. VOLUSEFULBIO = VOLRBIOREA / 1.15 'Useful Volume (m^3)
393. '=====
394. 'ADB CSTR'
395. '=====
396. CSTRBD2 = (VOLRBIOREA * 2 / 3.14) ^ (1 / 3) 'Diameter of CSTR (m)
397. CSTRBH2 = CSTRBD2 * 2 'Height of CSTR (m)
398. CSTRBA2 = (2 * 3.14 * (CSTRBD2 / 2) * CSTRBH2) + (2 * 3.14 * ((CSTRBD2 / 2) ^ 2)) 'Area of CSTR (m2)'to be print'
399. 'Cells..... CSTR
400. Cells(26, 16) = CSTRBD2 'Diameter of CSTR (m)
401. Cells(27, 16) = CSTRBH2 'Height of CSTR (m)
402. '=====
403. ' ADB MIXER (CSTR)
404. '=====
405. C6H12O6MOL = 180.156 'g/mol
406. MMIXG = MMIX * 1000 'INPUT FLOW OF WASTE in (g/day)
407. FAOQ = MMIXG / C6H12O6MOL
408. NUMTANKAB = VOLUSEFULBIO / MAXVOL 'Number Of Tanks
409. If NUMTANKAB < 1 Then
410. NUMTANKAB = 1
411. Else
412. End If
413. Cells(35, 19) = NUMTANKAB
414. '=====
415. ' TANK DESIGN (ADB MIXER)
416. '=====
417. '..... X1 From above (Dark Fermenter)Line 238
418. '....RATE
419. X2 = (1 - (VSEG / VSE)) 'Conversion Aaerobic
420. RA2 = -((FAO * (X2 - X1)) / (VOLUSEFULBIO)) 'Total reaction rate
421. 'AGITATOR DIMENSIONS FOR ADB'
422.
423. 'DENSITY OF THE EFFLUENT GOING TO COMPOST'
424. DENRTP = (DENDARK7 * 4.4) / (8.98)
425. '=====
426. IMPDA = (CSTRBD2 / (3)) 'Impeller diameter(m)
427. EMDA = IMPDA 'Impeller height above vessel floor(m)
428. LMPDA = (IMPDA / (4)) 'Length of Impeller blade(m)
429. WMPDA = (IMPDA / (5)) 'Width of Impeller blade(m)
430. QWPDA = (CSTRBD2 / (10)) 'Width of baffle(m)'
431. NOIMP = 3 'Number of impellers
432. NOBLAD = 6 'Number of impeller blades
433. 'SHAPE FACTORS OF BLADES AS FOLLOWS 6BLADE'
434. DISTB = IMPDA 'Distance between two consecutive impellers (m)'
435. S1BIO = IMPDA / CSTRBD2 'Shape Factor(m)
436. S2BIO = EMDA / CSTRBD2 'Shape Factor(m)
437. S3BIO = LMPDA / IMPDA 'Shape Factor(m)
438. S4BIO = WMPDA / IMPDA 'Shape Factor(m)
439. S5BIO = QWPDA / CSTRBD2 'Shape Factor(m)
440. S6BIO = CSTRBH2 / CSTRBD2 'Shape Factor(m)
441. 'Velocity of agitation
442. 'Density of Dark Mixture
443. FT5 = (RHOMIX * (0.733333))
444. FT0Y = (DENDARK7 * (1.5))
445. TIPVELO = 5 'Velocity of agitation
446. FT0Y = (DENDARK7 * (1.5))

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447. 'Speed of impellers'
448.   SPEIMP = ((TIPVELO) / (3.14 * IMPDA)) * 60 '(RPM)
449. 'Energy impellers HORSEPOWER'
450.   POWBIOA = (((NOBLAD) * (((SPEIMP) * (0.016)) ^ (3)) * ((IMPDA) ^ (5)) * (FT0Y)) / (2447.578)) * NUMTANKAB '(HP)
451.   POWBIOAN = POWBIOA 'Total Power for Total number of Vessels
452. 'IMPELLER EFFICIENCY'
453.   EFF1 = Cells(47, 19) 'Efficiency of impellers(%)<*****
454.   POWBIO = POWBIOA * ((EFF1 / 100)) 'Power by considering the efficiency of impeller
455. 'Baffle design'
456.   NOBLADQ = 6
457.   WBAFF = ((CSTRBD2) / (10)) 'width of baffle (m)
458.   HBAFF = CSTRBH2 'HEIGHT of baffle (m)
459. 'corrosion allowance'
460.   CORAL = ((2) * (10) ^ (-3)) 'Corrosion allowance (m)
461. 'Wall thickness'
462.   PSBIORAC = (RHOFW * (9.81) * CSTRBH) * 0.00000986 'Static pressure (atm)
463.   POP1 = 0.0144 'OPERATIONAL PRESSURE (atm)
464.   PTOTH = POP1 + PSBIORAC 'Maximum allowance pressure(atm)
465. 'Cells
466.   Cells(36, 19) = FAOQ 'INPUT FLOW OF WASTE in (g/day)
467.   Cells(37, 19) = X2 'Conversion Rate %
468.   Cells(38, 19) = IMPDA 'Impeller diameter (m)
469.   Cells(39, 19) = EMDA 'Impeller height above bottom of vessel(m)
470.   Cells(40, 19) = LMPDA 'Length of Impeller blade (m)
471.   Cells(41, 19) = WMPDA 'Width of Impeller blade(m)
472.   Cells(42, 19) = NOIMP 'Number of Propellers
473.   Cells(43, 19) = NOBLAD 'Number of impeller blades
474.   Cells(44, 19) = TIPVELO 'Velocity of agitation
475.   Cells(45, 19) = SPEIMP 'Rotation per minute (RPM)
476.   Cells(46, 19) = POWBIOAN 'Impeller Horse Power (HP)
477.   Cells(48, 19) = POWBIO 'Impeller Horse Power at EFFICIENCY (HP)
478.   Cells(49, 19) = NOBLADQ 'INumber of Baffles
479.   Cells(50, 19) = WBAFF 'Width of baffle (m)
480.   Cells(51, 19) = HBAFF 'HEIGHT of baffle (m)
481.   Cells(52, 19) = CORAL 'Corrosion allowance (m)
482.   Cells(53, 19) = PSBIORAC 'Static pressure (atm)
483.   Cells(54, 19) = POP1 'OPERATIONAL PRESSURE (atm)
484.   Cells(55, 19) = PTOTH 'Maximum allowance pressure(atm)
485. 'Shape Factor
486.   Cells(57, 19) = S1BIO
487.   Cells(58, 19) = S2BIO
488.   Cells(59, 19) = S3BIO
489.   Cells(60, 19) = S4BIO
490.   Cells(61, 19) = S5BIO
491.   Cells(62, 19) = S6BIO
492. '=====
493. ' TANK DESIGN (MIXER INOCULUM)
494. '=====
495.   INORESTIME = Cells(62, 4) 'Tank Residence Time (day)
496.   INOTIMFACTOR = 1.25 'TANK FACTOR
497.   INOTANKVOL = MMIX * (INORESTIME / RHOMIX) * INOTIMFACTOR 'Tank Volume (m^3)
498.   MAXVOL = 50 'Maximum Volume Allowed (m^3)
499.   INONUMBTANK = INOTANKVOL / MAXVOL 'Number Of Tanks
500.   If INONUMBTANK < 1 Then
501.     INONUMBTANK = 1
502.   Else
503.     End If
504.   INODISRATE = (MAXVOL * (INOTANKVOL / INONUMBTANK)) / (10) 'Discharge Rate (m^3/day)
505.   INODISRATE = ((INOTANKVOL / INONUMBTANK) / INODISRATE) 'Discharge Rate
506.   RTANKD = ((INOTANKVOL / INONUMBTANK) * 2 / 3.14) ^ (1 / 3) 'Diameter of Tank (m)
507.   RTANKH = RTANKD * 2 'Height of CSTR (m)
508. 'CELLS OUTPUT
509.   Cells(4, 20) = INOTANKVOL 'Tank Volume (m^3)
510.   Cells(5, 20) = INONUMBTANK 'NUMTANK
511.   Cells(6, 20) = RTANKD 'Diameter of Tank (m)/Tanks

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512. Cells(7, 20) = RTANKH 'Height of Tank (m) /Tanks
513. Cells(8, 20) = INODISRATE
514. 'Reactor Input Flow Rate
515. RRT = Cells(64, 17) 'Recycling Ratio (%)
516. TYUI = TOTVARGT - (MMIX / RHOMIX)
517. KGOUTR2 = TYUI * (RRT / 100) 'Amount of Recycled (kg/day)
518. '-----
519. 'Inoculum tank'
520. '-----
521. IMPDA0Y = RTANKD / 3
522. TIPVELO1Y = 5
523. 'Speed of impellers'
524. SPEIMP2Y = ((TIPVELO1Y) / (3.14 * IMPDA0Y)) * 60 '(RPM)
525. 'Energy impellers HORSEPOWER'
526. POWBIOAINOTANK = ((NOBLAD) * ((SPEIMP2Y) * (0.016) ^ (3)) * ((IMPDA0Y) ^ (5)) * (RHOMIX)) / (2447.578) '(HP)
527. POWBIOAINOTANKTOT = POWBIOAINOTANK * INONUMBANK
528. 'IMPELLER EFFICIENCY'
529. POWBIO5U = POWBIOAINOTANKTOT * ((EFF1 / 100)) 'Power by considering the efficiency of impeller
530. Cells(64, 12) = SPEIMP2Y
531. Cells(65, 12) = POWBIO5U
532. 'K constant
533. KM = ((1 / HRTB) * (-Logn(VSEG / VSE))) 'First Order Constant for CH4 (1/day)
534. SRTB = 1 / KM
535. Cells(51, 4) = KM
536. 'OLR
537. OLRB = VSEG * KM * VSE / (VSE - VSEG) 'OLR-Organic Loading Rate (kgVS/m^3. d)
538. 'SB, MU, and Organic Loading Rate (OLR)
539. 'Experimental Yield (m^3/kgVS)
540. MUB = 0.83 - (0.028 * VSEPB)
541. SGP = (MUB * KM * VSEG) / OLRB 'Specific Gas Production
542. SB = OLRB * HRTB 'Amount of Substract(kgVS/m^3)
543. GPRB = (OLRB * SGP) 'Gas Productio Rate (m3/m3.d)
544. QBIOGAD = MMIX * SGP
545. CH4PERBIO = CH4BIORAC
546. H2SPERBIO = H2SP
547. NH3PERBIO = NH3P
548. TOTALPERBIO = 100
549. CO2PERBIO = TOTALPERBIO - (H2SP + NH3P + CH4PERBIO)
550. 'Rate of Biogas OUT
551. YEXCH4 = (CH4PERBIO / 100) * SGP
552. YEXH2S = (H2SPERBIO / 100) * SGP
553. YEXNH3 = (NH3PERBIO / 100) * SGP
554. YEXCO2 = SGP - YEXCH4 - YEXH2S - YEXNH3
555. YEXCO2 = (CO2PERBIO / 100) * SGP
556. Total = YEXCH4 + YEXCO2 + YEXH2S + YEXNH3
557. 'Cells OUTPUT
558. Cells(29, 13) = YEXCH4
559. Cells(30, 13) = YEXCO2
560. Cells(31, 13) = YEXH2S
561. Cells(32, 13) = YEXNH3
562. Cells(33, 13) = YEXPE
563. CH4RATE = (QBIOGAD * CH4BIORAC) / 100 'CH4 OUT (m^3/day)<-----
564. H2SRATE = QBIOGAD * H2SP / 100 'H2O OUT (m^3/day)<-----
565. NH3RATE = QBIOGAD * NH3P / 100
566. CO2RATE = QBIOGAD - CH4RATE - H2SRATE 'CO2 OUT (m^3/day)<-----
567. TOTALB = CH4RATE + CO2RATE + H2SRATE + NH3RATE
568. '*****
569. 'Cells OUTPUT
570. Cells(29, 16) = CH4PERBIO 'CH4 (%)
571. Cells(30, 16) = CO2PERBIO 'CO2(%)
572. Cells(31, 16) = H2SPERBIO 'H2S (%)
573. Cells(32, 16) = NH3PERBIO 'NH3 (%)
574. Cells(33, 16) = TOTALPERBIO 'Total (%)
575. '*****
576. 'Cells OUT

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577. Cells(29, 20) = CH4RATE 'CH4 OUT (m^3/day)
578. Cells(30, 20) = CO2RATE 'CO2 OUT (m^3/day)
579. Cells(31, 20) = H2SRATE 'H2S OUT (m^3/day)
580. Cells(32, 20) = NH3RATE 'NH3 OUT (m^3/day)
581. TOTALB = CH4RATE + CO2RATE + H2SRATE + NH3RATE
582. Cells(33, 20) = TOTALB 'Total (m^3/day)
583. '*****
584. 'Cells
585. 'Cells(50, 4) = HRTB 'Hydrolic Residence Time (day)
586. Cells(22, 16) = VOLUSEFULBIO
587. Cells(23, 16) = SRTB
588. Cells(24, 16) = OLRB 'OLR-Organic Loading Rate (kgVS/m^3. d)
589. Cells(25, 16) = MUB
590. 'Cells
591. Cells(27, 12) = VRR 'Recycled Volume (m^3/day)
592. 'YIELD
593. Cells(27, 10) = TSREC 'TS RECYCLED (%)
594. Cells(29, 10) = GPRB 'Gas Productio Rate (m3/m3.d)
595. Cells(30, 10) = QBIOGAD 'Rate of Biogas OUT (m^3/day)
596. Cells(31, 10) = SGP 'Experimental Yield of CH4 (m^3/kgVS)
597. TKH5 = SGP
598. Cells(33, 13) = TKH5
599. '*****
600. ' OUTPUT FOR EMS
601. '*****
602. T = TEMPA
603. RHOH2S = 1.4341 'Density of H2S (kg/m^3)
604. RHOC02 = CO2DENSITY(T) 'CO2 Density T=oC,Kg/m^3
605. RHOCH4 = CH4DENSITY(T) 'CH4 Density T=oC,Kg/m^3
606. RHONH3 = NH3DENSITY(T) 'NH3 Density T=oC,Kg/m^3
607. CH4AK = CH4RATE * RHOCH4 'CH4 OUT From ADB (kg/day)
608. CO2AK = CO2RATE * RHOC02 'CO2 OUT From ADB (kg/day)
609. H2SAK = H2SRATE * RHOH2S 'H2S OUT From ADB (kg/day)
610. NH3AK = 0.00021
611. TOTALGASOUTADB = CH4AK + CO2AK + H2SAK + NH3AK 'Total gas out (Kg/day)'
612. DENBIOGASAD = TOTALGASOUTADB / (CH4RATE + CO2RATE + H2SRATE + NH3RATE) 'Density of biogas from AD'
613. MASSTOTRTQ = DENBIOGASAD * TOTALB
614. Cells(26, 20) = MASSTOTRTQ
615. RTFDDE = (CH4PERBIO / 100) * 16
616. RTFDDECO2 = (CO2PERBIO / 100) * 44
617. RTFDDEH2S = (H2SPERBIO / 100) * 34.1
618. RTFDDENH3 = (NH3PERBIO / 100) * 17.03
619. TREO0 = RTFDDE + RTFDDECO2 + RTFDDEH2S + RTFDDENH3
620. FTUU00I = RTFDDE / TREO0
621. FTUU00ICO2 = RTFDDECO2 / TREO0
622. FTUU00IH2S = RTFDDEH2S / TREO0
623. FTUU00INH3 = RTFDDENH3 / TREO0
624. FTTRREEQ = MASSTOTRTQ * FTUU00I
625. FTTRREEQCO2 = MASSTOTRTQ * FTUU00ICO2
626. FTTRREEQH2S = MASSTOTRTQ * FTUU00IH2S
627. FTTRREEQNH3 = MASSTOTRTQ * FTUU00INH3
628. Cells(22, 20) = FTTRREEQ 'CH4 OUT From ADB (kg/day)
629. Cells(23, 20) = FTTRREEQCO2 'CO2 OUT From ADB (kg/day)
630. Cells(24, 20) = FTTRREEQH2S 'H2S OUT From ADB (kg/day)
631. Cells(25, 20) = FTTRREEQNH3 'NH3 OUT From ADB (kg/day)
632. FTC3 = QBIOL - TOTALGASOUTADB
633. '=====
634. '***** RECYCLING *****
635. '=====
636. '.....MASS BALANCE WITHOUT RECYCLING
637. KGOUTADB = MMIX - TOTALGDKF - MASSTOTRTQ 'Total kg out of ADB wiyhout recycling
638. KGOUTDF = MMIX - TOTALGDK 'Total out of Dark Fermenter (kg/day)
639. KGINADB = KGOUTDF 'Total Flow into ADB (kg/day)
640. KGOUTADB = KGOUTDF - MASSTOTRTQ 'Total Flow OUT ADB (kg/day)
641. MMIXCV = MMIX

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642. '...DATA OUT
643.   Cells(67, 10) = MMIXCV      'Input flow to DARK Reactor (kg/day)
644.   Cells(68, 10) = TOTALGDKF  'Gas out of DF Dark Fermenter [H2,CO2] (kg/day)
645.   Cells(69, 10) = KGOUTDF    'Total out of Dark Fermenter (kg/day)
646.   Cells(70, 10) = KGINADB    'Total Flow into ADB (kg/day)
647.   Cells(71, 10) = MASSTOTRTQ 'Gas out of ADB [CH4,CO2] (kg/day)
648.   Cells(72, 10) = KGOUTADB   'Total Flow out of ADB (kg/day)
649. '.....Mass BALANCE WITH RECYCLING at RRAT % Recycling Ratio
650. '...DATA IN
651.   RRT = Cells(64, 17)          'Recycling Ratio (%)
652. '....
653.   KGOUTR = KGOUTADB * (RRT / 100) 'Amount of Recycled (kg/day)
654.   KGOUTCOM = KGOUTADB - KGOUTR   'Amount of compost Rejected (kg/day)
655. '...Recycling for DB ...
656.   KGINDARK = MMIX + KGOUTR       'Amount of kg into Dark with recycling (kg/day)
657.   KGGASOUTDFR = TOTALGDKF       'Amount of GAS out of DF (kg/day)
658. ' kg OUT of DF
659.   KGOUTDFR = KGINDARK - TOTALGDKF 'Amount of liquid kg out of DF
660. '...Recycling for ADB ...
661. 'kg OUT of DF into ADB
662.   KGINADBR = KGINADB            'Amount of liquid kg into ADB from DF
663. ' Recycling is transformed into ADB gas
664.   GASOUTADBR = MASSTOTRTQ + KGOUTR 'Amount of gas out of ADB (kg/day)
665. 'kg out of ADB
666.   KGOUTADBR = KGINADB - GASOUTADBR
667. '...DATA OUT
668.   Cells(33, 9) = KGOUTR        'Amount of Recycled (kg/day)
669.   Cells(33, 11) = KGOUTCOM     'Amount of compost Rejected (kg/day)
670.   Cells(65, 17) = KGOUTR      'Amount of Recycled (kg/day)
671.   Cells(65, 19) = KGOUTCOM     'Amount of compost Rejected (kg/day)
672.   Cells(67, 17) = KGINDARK    'Amount of kg into Dark with recycling (kg/day)
673.   Cells(68, 17) = TOTALGDKF   'Amount of Gas out of DF Dark Fermenter [H2,CO2] (kg/day)
674.   Cells(69, 17) = KGOUTDFR    'Amount of liquid kg out of DF
675.   Cells(70, 17) = KGINADBR    'Amount of liquid kg into ADB DF
676.   Cells(71, 17) = GASOUTADBR  'Amount of gas out of ADB (kg/day)
677.   Cells(72, 17) = KGOUTADBR   'Amount of gas out of ADB (kg/day)
678. '=====
679. 'DISCHARGED TANK'
680. '=====
681. TANKV98B = KGOUTADBR * (1 / FT0Y) * 1.25
682. NUMTANK0 = TANKV98B / 113.562
683. If NUMTANK0 < 1 Then
684.   NUMTANK0 = 1
685. Else
686.   End If
687. DISCHRATE0 = ((300) * (TANKV98B / NUMTANK0)) / (10) 'Discharge Rate (m^3/day)
688. DISCHRATE5I = ((TANKV98B / NUMTANK0) / (DISCHRATE0)) 'Discharge Rate (m^3/sec)
689. '=====
690. RTANKD0 = (((TANKV98B / NUMTANK0) * (2)) / (3.14)) ^ (1 / 3) 'Diameter of Tank (m)
691. RTANKH0 = (RTANKD0 * (2)) 'Height of CSTR (m)
692. 'Cells
693.   Cells(4, 18) = TANKV98B      'Tank Volume (m^3)
694.   Cells(5, 18) = NUMTANK0     'NUMTANK
695.   Cells(6, 18) = RTANKD0      'Diameter of Tank (m)/Tanks
696.   Cells(7, 18) = RTANKH0      'Height of Tank (m) /Tanks
697.   Cells(8, 18) = DISCHRATE5I  'Discharge Rate (m^3/sec)
698. '=====
699. 'SLUDGE PUPMPS
700. '=====
701. 'To Dark
702. '...INPUT DATA
703.   GR = 9.81
704.   PRESHEAD = (CSTRDARKH / NUMTANKD) + 0.5
705.   Cells(65, 4) = PRESHEAD
706.   Cells(66, 4) = RHOMIX

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707. Cells(67, 4) = MMIX
708. '...DATA OUT
709. SLUDGFR1 = (((MMIX / RHOMIX) / 86400) * GR * PRESHEAD * RHOMIX) 'SLUDGE Flow Rate (L/sec)
710. POWER1 = (SLUDGFR1) / 1000 'KW
711. WATT3 = 1000 * POWER1
712. Cells(68, 4) = POWER1 'Watt
713. Cells(69, 4) = WATT3 'HP
714. 'To Bioreactor
715. PRESHEAD2 = (CSTRBH2 / NUMTANKAB) + 0.5
716. Cells(71, 4) = PRESHEAD2
717. Cells(72, 4) = FT5
718. Cells(73, 4) = KGINADB
719. SLUDGFR2 = (((KGINADB / FT5) / 86400) * GR * PRESHEAD2 * FT5)
720. POWER12 = (SLUDGFR2) / 1000 'KW
721. WATT4 = 1000 * POWER12
722. Cells(74, 4) = POWER12 'Watt
723. Cells(75, 4) = WATT4
724. '*****
725. '
726. '=====  

727. 'Cells OUT
728. CONVERS = ((MMIX - KGOUTCOM) / (MMIX)) 'conversion without recycling (%)
729. OVERALLCONV = ((CONVERS) * (1 + RRT)) / ((1 + (RRT * CONVERS))) 'Overall conversion of the system'
730. Cells(63, 4) = CONVERS 'conversion without recycling (%)
731. Cells(63, 6) = OVERALLCONV 'Overall conversion of the system'
732. '=====  

733. '
734. '=====  

735. GACC = 9.81 'Gravity Acceleration
736. RHOCH4 = 0.656 'kg/m3
737. RHOCO2 = 1.98 'kg/m3
738. RHOGAS = RHOCH4 * (CH4PERBIO / 100) + RHOCO2 * (CO2PERBIO / 100)
739. GASFR = (TOTALB / 24) / 3600 'GAS Flow Rate OUT(m3/sec)
740. IPSPEED = 5000
741. '...DATA IN
742. Cells(78, 4) = GASFR
743. Cells(79, 4) = PDFB 'INLET Pressure (Atm.)
744. POUT = Cells(80, 4) 'OUTLET Pressure (Atm.)
745. EXITPIPARE = Cells(81, 4) 'Exit Pipe AREA (m)
746. IPSPEED = Cells(82, 4) 'Impeller Specific Speed (RPM)
747. '...DATA OUT
748. VDISCH = GASFR / EXITPIPARE '
749. HEADCH = POUT / (RHOGAS * GACC) + VDISCH ^ 2 / (GACC * 2) - PIN / (RHOGAS * GACC)
750. POWERFAN = (RHOGAS * GASFR * GACC * HEADCH) * 10000 'Watt
751. NS = (IPSPEED * GASFR ^ 0.5) / (HEADCH ^ (3 / 4))
752. Cells(83, 4) = VDISCH
753. Cells(84, 4) = NS
754. Cells(85, 4) = POWERFAN '(W)
755. '=====  

756. '=====  

757. '
758. '=====  

759. '.....Required Heat for DARK HEAT EXCHANGER N09
760. '=====  

761. 'Waste Specific Heat=2629.425 J/kg.K
762. TL = Cells(92, 4) 'Tube Length (m)
763. TOD = Cells(93, 4) 'Tube Outside Diameter (m)
764. '.....
765. TH1 = H2OTEMPXX + 273 'Steam Temperature(K)
766. TC1 = 2 + 273 'Waste IN Temperature (K)
767. TC2 = 90 + 273 'Waste OUT Temperature (K)
768. 'TH2 = ?
769. H2OTEMP = TH1
770. SCH20 = WATERSPECIFICHEAT(H2OTEMP) 'H2O SPECIFICHEAT (kJ/kg.K)
771. SCWASTE = 2629.425 / 1000 'WASTE Specific Heat Capacity (kJ/kg.K)

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772.   CWASTED = SCWASTE * ((MMIX / 24) / 3600) 'WASTE Heat Capacity (kW/sec.K)
773.   QWASTED = CWASTED * (TC2 - TC1)          '(kW)
774. 'STEAM
775. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
776.   FLAG = 1
777.   U = 0.227
778.   CCOLD = CWASTED: Q = QWASTED: SCHOT = SCH20: SCCOLD = SCWASTE
779.   Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN
GER
780. '
781. 'OUTPUT
782.   STEAMFR = HFR
783.   Cells(88, 4) = H2OTEMPXX          'Steam Temperature In (oC)
784.   Cells(89, 4) = TH2 - 273          'Steam Temperature OUT (°C)
785.   Cells(90, 4) = TC1 - 273          'Waste Temperature In (°C)
786.   Cells(91, 4) = TC2 - 273          'Waste Temperature OUT (°C)
787.   Cells(94, 4) = NTU                'Number of Tubes
788.   Cells(95, 4) = AREAHEX            'Shell Area (m^2)
789.   Cells(96, 4) = EPS * 100          'Effectiveness
790.   Cells(97, 4) = QEFF               'Heat Transfer (W)
791.   Cells(98, 4) = STEAMFR            'Steam Flow Rate (kg/day)
792.   WASTETEMOUT = TH2
793. '=====
794. '.....Required cold for DARK CONDENSER No3
795. '=====
796. 'Waste Specific Heat=2629.425 J/kg.K
797.   TL = Cells(79, 11) 'Tube Length (m)
798.   TOD = Cells(80, 11) 'Tube Outside Diameter (m)
799.   THH = Cells(91, 4)
800.   TH1 = THH + 273 'Waste IN Temperature (K)
801.   TH2 = 55 + 273 'Waste OUT Temperature (K)
802.   TC1 = 25 + 273 'Air IN Temperature (K)
803.   AIRTK = TC1
804.   SCAIR = AIRSPECIFICHEAT(AIRTK) 'AIRSPECIFICHEAT (kJ/kg.K)
805. '....
806.   SCWASTE = 2629.425 / 1000 'WASTE Specific Heat Capacity (kJ/kg.K)
807.   CWASTEDB = SCWASTE * (KGINDARK / 24) / 3600 'WASTE Heat Capacity (kW/sec.K)
808.   QWASTEDB = CWASTEDB * (TH1 - TH2)          '(kW)
809. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
810.   FLAG = 2
811.   U = 0.227
812.   CHOT = CWASTEDB: Q = QWASTEDB: SCHOT = SCWASTE: SCCOLD = SCAIR
813.   Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN
GER
814.   AIRFRDB = HFR
815.   Cells(75, 11) = TC1 - 273 'Air Temperature In (°C)
816.   Cells(76, 11) = TC2 - 273 'Air Temperature OUT (°C)
817.   Cells(77, 11) = TH1 - 273 'Waste Temperature In (°C)
818.   Cells(78, 11) = TH2 - 273 'Waste Temperature OUT (°C)
819.   Cells(81, 11) = NTU        'Number of Tubes
820.   Cells(82, 11) = AREAHEX    'Shell Area (m^2)
821.   Cells(83, 11) = EPS * 100  'Effectiveness
822.   Cells(84, 11) = QEFF       'Heat Transfer (W)
823.   Cells(85, 11) = AIRFRDB    'Steam Flow Rate (kg/day)
824. '=====
825. '.....Required cold for ADB CONDENSER No3
826. '=====
827. 'Waste Specific Heat=2629.425 J/kg.K
828.   TL = Cells(79, 18) 'Tube Length (m)
829.   TOD = Cells(80, 18) 'Tube Outside Diameter (m)
830.   TH1 = 55 + 273 'Waste IN Temperature (K)
831.   TH2 = 35 + 273 'Waste OUT Temperature (K)
832.   TC1 = 25 + 273
833.   SCAIR = AIRSPECIFICHEAT(AIRTK) 'AIRSPECIFICHEAT (kJ/kg.K)
834. '....

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835.   SCWASTE = 1.01 'WASTE Specific Heat Capacity (kJ/kg.K)
836.   CWASTEADB = SCWASTE * (KGINADBR / 24) / 3600 'WASTE Heat Capacity (kW/sec.K)
837.   QWASTEADB = CWASTEADB * (TH1 - TH2) '(kW)
838. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
839.   FLAG = 2
840.   U = 0.227
841.   CHOT = CWASTEADB: Q = QWASTEADB: SCHOT = SCWASTE: SCCOLD = SCAIR
842. 'Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN
GER
843.   Cells(75, 18) = TC1 - 273 'Air Temperature In (oC)
844.   Cells(76, 18) = TC2 - 273 'Air Temperature OUT (oC)
845.   Cells(77, 18) = TH1 - 273 'Waste Temperature In (oC)
846.   Cells(78, 18) = TH2 - 273 'Waste Temperature OUT (oC)
847.   Cells(81, 18) = NTU 'Number of Tubes
848.   Cells(82, 18) = AREAHEX 'Shell Area (m^2)
849.   Cells(83, 18) = EPS * 100 'Effectiveness
850.   Cells(84, 18) = QEFF 'Heat Transfer (W)
851.   Cells(85, 18) = HFR 'Steam Flow Rate (kg/day)
852. '=====
853. 'Heat LOSS
854. '=====
855. 'Dark fermentation heat loss'
856.
857.   TEMPDK = TEMPD + 273
858.   ANARDAR1 = CSTRDARKH * 2 * Pi * (CSTRDARKD / 2)
859.   ANARDAR2 = 2 * Pi * ((CSTRDARKD / 2) ^ 2)
860.   QUPDAR = (0.3 * ANARDAR1 * (TEMPDK - TAMBK)) / 1000 'Heat loss 1 (kW)'
861.   QUPDAR1 = (0.34 * ANARDAR1 * (TEMPDK - TAMBK)) / 1000 'Heat loss 2 (kW)'
862.   QUPDAR2 = (0.15 * ANARDAR2 * (TEMPDK - TAMBK)) / 1000 'Heat loss 3 (kW)'
863.   QUPDAR3 = (2.08 * ANARDAR2 * (TEMPDK - TAMBK)) / 1000 'Heat loss 4 (kW)'
864.   QUPDAR4 = (0.32 * ANARDAR1 * (TEMPDK - TAMBK)) / 1000 'Heat loss 5 (kW)'
865. 'TOTAL For Dark
866.   QUPTOTDARK = (QUPDAR + QUPDAR1 + QUPDAR2 + QUPDAR3 + QUPDAR4) * NUMTANKD 'Total heat loss (kW)'
867. '
868. 'Anaerobic digestion heat loss'
869.   ANAR1 = CSTRBH2 * 2 * Pi * (CSTRBD2 / 2)
870.   ANAR2 = 2 * Pi * ((CSTRBD2 / 2) ^ 2)
871.   QUP = (0.3 * ANAR1 * ((TEMPA + 273) - TAMBK)) / 1000 'Heat loss 1 (kW)'
872.   QUP1 = (0.34 * ANAR1 * ((TEMPA + 273) - TAMBK)) / 1000 'Heat loss 2 (kW)'
873.   QUP2 = (0.15 * ANAR2 * ((TEMPA + 273) - TAMBK)) / 1000 'Heat loss 3 (kW)'
874.   QUP3 = (2.08 * ANAR2 * ((TEMPA + 273) - TAMBK)) / 1000 'Heat loss 4 (kW)'
875.   QUP4 = (0.32 * ANAR1 * ((TEMPA + 273) - TAMBK)) / 1000 'Heat loss 5 (kW)'
876. 'TOTAL For ANAEROBIC
877.   QUPTOT = (QUP + QUP1 + QUP2 + QUP3 + QUP4) * NUMTANKAB 'Total heat loss (kW)'
878. 'Cells Output
879.   Cells(100, 4) = QUPTOTDARK
880.   Cells(101, 4) = QUPTOT
881. '===== TANKS HEAT LOSSES =====
882. 'heat loss Tank 1'(Before AD)
883.   TEMPA00 = 90 + 273 'ADB Temprature (K)
884.   CHT = 0.1 'W/m^2.K
885.   TIMCONV = 86400 '=> (3600) * (24)
886.   ANAWGH1 = 2 * RTANKH0 * Pi * (RTANKD0 / 2)
887.   ANAWGH2 = 2 * Pi * ((RTANKD0 / 2) ^ 2)
888.   ATWER56 = ANAWGH1 + ANAWGH2
889.
890.   QUPTFERT4 = ((ATWER56 * (308 - TAMBK)) / CHT) / 1000
891.   QUPTOTV4 = QUPTFERT4 * NUMTANK0 'Total heat loss (kW)'
892. 'Heat Loss Tank 2'(After DF)
893.   ANARDARW1 = 2 * RTANKH * Pi * (RTANKD / 2)
894.   ANARDARW2 = 2 * Pi * ((RTANKD / 2) ^ 2)
895.   ATRE12KL = ANARDARW2 + ANARDARW1
896.   QUPDARWEYT = ((ATRE12KL * (TEMPA00 - TAMBK)) / CHT) / 1000
897.   QUPTOTDARFKX1 = QUPDARWEYT * INONUMBANK 'Total heat loss (kW)'
898. 'Cells OUTPUT

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899. Cells(102, 4) = QUPTOTV4
900. Cells(103, 4) = QUPTODARFKX1
901. '=====
902. TVELAGDXTAN = 6
903. IMPDADXTAN = (RTANKD / 3) 'Impeller diameter (m)
904. SPEIMPDX TAN = ((TVELAGDXTAN) / (3.14 * IMPDADXTAN)) * 60 '(RPM)'Impeller speed'
905. IMPHPDX TAN = (((NOIMBPLD) * ((SPEIMPD) ^ (3)) * (0.016)) * ((IMPDADXTAN) ^ (5)) * (RHOMIX)) / (2447.578) '(HP)'impeller Power'
906. POWBIO5XTAN = IMPHPDX TAN * INONUMB TANK
907. TVELAGDXTAN = Cells(4, 23)
908. Cells(5, 23) = IMPDADXTAN
909. Cells(6, 23) = SPEIMPDX TAN
910. Cells(7, 23) = IMPHPDX TAN
911. Cells(8, 23) = POWBIO5XTAN
912. '=====
913. ' PUMP for Digested Sludge KGOUTADB
914. '=====
915. PRESHEAD3 = (RTANKD0 / NUMTANK0) + 0.5
916. Cells(105, 4) = PRESHEAD3
917. Cells(106, 4) = FT5
918. Cells(107, 4) = KGINADB
919. SLUDGFR23 = (((KGINADB / FT5) / 86400) * GR * PRESHEAD3 * FT5)
920. POWER123 = (SLUDGFR23) / 1000 'KW
921. WATT45 = 1000 * POWER123
922. Cells(108, 4) = POWER123 'Watt
923. Cells(109, 4) = WATT45
924. '=====
925. 'Dewatering the Digested Sludge'
926. '=====
927. DENSOLID = (FT5 / 34.429) / 1000 'Density of solid (Cake) (kg/liter)'
928. RTEW2 = 100 - TSOUT 'Moisture content%'
929. MOISTCONT = KGOUTCOM * (RTEW2 / 100) 'MOISTURE CONTENT (kg/day)'
930. SOLIDRT3 = KGOUTCOM - MOISTCONT ' Solid content (kg/day)'
931. 'FILTERFLUX = KGOUTCOM / 92 'Flux of Digested Sludge from Filter Press'(kg/day.m2)'https://www.environmental-
expert.com/files/19732/download/737034/2-Filter-Press-DRACO-Toro-Equipment-ENG.pdf'
932. VOLUY = (KGOUTCOM / FT5) * 1000 '(liter/day) to be dewatered'
933. DFREWQ = (VOLUY * (TSOUT)) / (100) 'Liter of solid'
934. HOYOU = (VOLUY * (TSOUT * 10)) / 1000 '(gram/day) of Solid (For sizing of the filter press)'
935. SFCAKE = ((HOYOU) / KGOUTCOM) * 100 'Dryness of the cakes produced (wet/dry)%'
936. VOLFILT = (100 * HOYOU) / (SFCAKE * (DENSOLID)) 'Daily volume of cake produced (Liter/day)'
937. VOLB023 = VOLFILT / 3.2
938. VOLB023HYD = (VOLB023 * SFCAKE * 1000 * DENSOLID) / (TSOUT * 1000) 'Total haydraulic volume to be pumped (Liters)'
939. VOLPUMPF R = VOLB023HYD / 1440 'flow to be pumped (Liter/min)'
940. BNM = ((1.55 * VOLB023HYD) / 2.25) / 60 'Initial flow rate of membrane pump (Liter/min)'
941. FLOWRATE = BNM
942. PUPMPOWER = FILTERPUMPPOWER(FLOWRATE) '(kw)
943. 'HYDROLIC PRESSING MOTOR POWER
944. If VOLUY <= 5100 Then
945. HYDROLICPOW = 4
946. End If
947. If VOLUY > 5100 Then
948. HYDROLICPOW = 7.5
949. End If
950. If VOLUY > 8000 Then
951. HYDROLICPOW = 7.5
952. End If
953. If VOLUY > 10660 Then
954. HYDROLICPOW = 11
955. End If
956. If HYDROLICPOW > 17800 Then
957. HYDROLICPOW = 15
958. End If
959. 'OUTPUT CELLS
960. Cells(111, 4) = VOLUY 'Wet Volume of Sludge (L/min)
961. Cells(112, 4) = RTEW2 'Sludge Moisture Contents (%)
962. Cells(113, 4) = VOLFILT 'Daily volume of cake produced (Liter/day)

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963. Cells(114, 4) = SFOCAKE 'Final Solid Moisture Content (%)
964. Cells(115, 4) = BNM 'Final Solid Moisture Content (%)
965. Cells(116, 4) = PUMPOWER 'Pump Power (kW)
966. Cells(117, 4) = HYDROLICPOW 'Hydraulic Pressing Motor (kW)
967. ss = ss
968. End Sub
969. Static Function Logn(X)
970. Logn = Log(X) / Log(2.718282)
971. End Function
972. Private Static Function H2DENSITY(T) 'T= °C,Kg/m^3 1Atm
973. A = 0.041236128: B = 11.271649
974. H2DENSITY = 1 / ((A * T) + B)
975. End Function
976. Private Static Function CO2DENSITY(T) 'T= °C,Kg/m^3
977. A = 0.50649907: B = 0.0019289299: C = 1.0174749
978. CO2DENSITY = (A + B * T) ^ (-1 / C)
979. End Function
980. Private Static Function CH4DENSITY(T) 'T= °C,Kg/m^3
981. A = 0.70822045: B = 269.39972: C = -0.00035602407: D = 0.99821142
982. CH4DENSITY = (A * B + C * (T) ^ D) / (B + (T) ^ D)
983. End Function
984. Private Static Function NH3DENSITY(T) 'T= °C,Kg/m^3
985. A = 1.3112907: B = 0.0054825167: C = 0.98156027
986. NH3DENSITY = 1 / (A + B * (T) ^ C)
987. End Function
988. Private Static Function WATERSPECIFICHEAT(H2OTEMP) 'WATER SPECIFIC HEAT kJ/Kg.K in oK
989. WATERSPECIFICHEAT = 1.224986 + 0.0014072339 * H2OTEMP - 0.00000039722778 * H2OTEMP ^ 2 + 5.3431749E-11 * H2OTEMP ^ 3 + -2.7473115E-
15 * H2OTEMP ^ 4
990. End Function
991. Private Static Function AIRSPECIFICHEAT(AIRTK) 'AIRSPECIFICHEAT kJ/Kg.K T=oK
992. TA = 1.0828694: TB = -0.00063119116: TC = 0.0000016253087: TD = -1.3949526E-09: TE = 5.3826153E-13: TF = -7.9021928E-17
993. AIRSPECIFICHEAT = TA + TB * AIRTK + TC * AIRTK ^ 2 + TD * AIRTK ^ 3 + TE * AIRTK ^ 4 + TF * AIRTK ^ 5
994. End Function
995. Private Static Sub HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'H
EAT EXCHANGER
996. AREAHEX = 3.14 * TOD * TL
997. 'DELTAB = TH2 - TC1
998. LMTD = Q / (U * AREAHEX)
999. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
1000. '----- HEATING -----
1001. If FLAG = 1 Then
1002. DELTAA = TH1 - TC2
1003.
1004. 'DELTAB = TH2 - TC1
1005. LMTD = Q / (U * AREAHEX)
1006. X1 = 1
1007. S1 = DELTAA / (LMTD - Logn(DELTAA))
1008. S2 = X1 / (LMTD - Logn(X1))
1009. If S2 >= S1 Then
1010. GoTo 400
1011. Else
1012. X1 = X1 + 0.1
1013. GoTo 300
1014. End If
1015. DELTAB = X1
1016. TH2 = DELTAB + TC1
1017. GoTo 700
1018. End If
1019. '-----
1020. '----- COOLING -----
1021. If FLAG = 2 Then
1022. 'DELTAA = TH1 - TC2
1023. DELTAB = TH2 - TC1
1024. LMTD = Q / (U * AREAHEX)
1025. X1 = 2

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1026. 500 S1 = Logn(X1) - X1 / LMTD
1027. S2 = Logn(DELTAB) - DELTAB / LMTD
1028. If S1 >= S2 Then
1029. GoTo 600
1030. Else
1031. X1 = X1 + 0.1
1032. GoTo 500
1033. 600 End If
1034. DELTAA = X1
1035. TC2 = TH1 - DELTAA
1036. End If
1037. '-----
1038. 700 P = (TC2 - TC1) / (TH1 - TC1)
1039. R = (TH1 - TH2) / (TC2 - TC1)
1040. If R > 1 Then
1041. R1 = 1 / R
1042. P1 = P * R
1043. Else
1044. P1 = P
1045. R1 = R
1046. End If
1047. A1 = (((R1) ^ 2 + 1) ^ 0.5) / (1 - R1)
1048. A2 = Logn((1 - R1 * P1) / Abs(1 - P1))
1049. A3 = 2 - P1 * (1 + R1 - (1 + (R1) ^ 2)) ^ 0.5 'up
1050. A4 = Abs(2 - P1 * (1 + R1 + (1 + (R1) ^ 2)) ^ 0.5) 'down
1051. A5 = Logn(A3 / A4)
1052. FCORF = (A1 * A2) / A5
1053. If Abs(FCORF) > 1 Then
1054. FCORF = 1
1055. End If
1056. If FLAG = 1 Then
1057. LMTD = Q / (U * AREAHEX * FCORF)
1058. CHOT = Q / (TH1 - TH2)
1059. HFR = CHOT * 24 * 3600 / SCHOT
1060. GoTo 800
1061. End If
1062. If FLAG = 2 Then
1063. LMTD = Q / (U * AREAHEX * FCORF)
1064. CCOLD = Q / (TH1 - TH2)
1065. HFR = CCOLD * 24 * 3600 / SCHOT
1066. End If
1067. 'EFFECTIVENESS
1068. 800 If CCOLD > CHOT Then
1069. CMIN = CHOT
1070. C1 = CHOT
1071. EPS = (C1 * (TC2 - TC1)) / (CMIN * (TH1 - TC1))
1072. GoTo 900
1073. Else
1074. CMIN = CCOLD
1075. C1 = CCOLD
1076. EPS = (C1 * (TH1 - TH2)) / (CMIN * (TH1 - TC1))
1077. 900 End If
1078. QEFF = EPS * CMIN * (TH1 - TC1)
1079. 'Number of ELEMENT
1080. NTU = U * AREAHEX / CMIN
1081. If NTU <= 1 Then
1082. NTU = 1
1083. Else
1084. End If
1085. End Sub
1086. Private Static Function FILTERPUMPPOWER(FLOWRATE)
1087. A = 6.1441296: B = 0.0277043
1088. FILTERPUMPPOWER = A * (1 - Exp(-B * FLOWRATE))
1089. End Function

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MFI membrane

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1. Sub Sheet4_Button1_Click()
2. '
3. ' =====
4. 'MFI (ZM)
5. '
6. '           From Output of Dark-Reactor
7. '
8. H2FR = ActiveWorkbook.Worksheets("DFB-ADB").Cells(10, 20) ' H2 mass flow (Kg/Day)
9. CO2FR = ActiveWorkbook.Worksheets("DFB-ADB").Cells(11, 20) ' CO2 mass flow (Kg/Day)
10. GASTEM = ActiveWorkbook.Worksheets("DFB-ADB").Cells(42, 4) 'Gas Temperature (°C)
11. PERCETVB = GASTEM = ActiveWorkbook.Worksheets("DFB-ADB").Cells(58, 4)
12. TOTALGAS = H2FR + CO2FR 'Total Gas Flow Rate (Kg/Day)
13.
14. 'INPUT GAS DATA
15. Cells(5, 4) = H2FR 'H2 mass flow (Kg / Day)
16. Cells(6, 4) = CO2FR 'CO2 mass flow (Kg / Day)
17. Cells(7, 4) = GASTEM 'Gas Temperature (oC)
18. PGAS = Cells(8, 4)
19. 'INPUT CELL DATA
20. TC1X = Cells(10, 4) 'Cell Temperature (oC)
21. '.....
22. If TC1X >= -1 Then
23. TC1X = -1
24. Cells(10, 4) = TC1X
25. End If
26. If TC1X <= (-39) Then
27. TC1X = -39
28. Cells(10, 4) = TC1X 'Cell Temperature
29. End If
30. '.....
31. PCI = Cells(11, 4) 'Inlet Cell Pressure (atm)
32. PERCREC1 = Cells(4, 15)
33. '.....
34. If PCI <= 3 Then
35. Cells(11, 4) = 3
36. PCI = 3
37. End If
38. If PCI >= 30 Then
39. Cells(11, 4) = 30
40. End If
41. '.....
42. PCO = Cells(12, 4) 'Outlet Cell Pressure (atm)
43. 'MBAREA = Cells(13, 4) 'Membrane Area (cm^2)
44. MBDA1 = Cells(14, 4) 'Membrane Diameter (mm)
45. MMTH1 = Cells(15, 4) 'Thickness (micron m)
46. PRSZ1 = Cells(16, 4) 'Porosity (micron %)
47. PRAD1 = Cells(17, 4) 'Pore Radius Size (micron m)
48. NTUBEM = Cells(18, 4) 'Number of Tubes / Module
49. LTUBE1 = Cells(19, 4) 'Tube Length (m)
50. MMTH = MMTH1 / 100000000 'Thickness (m)
51. MMTHCM = MMTH * (10) ^ -5 'Thickness (cm)
52. MWC02 = 44 / 1000 'g/mol 'CO2 molecular weight
53. MWH2 = 2 / 1000 'g/mol 'H2 molecular weight
54. '.....
55. If PCI <= 3 Then
56. Cells(11, 4) = 3
57. PCI = 3
58. End If
59. If PCI > 30 Then
60. Cells(11, 4) = 30
61. End If
62. '.....
63. '----- Constant -----

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64.   PORDIAM = PRAD1 * 2      'Pore diameter (micron-m)
65.   PERCREC = PERCREC1 / 100
66.   PRAD = PRAD1 / 1000    'Pore Radius in (cm)
67.   PRSZ = PRSZ1 / 100     '% Porosity
68.   MMTHCM = MMTH1 / 1000  'Membrane Thickness (cm)
69.   TCK = TC1X + 273       'Cell temperature in °K
70.   LTUBE = LTUBE1 * 100    'Tube length in cm
71.   '.....
72.   SIGMACO2 = 3.3          'CO2 Collision Diameter (Angstrom)
73.   SIGMAH2 = 2.89         'H2 Collision Diameter (Angstrom)
74.   KNS = 1.38 * (10) ^ -23
75.   NAV = 6.0221367E+23    'Avogadro Constant (1/mol)
76.   FA = 96485             'Faraday (Coulombs/mole)
77.   R = 8.3143             'Gas constant (J/mol.K)or (pa m^3/K.mol)
78.   R1 = 83143
79.   RA = 0.0821            'Gas constant (atm.L/mol.K)
80.   RM = 0.0000821        'Gas constant (atm.m^3/mol.K)
81.   ATPASC = 1.01325 * (10) ^ 5 ' 1 Atm = 101325 Pascal ----> 101.325 kPascal
82.   Pi = 3.1416
83.   '.....
84.   H2MW = 2 / 1000        'H2 Molecular weight
85.   CO2MW = 44 / 1000     'CO2 Molecular weight
86.   RHOCO2 = 1.98         'Density of CO2 (kg/m^3)
87.   NU = 0.22             'Gas aver. vis.
88.   CO2DP = 0.0000000052  'CO2 Molecular diameter (m)[Ang.or 5.2e-11 meter]
89.   H2DP = 0.00000000289  'H2 Molecular diameter (m) [Ang.or 5.2e-11 meter]
90.   H2VISC = 0.0087       'H2 Viscosity
91.   '===== TUBE AREA =====
92.   'TUBE AREA
93.   MBDA = MBDA1 / 10      'Tube Diameter in mm to(cm)
94.   LTUBE = LTUBE1 * 100   'Tube Legth from mm to cm)
95.   AREATUBE = 4 * 3.14 * MBDA * LTUBE1 'Tube Area in (m^2)
96.   AREATUBE = MBDA * Pi * LTUBE 'Area (cm^2)
97.   Cells(13, 4) = AREATUBE 'Tube AREA
98.   '
99.   '===== Kinetics Calculation =====
100.  T = TGAS
101.  RHOH2 = H2DENSITY(T)   'Density of H2 (kg/m^3)T=oC,Kg/m^3
102.  RHOCO2 = CO2DENSITY(T) 'Density of CO2 (kg/m^3)
103.  H2VF = H2FR / RHOH2   'H2 volumetric flow (m ^ 3 / day)
104.  CO2VF = CO2FR / RHOCO2 'CO2 volumetric flow (m ^ 3 / day)
105.  'Recycling
106.  H2KGREC = H2FR * PERCREC
107.  CO2KGREC = CO2FR - CO2FR * PERCREC
108.  ' Volume Fraction
109.  TOTALVOL = CO2VF + H2VF
110.  H2VFR = H2VF / TOTALVOL
111.  H2MOLIN = (H2FR + H2KGREC) / H2MW ' H2 mols (kgmols/day)
112.  CO2MOLIN = (CO2FR - CO2KGREC) / CO2MW ' CO2 mols (kgmols/day)
113.  TOTMOL = H2MOLIN + CO2MOLIN 'Total mols in gas (kgmols/day)
114.  CO2PERCI = CO2MOLIN / TOTMOL '% CO2 mols at Entrance
115.  CO2PPI = CO2PERCI * PCI 'CO2 Partial Pressure at Entrance in atm.
116.  CO2PPO = CO2PERCI * PCO 'CO2 Partial Pressure at Exit in atm.
117.  H2PERCI = H2MOLIN / TOTMOL '% H2 mols at Entrance
118.  H2PPI = H2PERCI * PCI 'H2 Partial Pressure at Entrance in atm.
119.  FCO2 = CO2MOLIN / TOTMOL 'CO2 m01%
120.  FH2 = H2MOLIN / TOTMOL 'H2 (mol%)
121.  CO2PCK = CO2FR / TOTALGAS 'CO2 (kg%)
122.  H2PCK = H2FR / TOTALGAS 'H2 (kg%)
123.  DELP = PCI - PCO 'DP Pressure (atm)
124.  '===== TEST FLUX with Knudsen Diffusion =====
125.  'Knudsen Number
126.  LAMDACO2 = RM * TCK / (Pi * NAV * CO2DP * PCI * (2) ^ 0.5)
127.  KN = LAMDACO2 / (2 * (PRAD / 2)) 'Since it is smaller than 1 KN<1 => viscous (POISEUILLE FLOW)
128.  '===== FLUX With POISEUILLE =====

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129. 'CO2 Viscosity and Concentration
130.     T = TC1X
131.     CO2VISC = CO2VISCOSITY(T) 'T=0C centipoise
132. 'CO2 Concentration [Ref:0-0-1-A-EXCELLENT-CRAWFORD-THESIS-2013, Page:44,48,
133.     CO2PERCOR = (CO2PERCI * PCO) / PCI 'CO2 Concentration OUT in RETENTATE (kgmol)
134.     CO2PERCOP = (CO2PERCI - CO2PERCOR) 'CO2 Concentration OUT in PERMATE (kgmol)
135.     DELPCO2 = CO2PERCOP - CO2PERCOR 'CO2 DELTA Concentration (IN-OUT)
136. 'CO2 FLUX with POISEUILLE (Ref: 0-0-1-A1-FORMULA-materials-09-00930(2))
137.     ALFACO2P = (PRSZ * ((PRAD / 2) ^ 0.5) * (DELPCO2 / 2)) / (8 * R * TCK * CO2VISC) 'Flux'
138.     JCO2P = ALFACO2P * (DELPCO2) / MMTHCM 'CO2 Flux (mols/sec.cm^2) for one tube
139. 'H2 Viscosity and Concentration [Ref:0-0-1-A-EXCELLENT-CRAWFORD-THESIS-2013,Page:44,48,
140.     H2PERCOR = (H2PERCI - CO2PERCOR) 'H2 Concentration OUT in RETENTATE (kgmol)
141.     H2PERCOP = H2PERCI - H2PERCOR 'H2 Concentration OUT in PERMATE (kgmol)
142.     DELPH2 = (H2PERCI - H2PERCOR) 'H2 DELTA Concentration (IN-OUT)
143. 'H2 FLUX with POISEUILLE
144.     ALFAH2P = (PRSZ * ((PRAD / 2) ^ 0.5) * (DELPH2 / 2)) / (8 * R * TCK * H2VISC)
145.     JH2P = ALFAH2P * (DELPH2) / MMTHCM 'H2 Flux (mol/sec.cm^2)
146. 'Flow Rate passing through one tube
147.     CO2FR1TUBE = JCO2P * AREATUBE 'mols/sec
148. 'Number of Tubes
149.     CO2MOLRATE = (CO2FR / MWC02) 'CO2 mole/day
150.     CO2MOLINSE = (CO2MOLRATE / 24) / 3600 'Total CO2 kgmol IN (mols/sec)
151. '=====
152.     REQAREA1 = (10 * CO2FR) / 300000 'AREA(m2)
153.     AREAREQ2 = REQAREA1 * 10000 '(cm2)
154.     TUBENUM = AREAREQ2 / AREATUBE
155.     If TUBENUM < 1 Then
156.         TUBENUM = 1
157.     End If
158.     AREAREQ = TUBENUM * AREATUBE
159. 'TOTAL CO2 Flux
160.     FLUXCO2 = JCO2P * TUBENUM 'Total CO2 Flux (mol/s.cm^2)
161. 'TOTAL CO2 Flux
162.     FLUXH2 = JH2P * TUBENUM 'Total H2 Flux (mol/s.cm^2)
163. '===== PERMEANCE =====
164. 'Cell Efficiency
165.     CEFF = (H2PERCOP / H2PERCI)
166.     H2PERCRET = CEFF * 100
167. 'CO2 PERMEANCE
168.     CO2PERMEANCE = JCO2P / (DELP) 'CO2 PERMEANCE (mol/sec.cm^2. atm)
169. 'H2 PERMEANCE
170.     H2PERMEANCE = JH2P / (DELP) 'H2 PERMEANCE (mol/sec.cm^2. atm)
171. 'CO2 PERMEABILITY
172.     CO2PERMABIL = (JCO2P * MMTHCM) / DELP 'CO2 Permeability (mol/sec.cm.atm)
173. 'H2 PERMEABILITY
174.     H2PERMABIL = (JH2P * MMTHCM) / DELP 'H2 Permeability (mol/sec.cm.atm)
175. 'Separation Factor
176.     SEPFAC = ((CO2PERCOP / H2PERCOR) / (CO2MOLIN / H2MOLIN)) 'Separation Factor
177.     SEPFAC = ((44 / 56) / (CO2PERCOP / H2PERCOR)) 'Separation Factor
178.     SELEC = (CO2PERMEANCE / H2PERMEANCE)
179. '===== Mass Balance OUT TEST =====
180. 'RETENTATE
181.     RETENTOTAL = CO2PERCOR + H2PERCOR
182.     PERMEATOTL = CO2PERCOP + H2PERCOP
183.     KOL = RETENTOTAL + PERMEATOTL
184. 'CO2 Kg/day in PERMEATE and RETENTATE
185.     CO2KGOUTP = CO2FR * CEFF
186.     CO2KGOUTR = CO2FR - CO2KGOUTP
187. 'H2 Kg/day in PERMEATE and RETENTATE
188.     H2KGOUTR = H2FR * CEFF
189.     H2KGOUTP = H2FR - H2KGOUTR
190. '===== AREA Calculation =====
191. 'Number of Modules
192.     NUMBMOD = TUBENUM / NTUBEM
193.     If NUMBMOD < 1 Then

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194. NUMBMOD = 1
195. End If
196. 'PERMEATE
197. CO2PERMEAB = JC02P * MMTHM 'CO2 PERMEABILITY
198. H2PERMEAB = JH2P * MMTHM 'H2 PERMEABILITY
199. -----
200. ' OUTPUT
201. Cells(4, 11) = CO2KGOUTP 'CO2 (kg/Day) at PERMEATE
202. Cells(5, 11) = CO2KGOUTR 'CO2 (kg/Day) at RETENTATE
203. Cells(6, 11) = H2KGOUTR 'H2 (kg/Day) at RETENTATE
204. Cells(7, 11) = H2KGOUTP 'H2 (kg/Day) at PERMEATE
205. Cells(8, 11) = FLUXCO2 'CO2 Flux (mol/sec.cm^2)
206. Cells(9, 11) = JH2P / 24 'H2 Flux (kg/h.m^2)
207. Cells(10, 11) = CO2PERMEANCE 'CO2 Permeance
208. Cells(11, 11) = H2PERMEANCE 'H2 Permeance
209. Cells(12, 11) = CO2PERMABIL 'CO2 PERMEABILITY
210. Cells(13, 11) = H2PERMABIL 'H2 PERMEABILITY
211. Cells(14, 11) = SEPFAC 'Separation Factor
212. Cells(15, 11) = H2PERCRET 'H2 % in RETENTATE
213. Cells(16, 11) = TUBENUM 'Number of tubes
214. Cells(17, 11) = AREAREQ 'Total Area required (cm^2)
215. Cells(5, 15) = SELEC
216. =====
217. Cells(3, 15) = NUMBMOD 'NUMBMOD
218. -----
219. '- Plot Temperature versus CO2 %
220. TCK = 310
221. For I = 1 To 9
222. CO2CON3 = THERMODYNAMIC(TCK)
223. Cells(65 + I, 1) = TCK
224. Cells(65 + I, 2) = CO2CON3 - 0.002
225. If TCK > 1.00001 Then
226. CO2CON3 = CO2CON1 / CO2CON3
227. End If
228. TCK = TCK - 10
229. Next I
230. '-Plot Flux Selectivity
231. TCK = 234
232. For I = 1 To 9
233. FLUX = FLUXDYNAMICS(TCK)
234. Cells(65 + I, 3) = TCK
235. Cells(65 + I, 4) = FLUX
236. TCK = TCK + 10
237. Next I
238. '===== ENERGY BALANCE ====='
239. '
240. '===== COMPRESSOR-1 (GAS FROM BIOGAS Reactor)=====
241. '...H2
242. RH2 = 4.1242 'Gas Constant (kJ/kg k)
243. H2ITK = GASTEM + 273
244. H2SPHEATP = H2SPEHEAT(H2ITK) ' Cp of H2 kJ/Kg K)
245. H2SPHEATC = H2SPHEATP - RH2 ' Cv of H2 kJ/Kg K)
246. H2VOL = H2FR / 0.735 'RHOH2 ' H2 Volume (m^3)
247. '...CO2
248. RCO2 = 0.1889 'Gas Constant (kJ/kg k)
249. GASTK = GASTEM + 273
250. CO2SPHEATP = CO2SPEHEAT(GASTK) ' Cp of CO2 kJ/Kg K)
251. CO2SPHEATC = CO2SPHEATP - RCO2 ' Cv of H2 kJ/Kg K)
252. CO2VOL = CO2FR / 1.586 'RHOCO2 ' CO2 Volume (m^3)
253. '...GAS
254. H2PERC = H2FR / TOTALGAS 'H2 Mass fraction
255. CO2PERC = CO2FR / TOTALGAS 'CO2 Mass fraction
256. RHOGAS = H2PERC * RHOH2 + CO2PERC * RHOCO2 'Gas Density
257. RMW1 = 44 * CO2PERC
258. RMW2 = 2 * H2PERC

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259. RMWMIXZ = RMW1 + RMW2
260. RMWS = RMW1 / RMWMIXZ 'CO2 percentage'
261. RMWS1 = RMW2 / RMWMIXZ 'H2 percentage'
262. MASSMIXCP = (0.88 * RMWS) + (14.1 * RMWS1) 'CP of mixture kj/kg.k
263. RCG = (RH2 * H2PERC + RCO2 * CO2PERC) * 1000
264. GASVOL = H2VOL * H2PERC + CO2VOL * CO2PERC 'm^3
265. GASVOLL = GASVOL * 1000 'Gas Volume(L/day)
266. GASVOL1 = (GASVOLL / 24) / 60 'Gas Volume (L/min)
267. GASSPHEATP = H2SPHEATP * H2PERC + CO2SPHEATP * CO2PERC 'CP of mixture kj/kg.k
268. GASSPHEATC = H2SPHEATC * H2PERC + CO2SPHEATC * CO2PERC 'CV of mixture kj/kg.k
269. GAMMA = GASSPHEATP / GASSPHEATC
270. COMPIP = PCO 'PCI
271. COMPOP = PCI 'PCO
272. ENTCC = 127 'RHOGAS * RCG ' * 100 '* Logn(COMPOP / COMPIP) 'Entropy Change Constant (J/K.m^3)
273. '...Data Input
274. Cells(21, 4) = GASVOL1
275. Cells(22, 4) = COMPIP
276. Cells(23, 4) = COMPOP
277. Cells(24, 4) = GASTEM
278. COMETREFF = Cells(25, 4)
279. SPHASVOL = Cells(26, 4)
280. MOTOREFF1 = Cells(27, 4)
281. THREPASEVOL = Cells(28, 4)
282. MOTOREFF3 = Cells(29, 4)
283. GASTEMPC = GASTEM ' + 273
284. OUTADIATEMP = ((GASTEMPC + 273) * ((COMPOP / COMPIP) ^ ((1.3 - 1) / 1.3))) - 273 ' OUTLET ADIABATIC TEMPERATURE
285. DRMOTWATT = ((OUTADIATEMP + 273) - (GASTEMPC + 273)) * MASSMIXCP * (TOTALGAS / 86400) / (MOTOREFF1 / 100) 'kW
286. Call COMPRESSOR(GASTEMPC, COMPOP, COMPIP, GAMMA, GASVOL, OUTADIATEMP, COMETREFF, WATT, ENTCC, DRMOTWATT, DRMOTHP, MOTOREFF1, MOTOREFF3, SPH
ASVOL, THREPASEVOL, CURRENT1, CURRENT3)
287. Cells(27, 11) = OUTADIATEMP
288. Cells(28, 11) = DRMOTWATT 'kW
289. Cells(29, 11) = DRMOTHP
290. Cells(30, 11) = CURRENT1
291. Cells(31, 11) = CURRENT3
292. '----- HEAT EXCHANGER -----
293. ' GAS
294. TL = Cells(44, 11)
295. TOD = Cells(45, 11)
296. GASFLOWRATE = H2FR + CO2FR
297. SCGAS = GASSPHEATP 'GAS Specific Heat (kJ/kg.K)
298. CGAS = ((GASFLOWRATE / 24) / 3600) * SCGAS 'GAS Heat capacity (KW/oK)
299. TH1 = OUTADIATEMP + 273 'GAS Hot Side (oK)
300. TH2 = 179 + 273 'GAS Cold Side (oK) (179 max. Temperature of refrigerent
301. QGAS = CGAS * (TH1 - TH2)
302. 'Air
303. TC1 = 25 + 273
304. AIRINTK = TIC
305. SCAIR = AIRSPECIFICHEAT(AIRINTK)
306. 'TC2=?
307. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
308. FLAG = 2
309. U = 0.02
310. CHOT = CGAS: Q = QGAS: SCHOT = SCGAS: SCCOLD = SCAIR = AIRSPECIFICHEAT(AIRINTK)
311. Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN
GER
312. 'DATA OUT
313. AIRFLR = HFR
314. Cells(40, 11) = OUTADIATEMP
315. Cells(41, 11) = TH2 - 273
316. Cells(42, 11) = TC1 - 273
317. Cells(43, 11) = TC2 - 273
318. Cells(46, 11) = NTU
319. Cells(47, 11) = AREAHEX
320. Cells(48, 11) = EPS * 100
321. Cells(49, 11) = QEFF

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322. Cells(50, 11) = AIRFLR
323. '===== INTERNAL BOX =====
324. '..... REFRIGERATOR UNIT .....
325. ' COMPRESSOR Input
326. CTIN = OUTADIATEMP
327. Cells(37, 4) = CTIN 'Compressor Input Temperature (oC)
328. CTOUT = Cells(38, 4) 'Compressor Output Temperature (oC)
329. RRATE = Cells(39, 4) 'Compressor Refrigerante Rate (Kg/sec)
330. CPIN = Cells(40, 4) 'Compressor Pressure In (MPa)
331. CPOUT = Cells(41, 4) 'Compressor Pressure Out (MPa)
332. CENT = Cells(42, 4) 'Compressor Enthalpy In (kJ/kg)--> (H1)
333. CENTO = Cells(43, 4) 'Compressor Enthalpy Out(kJ/kg)--> (H2)
334. CENTS = Cells(44, 4) 'Compressor Enthalpy (Steam) (kJ/kg)--->(H2S)
335. ' CONDENSER
336. TCN = Cells(46, 4) 'Condenser Input Temperature (oC)
337. PCN = Cells(47, 4) 'Condenser Pressure (MPa)
338. ENTCN = Cells(48, 4) 'Condenser Enthalpy (kJ/kg)---(H3)
339. ' VALVE
340. VTRP = Cells(50, 4) 'Valve Throttled Pressure (MPa)
341. ENTEV = Cells(51, 4) 'Valve Enthalpy (kJ/kg)----> (H4)
342. COREF = NUMBMOD * 1.08 'Correction Factor/module
343. 'Heat removal from Condenser(kW)
344. '===== REFRGERATION CHAMBER SIZE =====
345. LENGTHB = LTUBE / 100 'Length in (m)
346. WIDTHB = (LTUBE / 6.6) / 100 'Width in (m)
347. HEIGTHB = LENGTHB / 8 'Height in (m)
348. AREAB = LENGTHB * WIDTHB * HEIGTHB 'AREA in (m^3)/module
349. Cells(31, 4) = LENGTHB 'Length in (m)
350. Cells(32, 4) = WIDTHB 'Width in (m)
351. Cells(33, 4) = HEIGTHB 'Height in (m)
352. '=====
353. ' OUTPUT
354. Cells(19, 11) = QL
355. Cells(20, 11) = WC
356. Cells(21, 11) = ISEFF
357. Cells(22, 11) = COPR
358. Cells(23, 11) = COPHP
359. Cells(24, 11) = COOLoad
360. Cells(25, 11) = QH
361. '=====
362. '..... COMPRESSOT FOR CO2 TO UREA .....
363. '...INPUT
364. CO2VOL1 = ((CO2VOL * 1000) / 24) / 60 'CO2 Volume (L/min)
365. COMPIP = COMPOP
366. Cells(53, 4) = CO2VOL1
367. Cells(54, 4) = COMPIP
368. COMPOP = Cells(55, 4)
369. Cells(56, 4) = TC1
370. '...OUTPUT
371. GAMMA = CO2SPHEATP / CO2SPHEATC
372. ENTCC = (RCO2 * RHOCO2) * 1000
373. Call COMPRESSOR(GASTEMPC, COMPOP, COMPIP, GAMMA, GASVOL, OUTADIATEMP, COMETREFF, WATT, ENTCC, DRMOTWATT, DRMOTHP, MOTOREFF1, MOTOREFF3, SPH
ASVOL, THREPASEVOL, CURRENT1, CURRENT3)
374. Cells(33, 11) = OUTADIATEMP
375. Cells(34, 11) = DRMOTWATT / 1000 'kW
376. Cells(35, 11) = DRMOTHP
377. Cells(36, 11) = CURRENT1
378. Cells(37, 11) = CURRENT3
379. '=====
380. ' HEAT LOSS
381. '=====
382. '----- HEAT LOSS (HEAT IN)
383. H2ITK = GASTEM + 273 'For Emperical Equation of H2
384. GASTK = GASTEM + 273 'For Emperical Equation of CO2
385. H2FRGS = ((H2FR / 24) / 3600) 'H2 Flow Rate (kg/sec)

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386. CO2FRGS = ((CO2FR / 24) / 3600) 'CO2 Flow Rate (kg/sec)
387. GASFR = H2FRGS + CO2FRGS 'Total Gas Flow Rate (kg/day)
388. H2MPER = H2FRGS / GASFR 'H2 mass %
389. CO2PER = CO2FRGS / GASFR 'CO2 mass %
390. H2SPHEAT = H2SPECHEAT(H2ITK) 'H2 Specific HeatSPECIFIC HEAT (kJ/Kg K)
391. CO2SPHEAT = CO2SPEHEAT(GASTK) 'CO2 SPECIFIC HEAT ' Cp of CO2 (kJ/Kg K)
392. GASSPHEAT = H2MPER * H2SPHEAT + CO2PER * CO2SPHEAT 'Gas SPECIFIC HEAT SPECIFIC HEAT (kJ/kg K)
393. QGASIN = GASFR * GASSPHEAT * GASTK 'kW
394. '----- HEAT LOSS (HEAT OUT)
395.
396. H2ITK = TC1X + 273
397. GASTK = TC1X + 273
398. H2SPHEAT = H2SPECHEAT(H2ITK) 'H2 Specific HeatSPECIFIC HEAT (kJ/Kg K)
399. CO2SPHEAT = CO2SPEHEAT(GASTK) 'CO2 SPECIFIC HEAT ' Cp of CO2 (kJ/Kg K)
400. 'Heat from H2 OUT
401. H2OUTKGS = (H2KGOUTR / 24) / 3600 'H2 Flow Rate (kg/sec)
402. QH2 = H2OUTKGS * H2SPHEAT * H2ITK 'Heat from H2 (kJ/sec)
403. 'Heat from CO2 OUT
404. CO2OUTKGS = (CO2KGOUTP / 24) / 3600 'CO2 Flow Rate (kg/sec)
405. QC02 = CO2OUTKGS * CO2SPHEAT * GASTK 'Heat from CO2 (kJ/sec)
406. 'Total Heat OUT
407. QTOTOUT = QH2 + QC02 'Q total OUT (kJ/sec)
408. 'Q LOSS
409. QLOSS = QGASIN - QTOTOUT 'Q LOSS (kJ/sec)
410. 'DATA OUT
411. Cells(52, 9) = QGASIN
412. Cells(53, 9) = QTOTOUT
413. Cells(54, 9) = QLOSS
414. '=====
415. 'REFRIGRATION
416. '=====
417. Cells(37, 4) = 179 'Compressor Input Temperature (°C)
418. CTIN = 179
419. Cells(38, 4) = TC1X
420. COMPPRESSU1 = 0.535287441 'atm'
421. COMPTEMPU1 = CTIN + 273 'Celcuis'
422. ENTHALPYCOMP = 226.494 'KJ/Kg'
423. ENTROPYCOMP = 0.9668 'KJ/Kg.K'
424. COMPPRESSU2 = 5.21095 '9.86 'atm'
425. ADIATEMPCOM = 30 '54.96875 'Celcuis
426. ENTHALPYCOMP2 = 272.32 '288.01656 'KJ/kg'
427. MASSFLOW = 5 'kg/min'
428. CONDENSTEMP = 17.406 'Celcuis'
429. PRESSURECOND = 5.21095 'atm'
430. ISENTROPYCONDENS = 0.962 '0.96609355 'KJ/Kg.K
431. ENTHALPYCONDENS = 75.6104 'KJ/Kg'
432. Cells(39, 4) = MASSFLOW
433. Cells(40, 4) = COMPPRESSU1
434. Cells(41, 4) = COMPPRESSU2
435. Cells(42, 4) = ENTHALPYCOMP
436. Cells(43, 4) = ENTHALPYCOMP2
437. Cells(44, 4) = COMPPRESSU2
438. Cells(46, 4) = CONDENSTEMP
439. Cells(47, 4) = PRESSURECOND
440. Cells(48, 4) = ENTHALPYCONDENS
441. Cells(50, 4) = ISENTROPYCONDENS
442. Cells(51, 4) = ENTHALPYCONDENS 'Enthalpy of Expansion valve is the same as the output from the condensetr'
443. 'entropy=0.0054'KJ/Kg.K''FROM VALVE TO THE EVAPORATOR'
444. ENTALPMID = 260.198 '1.254'225.239 '286.612 'KJ/Kg''ENTROPY=0.969 from compressor to the condenser & pressure=0.8 'MPA''
445. 'POWER INPUT TO THE COMPRESSOR'
446. WORKCOMP = (ENTHALPYCOMP2 - ENTHALPYCOMP) * (MASSFLOW / 60) 'Kw'W*
447. WORKCOMPREF = (ENTHALPYCOMP - ENTHALPYCONDENS) * (MASSFLOW / 60) 'QL'Kw''EVAPORATOR'*
448. EFFECREF = (ENTALPMID - ENTHALPYCOMP) / (ENTHALPYCOMP2 - ENTHALPYCOMP) '%'
449. CONDENSWORK = (ENTHALPYCOMP2 - ENTHALPYCONDENS) * (MASSFLOW / 60) 'Kw'
450. COPRREF = WORKCOMPREF / WORKCOMP 'COPr*'

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451. COPRSREFRT = CONDENSWORK / WORKCOMP 'COP
452. Cells(19, 11) = WORKCOMPREF
453. Cells(20, 11) = WORKCOMP
454. Cells(21, 11) = EFFECREF * 100
455. Cells(22, 11) = COPRSREF
456. Cells(23, 11) = COPRSREFRT
457. End Sub
458. Static Function Logn(X)
459.     Logn = Log(X) / Log(2.718282)
460. End Function
461. Function Log10(XX)
462.     Log10 = Log(XX) / Log(10)
463. End Function
464. Private Static Function CO2PARPRES(TC)
465.     CO2PARPRES = -8.0090945 * 10 ^ 8 / (1 - 24806707 * Exp(-0.02744426 * TC))
466. End Function
467. Private Static Function CO2DENSITY(T)
468.     A = 0.50649907: B = 0.0019289299: C = 1.0174749
469.     CO2DENSITY = (A + B * T) ^ (-1 / C)
470. End Function
471. Private Static Function H2PARPRES(TCK)
472.     H2PARPRES = 3.54314 - (99.395 / (TCK + 7.726))
473. End Function
474. Private Static Function H2DENSITY(T) 'T=oC,Kg/m^3 10 ATM.
475.     A = 1.1338296: B = 0.00414983: C = 1.0033354
476.     H2DENSITY = (A + B * T) ^ (-1 / C)
477. End Function
478. Private Static Function ALFADPL(JCO2)
479.     ALFADPL = (229.86086) / (1 + Exp(-20.968662 + 0.040633684 * JCO2) ^ 1 / 0.015843568)
480. End Function
481. Private Static Function FLUXDYNAMICS(TCK)
482.     FLUXDYNAMICS = (428.53071) / (1 + Exp(59.137653 - 0.21830436 * TCK) ^ 1 / 42.291375)
483. End Function
484. Private Static Function THERMODYNAMIC(TCK)
485.     THERMODYNAMIC = (Exp(6.703717 - 57.793114 / TCK - 0.33932743 * Logn(TCK))) / 100 'in function of vapor pressure
486. End Function
487. Private Static Sub COMPRESSOR(GASTEMPC, COMPOP, COMPIP, GAMMA, GASVOL, OUTADIATEMP, COMETREFF, WATT, ENTCC, DRMOTWATT, DRMOTHP, MOTOREFF1, MOTO
    REFF3, SPHASVOL, THREPASEVOL, CURRENT1, CURRENT3)
488. End Sub
489. Private Static Function H2SPECHEAT(H2ITK) '(kJ/Kg K)
490.     ZA = 8.3580785: ZB = 0.046774926: ZC = -0.00014346423: ZD = 0.00000023506381: ZE = -2.3076196E-10: ZF = 1.4608608E-13
491.     ZG = -6.1673082E-17: ZH = 1.7508367E-20: ZI = -3.2962768E-24: ZJ = 3.9405226E-28: ZK = -2.7046605E-32: ZL = 8.1083083E-37
492.     H2SPECHEAT = ZA + ZB * H2ITK + ZC * H2ITK ^ 2 + ZD * H2ITK ^ 3 + ZE * H2ITK ^ 4 + ZF * H2ITK ^ 5 + ZG * H2ITK ^ 6 + ZH * H2ITK ^ 7 + ZI * H2ITK
        ^ 8 + ZJ * H2ITK ^ 9 + ZK * H2ITK ^ 10 + ZL * H2ITK ^ 11
493. End Function
494. Private Static Function CO2SPEHEAT(GASTK) 'CO2 SPECIFIC HEAT ' Cp of CO2 kJ/Kg K)
495.     Z1 = 0.51476288
496.     Z2 = 5820.1918
497.     Z3 = 1.4877831
498.     Z4 = 1.404349
499.     CO2SPEHEAT = (Z1 * Z2 + Z3 * GASTK ^ 24) / (Z2 + GASTK ^ 24)
500. End Function
501. Private Static Function DPLALFA(X)
502.     A = 1074916.6: B = -33782.296: C = 353.9222: D = -1.2355557
503.     DPLALFA = A + B * X + C * X ^ 2 + D * X ^ 3
504. End Function
505. Private Static Function CO2VISCOSITY(T) 'T=oC and Centipoise
506.     A = 0.013830936: B = 0.000050308039: C = 0.00000028002318: D = 7.0996286E-10
507.     CO2VISCOSITY = A + B * T + C * (T) ^ 2 + D * (T) ^ 3
508. End Function
509. Private Static Function AIRSPECIFICHEAT(AIRINK) 'T=oK
510.     TA = 1.0828694: TB = -0.00063119116: TC = 0.0000016253087: TD = -1.3949526E-09: TE = 5.3826153E-13: TF = -7.9021928E-17
511.     AIRSPECIFICHEAT = TA + TB * AIRINK + TC * AIRINK ^ 2 + TD * AIRINK ^ 3 + TE * AIRINK ^ 4 + TF * AIRINK ^ 5
512. End Function

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513. Private Static Sub HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'H
    EAT EXCHANGER
514.     AREAHEX = 3.14 * TOD * TL
515.     'DELTAB = TH2 - TC1
516.     LMTD = Q / (U * AREAHEX)
517.     'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
518.     '----- HEATING -----
519.     If FLAG = 1 Then
520.         DELTAA = TH1 - TC2
521.         'DELTAB = TH2 - TC1
522.         LMTD = Q / (U * AREAHEX)
523.         X1 = 1
524. 300 S1 = DELTAA / (LMTD - Logn(DELTAA))
525.         S2 = X1 / (LMTD - Logn(X1))
526.         If S2 >= S1 Then
527.             GoTo 400
528.         Else
529.             X1 = X1 + 0.1
530.             GoTo 300
531. 400 End If
532.         DELTAB = X1
533.         TH2 = DELTAB + TC1
534.         GoTo 700
535.     End If
536.     '----- COOLING -----
537.     '----- COOLING -----
538.     If FLAG = 2 Then
539.         'DELTAA = TH1 - TC2
540.         DELTAB = TH2 - TC1
541.         LMTD = Q / (U * AREAHEX)
542.         X1 = 2
543. 500 S1 = Logn(X1) - X1 / LMTD
544.         S2 = Logn(DELTAB) - DELTAB / LMTD
545.         If S1 >= S2 Then
546.             GoTo 600
547.         Else
548.             X1 = X1 + 0.1
549.             GoTo 500
550. 600 End If
551.         DELTAA = X1
552.         TC2 = TH1 - DELTAA
553.     End If
554.     '-----
555. 700 P = (TC2 - TC1) / (TH1 - TC1)
556.         R = (TH1 - TH2) / (TC2 - TC1)
557.         If R > 1 Then
558.             R1 = 1 / R
559.             P1 = P * R
560.         Else
561.             P1 = P
562.             R1 = R
563.         End If
564.         A1 = (((R1) ^ 2 + 1) ^ 0.5) / (1 - R1)
565.         A2 = Logn((1 - R1 * P1) / Abs(1 - P1))
566.         A3 = 2 - P1 * (1 + R1 - (1 + (R1) ^ 2)) ^ 0.5 'up
567.         A4 = Abs(2 - P1 * (1 + R1 + (1 + (R1) ^ 2)) ^ 0.5) 'down
568.         A5 = Logn(A3 / A4)
569.         FCORF = (A1 * A2) / A5
570.         If Abs(FCORF) > 1 Then
571.             FCORF = 1
572.         End If
573.         If FLAG = 1 Then
574.             LMTD = Q / (U * AREAHEX * FCORF)
575.             CHOT = Q / (TH1 - TH2)
576.             HFR = CHOT * 24 * 3600 / SCHOT

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577.   GoTo 800
578.   End If
579.   If FLAG = 2 Then
580.     LMTD = Q / (U * AREAHEX * FCORF)
581.     CCOLD = Q / (TH1 - TH2)
582.     HFR = CCOLD * 24 * 3600 / SCHOT
583.   End If
584. 'EFFECTIVENESS
585. 800 If CCOLD > CHOT Then
586.   CMIN = CHOT
587.   C1 = CHOT
588.   EPS = (C1 * (TC2 - TC1)) / (CMIN * (TH1 - TC1))
589.   GoTo 900
590. Else
591.   CMIN = CCOLD
592.   C1 = CCOLD
593.   EPS = (C1 * (TH1 - TH2)) / (CMIN * (TH1 - TC1))
594. 900 End If
595.   QEFF = EPS * CMIN * (TH1 - TC1)
596. 'Number of ELEMENT
597.   NTU = U * AREAHEX / CMIN
598.   If NTU <= 1 Then
599.     NTU = 1
600.   Else
601.   End If
602. End Sub

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ITM membrane

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1. Sub Sheet5_Button1_Click()
2. '
3. ' (ITM)
4. '
5. 1 N2EMS = ActiveWorkbook.Worksheets("EMS").Cells(6, 11) 'N2 Needed for EMS (Kg/day)
6. CH4FRK = ActiveWorkbook.Worksheets("DFB-ADB").Cells(22, 20) 'Mass of CH4 (Kg/day)
7. CO2FRK = ActiveWorkbook.Worksheets("DFB-ADB").Cells(23, 20) 'Mass of CO2 (Kg/day)
8. H2SFRK = ActiveWorkbook.Worksheets("DFB-ADB").Cells(24, 20) 'Mass of H2S (Kg/day)
9. NH3FRK = ActiveWorkbook.Worksheets("DFB-ADB").Cells(25, 20) 'Mass of H2 (Kg/day)
10. H2TEMP = ActiveWorkbook.Worksheets("SOFC").Cells(31, 4) 'HOT WATER(STEAM)Temperature (°C)
11. H2TEMPXX = ActiveWorkbook.Worksheets("HEAT BALANCE").Cells(42, 11) 'HOT WATER(STEAM)Temperature (°C)
12. N2SSAS = Cells(7, 4) 'Total N2 Needed for the system(Kg/Day)ASSUMPTION According to hand calculations
13. TGFR1 = CH4FRK + CO2FRK + H2SFRK + NH3FRK 'TOTAL GAS FLOW RATE (Kg/day)
14. AIRIN = H2TEMPXX
15. ' INPUT
16. AIRFR = N2SSAS / 0.79
17. AIRFR = Cells(5, 4) 'Mass of Air ((kg/day)
18. O2FMRATE1 = AIRFR * 0.21 'O2 Kg/day(Standard % = 0.21)
19. N2FMRATE1 = AIRFR * 0.79 'N2 Kg/day(Standard % = 0.79)
20. TOTAIR = O2FMRATE1 + N2FMRATE1
21. Cells(6, 4) = O2FMRATE1 'Oxygen flow Rate (Kg/day)
22. Cells(7, 4) = N2FMRATE1 'N2 flow Rate (Kg/day)
23. AITC = Cells(8, 4) 'Air Inlet Temperature oC
24. IP = Cells(9, 4) 'Air Inlet Pressure (atm)
25. '.... Cell Side
26. CT = Cells(11, 4) 'Cell Temperature (oC)
27. '----- LIMIT OF TEMPERATURE
28. If CT < 800 Then
29. Cells(11, 4) = 800
30. End If
31. If CT > 900 Then
32. Cells(11, 4) = 950
33. End If
34. '-----
35. CPIN = Cells(12, 4) 'Cell Pressure [Cathode Shell Side] (atm)
36. ORAD1 = Cells(13, 4) 'Outer Radius (mm)

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37.   IRAD1 = Cells(14, 4)  'Inner Radius (mm)
38.   CTL = Cells(15, 4)  'Cell Tube Length (cm)
39.   'Membrane Thickness
40.   ORAD = ORAD1 / 10    'Outer Radius (cmm)
41.   IRAD = IRAD1 / 10    ''Inner Radius (cm)
42.   MEMTH = (ORAD - IRAD) / (Logn(ORAD / IRAD)) 'Membrane Thickness (cm)
43.   'Unit Surface Area
44.   MAUT = 2 * 3.1416 * CTL * MEMTH 'Membrane area / unit tube (m^2/u.t)
45.   Cells(16, 4) = MAUT  'Membrane area / unit tube (m^2/u.t)
46.   NTPU = Cells(17, 4)  'Number of tube /Units
47.   CPOUT = Cells(19, 4) 'Oxygen Pressure at Permeate
48.   ' Constant
49.   'FUEF = FUEF1 / 100
50.   MW02 = 32            'O2 Molecular Weight
51.   AIRITK = AITC + 273
52.   FA = 96485          'coulombs/mole
53.   CTK = CT + 273     'Cell Temperature in oK
54.   R = 8.314          'J/K.mol
55.   O2DEN = 1.429      'Oxygen Density(g/L)
56.   CD = 3.5 * 10 ^ 4  'Constant for Nernst Potential
57.   ED = 282.8         'Effective dissociation energy (kJ/mole)
58.   BOLTZCON1 = 1.38064852E-23 'Boltzmann Constant (m^2.Kg/s.K)
59.   BOLTZCON = 1.380658 * 10 ^ -3 'Boltzmann Constant (J/K)
60.   O2DV = 0.00498     'Lattice vacancy diffusion (cm^2/s)
61.   '
62.   '===== CALCULATIONS =====
63.   'N2 Balance
64.   N2FMRATER = N2FMRATE1 'N2 at RETENTATE IN (Cathode)(Kg/Day)
65.   'O2 Balance
66.   O2FMRATERI = O2FMRATE1 'O2 at RETENTATE IN (Cathode)(Kg/Day)
67.   ' Partial Pressure
68.   '
69.   O2MOLES = ((O2FMRATERI / 32) * 1000) 'Moles of O2 IN (gMOLE/day)at RETENTATE
70.   N2MOLES = ((N2FMRATER / 28) * 1000) 'Moles of N2 IN (gMOLE/day)at RETENTATE
71.   TOTMOLES = O2MOLES + N2MOLES        'Total Moles IN (gMOLE/day)at RETENTATE (Cathode)
72.   N2MPERCI = N2MOLES / TOTMOLES       'Mole % of N2 at INLET at RETENTATE (Cathode)
73.   O2MPERCI = O2MOLES / TOTMOLES       'Mole % of O2 at INLET at RETENTATE (Cathode)
74.   O2CPOUT = (CPIN * 0.21) / CPOUT     'Cell Pressure OUT O2 at PERMEATE (anode)side (atm)
75.   N2PPIN = N2MPERCI * CPIN            'N2 IN Partial Pressure at RETENTATE (Cathode) (atm)
76.   O2PPIN = O2MPERCI * CPIN           'O2 IN Partial Pressure at RETENTATE (Cathode) (atm)
77.   O2PPOUT = (O2MOLES / O2MOLES) * O2CPOUT 'O2 OUT Partial Pressure at PERMEATE (anode)(atm)
78.   N2PPOUT = (CPIN * 0.79) / CPOUT    'N2 Pressure OUT at PERMEATE (anode)side (atm)
79.   '...Volumetric Flow Rate
80.   'Air
81.   T = CT
82.   RHOAIR = AIRDENSITY(T) 'Air density (KG/m^3) 'Temperature in oC and kg/m^3
83.   VOLAIR = AIRFR * RHOAIR 'Volume of Air (m^3/day)
84.   'O2 Volumetric Flow
85.   O2DEN = O2DENSITY(TC) 'O2 Density (kg/m^3)
86.   O2VOLFM = O2FMRATERI / O2DEN 'O2 Volumetric Flow (m^3/day) at RETENTATE
87.   O2VOLF = O2VOLFM * 1000000 'O2 Volumetric Flow (cm^3/day) at RETENTATE
88.   O2VOLFSR = (O2VOLF / 24) / 3600 'O2 Volumetric Flow (cm^3/sec) at RETENTATE
89.   'N2 Volumetric Flow
90.   N2DEN = N2DENSITY(TC) 'N2 Density (kg/m^3)
91.   N2VOLF = N2FMRATEP / N2DEN 'N2 Volumetric Flow (m^3/day) at RETENTATE
92.   'O2 INPUT Concentration Cv'
93.   O2CVR = O2VOLFM / VOLAIR 'Cv' O2% Volumetric Concentrarion at RETENTATE
94.   'N2 INPUT Concentration Cv'
95.   N2CVR = N2VOLF / VOLAIR 'Cv N2% Volumetric Concentrarion at RETENTATE
96.   '
97.   '...INPUT PARAMETERS
98.   '
99.   '===== FLUX =====
100. 'Diffusivity of oxygen vacancy (cm2/s) ...Ref:0-1-coal_igcc-rport Page:37
101.   DV = (1.58 * (10) ^ -2 * Exp(-8852.5 / CTK)) '(cm^2/sec)

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102. 'Foward Reaction Rate Constant (cm/(atm^0.5)*s)'\...Ref:0-1-coal_igcc-rport Page:37
103.   KF = 5.9 * (10) ^ 6 * Exp(-27291 / CTK) '(cm/(atm^0.5).sec)
104. 'Reverse reaction rate constant (mol/cm^2*s)'\... Ref:0-1-coal_igcc-rport Page:37
105.   KR = (2.07 * (10) ^ 4 * Exp(-29023 / CTK)) '(mol/cm^2.sec)
106. 'Local oxygen permeation flux through the hollow fiber membranes
107. 'Reference: itm66 Page-10 or eee551fa593cae9fd2a3d0f79407c9e50ee7 Page-24,63,46 Ref: you1 Page:249
108.   NUM = DV * KR * ((O2PPIN) ^ 0.5 - (O2PPOUT) ^ 0.5)
109.   DENOM1 = 2 * MEMTH * KF * (O2PPIN * O2PPOUT) ^ 0.5
110.   DENIM2 = DV * ((O2PPIN) ^ 0.5 + (O2PPOUT) ^ 0.5)
111.   FLUXO2 = NUM / (DENIM2 + DENOM1) 'OXYGEN FLUX (mole/cm^2.s)
112.   FLUXO2KGS = FLUXO2 * MW02 'OXYGEN FLUX (kg/cm^2.s)
113.   FLUXO2KGM2 = (FLUXO2 * MW02 * ((10) ^ 4) * 3600 * 24) '(kg/m^2.day)
114. '
115. '===== CONCENTRATION OUT =====
116. 'O2 Concentration OUT at Permeate [YOU1-Page:249 or itm66-Page:10
117.   O2VOLFSR = -((FLUXO2KGS * MEMTH) / DV) + O2VOLFSR 'CO2 OUT in PERMEATE (cm^3/sec)
118.   O2VOLCMS = O2VOLFSR / 1000000 'CO2 OUT in PERMEATE (m^3/sec)
119.   O2MASFOP = O2VOLCMS * O2DEN * 24 * 3600 'CO2 OUT in PERMEATE (kg/day)
120. 'O2 Flow Rate OUT at RETENTATE
121.   O2MASOR = O2FMRATERI - O2MASFOP 'CO2 OUT in RETENTATE (kg/day)
122. 'Cell Efficiency
123.   CELEFF = O2MASFOP / O2FMRATE1 'Cell Efficiency %
124. 'N2 Flow Rate OUT at RETENTATE
125.   N2MASOR = N2FMRATER * CELEFF 'N2 OUT in RETENTATE (kg/day)
126. 'N2 Flow Rate OUT at PERMEATE
127.   N2MASOP = N2FMRATE1 - N2MASOR 'N2 OUT in PERMEATE (kg/day)
128. '
129. '===== PERMEABILITY-PERMEANCE =====
130. 'REFERENCE: 0-0-1-A-EXELLENT-CRAWFORD-THESIS-2013, Page:41,49
131. 'O2 Permeability
132.   O2PERMAB = (FLUXO2 * MEMTH) / (CPIN - O2CPOUT) '(mol/cm.sec.atm)
133. 'O2 Permeance
134.   O2PERMAC = O2PERMAB / MEMTH '(mol/cm^2.sec.atm)
135. 'Selectivity
136.   SELECFACT = ((N2MASOR / N2FMRATER) / (O2FMRATERI / O2MASFOP)) * 100
137. '===== Unit Tube Area =====
138. 'Area per Tubes
139.   UTA = 2 * 3.14 * (ORAD / 1000) * (CTL / 100) ' UNIT TUBE AREA (m^2)
140. 'Cell Area Required
141.   CELLAREAREQ = O2FMRATE1 / FLUXO2KGM2
142. 'Number of Tubes
143.   TUBENUM = CELLAREAREQ / UTA
144. 'NUMBER OF UNITS
145.   NUMUN = TUBENUM / NTPU
146.   If NUMUN < 1 Then
147.     NUMUN = 1
148.   End If
149. '===== Total Voltage =====
150. 'Voltage
151.   EVOLT = (R * CTK / (4 * FA)) * Logn(O2PPIN / O2PPOUT) 'Voltage per Tubes
152. ' Total Voltage
153.   VOLTOT = EVOLT * TUBENUM
154. 'Pressure Ratio of O2
155.   O2PRERAT = Logn(CPIN / O2CPOUT)
156. 'IONIC CONDUCTIVITY ref 0-1-coal_igcc-report...Page 28
157.   NUM1 = 4 * (MEMTH) * ((2) ^ 2) * ((FA) ^ 2) * (FLUXO2)
158.   DENUM1 = R * CTK * O2PRERAT
159.   IONCON = (NUM1 / DENUM1) 'Conductivity (1/cm.Ohm) = S/cm
160. 'Resistance
161.   RESISTOT = MEMTH * IONCON * NUMUN
162.   INVRESISTOT = 1 / RESISTOT
163.   UNITRESI = INVRESISTOT / TUBENUM 'Init Resistance (ohm)
164.   UNITCURRE = EVOLT / UNITRESI
165.   CURRENTS = EVOLT / UNITRESI 'Total current (amps)'
166.   TOTCURENT = CURRENTS * TUBENUM

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167.     POWERTOT = ((UNITCURRE * EVOLT * TUBENUM) / (1000))           'TOTAL POWER(KW)'
168. '===== N2 AVAILABILY CALCULATIONS ====='
169. 'N2 Calculations
170.     N2AVAILABLE = N2MASOR - N2EMS
171.     Cells(22, 4) = N2AVAILABLE 'N2 Available (Kg/day)
172.     Cells(23, 4) = N2EMS       'N2For EMS(Kg/day)
173.     If N2AVAILABLE <= 0 Then
174.         Cells(22, 6) = "TOO LOW"
175.         Cells(9, 7) = "ERROR"
176.         Cells(10, 7) = "N2<=0"
177.     End
178.     Else
179.         Cells(22, 6) = " "
180.         Cells(9, 7) = " "
181.         Cells(10, 7) = " "
182.     End If
183. 'Cells OUTPUT
184. '           OUTPUT
185.     Cells(20, 4) = CELEFF * 100
186.     Cells(4, 11) = DV           'Diffusivity of Oxygen (cm^2/S)
187.     Cells(5, 11) = KF           'Foward Reaction Rate (cm/atm^0.5*S)
188.     Cells(6, 11) = KR           'Reverse Reaction Rate (mole/cm^2*S)
189.     Cells(7, 11) = FLUXO2       'Oxygen Flux (mol/cm^2*s)
190.     Cells(8, 11) = N2FMRATER    'N2 IN Cathode Side (Kg/day)
191.     Cells(9, 11) = O2FMRATERI   'O2 IN Cathode side (Kg/day)
192.     Cells(10, 11) = N2MASOR     'N2 OUT RETENTEDT Anode side (Kg/day)
193.     Cells(11, 11) = O2MASFOP    'O2 OUT Anode side (Kg/day)
194.     Cells(12, 11) = CELLAREAREQ 'Area of Cell required (m^2)
195.     Cells(13, 11) = TUBENUM     'Number of Tubes
196.     Cells(14, 11) = NUMUN       'Number of Units
197.     Cells(15, 11) = MEMTH * 10  'Cell Membrane Thickness (mm)
198.     Cells(16, 11) = O2CPOUT     'O2 Pressure at Anode (atm)
199.     Cells(17, 11) = CPIN        'N2 Pressure at Anode (atm)
200.     Cells(18, 11) = O2PERMAC    'O2 Permeance (mole/cm^2*S.atm)
201.     Cells(19, 11) = O2PERMAB    'O2 Permeability (mole/cm*S.atm)
202.     Cells(20, 11) = SELECFACT   'Selectivity Factor
203.     Cells(21, 11) = EVOLT       'Cell Voltage/Tubes Out (Volt)
204.     Cells(22, 11) = VOLTOT      'Total Voltage OUT (Volt)
205.     Cells(23, 11) = IONCON      'IONIC CONDUCTIVITY(s/cm)
206.     Cells(24, 11) = RESISTOT    'Total resistance OHM
207.     Cells(25, 11) = TOTCURENT   'Total current (amps)
208.     Cells(26, 11) = POWERTOT    'TOTAL POWER(KW)
209. '===== PLOTS =====
210. 'Flux vs. Temperature
211.     CTK1 = CTK
212.     For I = 1 To 10
213.         DV = 1.58 * (10) ^ -2 * Exp(-8852.5 / CTK1)
214.         KF = 5.9 * (10) ^ 5 * Exp(-27291 / CTK1)
215.         KR = 2.07 * (10) ^ 4 * Exp(-27291 / CTK1)
216.         NUM = DV * KR * ((O2PPIN) ^ 0.5 - (O2PPOUT) ^ 0.5)
217.         DENOM1 = 2 * MEMTH * KF * (O2PPIN * O2PPOUT) ^ 0.5
218.         DENIM2 = DV * ((O2PPIN) ^ 0.5 + (O2PPOUT) ^ 0.5)
219.         FLUXO2 = NUM / (DENOM1 - DENOM2) 'OXYGEN FLUX (mole/cm^2.s)
220.         Cells(70 + I, 1) = CTK1 - 50
221.         Cells(70 + I, 2) = FLUXO2
222.         CTK1 = CTK1 - 50
223.     Next I
224. 'Preaure vs. O2 production
225.     CTK2 = CTK
226.     For I = 1 To 10
227.         DV = 1.58 * (10) ^ -2 * Exp(-8852.5 / CTK2)
228.         KF = 5.9 * (10) ^ 5 * Exp(-27291 / CTK2)
229.         KR = 2.07 * (10) ^ 4 * Exp(-27291 / CTK2)
230.         NUM = DV * KR * ((O2PPIN) ^ 0.5 - (O2PPOUT) ^ 0.5)
231.         DENOM1 = 2 * MEMTH * KF * (O2PPIN * O2PPOUT) ^ 0.5

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232. DENIM2 = DV * ((O2PPIN) ^ 0.5 + (O2PPOUT) ^ 0.5)
233. FLUXO2 = NUM / (DENOM1 - DENOM2) 'OXYGEN FLUX (mole/cm^2.s)
234. O2GF = FLUXO2 * MW02 * (10) ^ 4 * 24 * 60 * 60
235. Cells(70 + I, 3) = CTK2 - 50
236. Cells(70 + I, 4) = O2GF
237. CTK2 = CTK2 - 50
238. Next I
239. TOD = Cells(36, 4) ' Tube Outside Diameter (m)<=====
240. TL = Cells(35, 4)
241. '---TEMPERATURE
242. TC1 = AIRIN + 273 'AIR IN (K)
243. TC2 = CT + 273 'AIROUT (K)
244. TH1 = H2OTEMP + 273 'WATER IN (K)
245. ' TH2=? 'WATER OUT (K)
246. 'SPECIFIC HEAT
247. AIRTK = TC1
248. SCAIR = AIRSPECIFICHEAT(AIRTK) 'Air Specific Heat (kJ/kg.K)
249. H2OTEMP = TH1
250. SCH2O = WATERSPECIFICHEAT(H2OTEMP) 'Water Specific Heat (kJ/kg.K)
251. SCAIR = (AIRFR / 24) / 3600 * SCAIR 'Air Heat Capacity kW/oK
252. 'CALCULATIONS
253. CAIR = ((AIRFR / 24) / 3600) * SCAIR 'Air Heat Capacity kW/oK
254. QAIR = CAIR * (TC2 - TC1) 'Q-Air (kW)
255. Q = QAIR
256. U = 0.02
257. 'FLAG=1 for HEATING and FLAG=0 for COOLING
258. FLAG = 1
259. SCHOT = SCH2O: SCCOLD = SCH2O: CCOLD = CAIR
260. 'SUB
261. Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN
GER
262. '=====
263. H2OR = HFR:
264. '===== HEAT EXCHANGER OUTPUT =====
265.
266. Cells(26, 4) = H2OR 'Water Flow Rate Needed(Kg)
267. Cells(27, 4) = CAIR 'Air Heat Capacity (kW/oK)
268. Cells(28, 4) = CHOT 'Water Heat Capacity (kW/oK)
269. Cells(29, 4) = TH1 - 273 'H2O Temperature IN (oC)
270. Cells(30, 4) = TH2 - 273 'H2O Temperature Out (oC)
271. Cells(31, 4) = TC1 - 273 'N2 Temperature Out (oC)
272. Cells(32, 4) = TC2 - 273 'O2 Temperature Out (oC)
273. Cells(33, 4) = NTU 'Number of Tubes
274. Cells(34, 4) = AREAHEX 'Shell Area (m^2)
275. ' Cells(35, 4) = LEX 'Heat Exchanger Length (m)
276. 'Cells(36, 4) = TDO ' Tube Outside Diameter (m)
277. Cells(37, 4) = EPS * 100 'Effectiveness
278. Cells(38, 4) = QEFF 'Effective Heat Transfer Rate Q (kW)
279. Cells(39, 4) = AREAHEX 'Air Temperature from compressor (oC)
280. '=====
281. ' HEAT LOSS
282. '=====
283. '----- Heat from Air IN
284.
285. '...AIR
286. AIRTK = CT + 273 'Cell Temperature (oK)
287. AIRFLOW = (AIRFR / 24) / 3600 'O2 Flow Rate OUT (kg/sec.)
288. CPAIR = AIRSPECIFICHEAT(AIRTK) 'AIRSPECIFICHEAT (kJ/kg.K)
289. QOAIRT = AIRFLOW * CPAIR * AIRTK 'QO2 OUT (kW)
290.
291. '----- Heat from GAS OUT
292. '...O2
293. CP02 = CTK 'Cell Temperature (oK)
294. O2FRS = (O2MASFOP / 24) / 3600 'O2 Flow Rate OUT (kg/sec.)
295. CP02 = OXYGENSPECIFICHEAT(O2TEMP) 'Cp O2 (kJ/Kg.K T=oK)

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296. QO2OUT = O2FRS * CPO2 * CTK      'QO2 OUT (kJ/sec)
297. '...N2
298. 'TK = CTK
299. N2FRS = (N2MASOR / 24) / 3600    'N2 Flow Rate OUT (kg/sec.)
300. CPN2 = NITROGENSPECIFICHEAT(TK) 'Cp N2(kJ/kg.K)
301. QN2OUT = N2FRS * CPN2 * CTK     'QN2 OUT (kJ/sec)
302. 'Q OUT
303. QOUT = QO2OUT + QN2OUT + (POWERTOT) 'Q OUT (kJ/sec)
304. 'Q LOSS
305. QLOSS = QOAIRT - (QOUT) 'Q Total AOUT
306. 'Cells Output
307. Cells(41, 4) = QLOSS
308. Cells(42, 4) = QOUT
309. Cells(43, 4) = QOAIRT
310. End Sub
311. Static Function Logn(X)
312. Logn = Log(X) / Log(2.718282)
313. End Function
314. Private Static Function AIRDENSITY(T) 'Temperature in oC, kg/m^3
315. A = 1.2910739: B = 279.63468: C = 0.0036989433: D = 1.0050404
316. AIRDENSITY = (A * B + C * (T) ^ D) / (B + (T) ^ D)
317. End Function
318. Private Static Function O2DENSITY(TC) 'Temperature TC in oC g/L
319. A = 0.70879975: B = 0.0026206143: C = 0.9987447
320. O2DENSITY = 1 / (A + B * (TC) ^ C) '(A * B + C * (TC) ^ (D)) / (B + (TC) ^ (D))
321. End Function
322. Private Static Function N2DENSITY(TC)
323. A = 0.0029664293: B = 0.80793387
324. N2DENSITY = 1 / (A * TC + B)
325. End Function
326. Private Static Function AIRSPECIFICHEAT(AIRTK) 'AIRSPECIFICHEAT (kJ/kg.K)
327. TA = 1.0828694: TB = -0.00063119116: TC = 0.0000016253087: TD = -1.3949526E-09: TE = 5.3826153E-13: TF = -7.9021928E-17
328. AIRSPECIFICHEAT = TA + TB * AIRTK + TC * AIRTK ^ 2 + TD * AIRTK ^ 3 + TE * AIRTK ^ 4 + TF * AIRTK ^ 5
329. End Function
330. Private Static Function WATERSPECIFICHEAT(H2OTEMP) 'WATER SPECIFIC HEAT (kJ/kg.K)
331. WATERSPECIFICHEAT = 1.224986 + 0.0014072339 * H2OTEMP - 0.00000039722778 * H2OTEMP ^ 2 + 5.3431749E-11 * H2OTEMP ^ 3 + -2.7473115E-
15 * H2OTEMP ^ 4
332. End Function
333. Private Static Sub HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'H
EAT EXCHANGER
334. AREAHEX = 3.14 * TOD * TL
335. 'DELTAB = TH2 - TC1
336. LMTD = Q / (U * AREAHEX)
337. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
338. '----- HEATING -----
339. If FLAG = 1 Then
340. DELTAA = TH1 - TC2
341. 'DELTAB = TH2 - TC1
342. LMTD = Q / (U * AREAHEX)
343. X1 = 1
344. S1 = DELTAA / (LMTD - Logn(DELTAA))
345. S2 = X1 / (LMTD - Logn(X1))
346. If S2 >= S1 Then
347. GoTo 400
348. Else
349. X1 = X1 + 0.1
350. GoTo 300
351. 400 End If
352. DELTAB = X1
353. TH2 = DELTAB + TC1
354. GoTo 700
355. End If
356. '-----
357. '----- COOLING -----
358. If FLAG = 2 Then

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359. DELTAB = TH2 - TC1
360. LMTD = Q / (U * AREAHEX)
361. X1 = 2
362. 500 S1 = Logn(X1) - X1 / LMTD
363. S2 = Logn(DELTAB) - DELTAB / LMTD
364. If S1 >= S2 Then
365.     GoTo 600
366. Else
367.     X1 = X1 + 0.1
368.     GoTo 500
369. 600 End If
370. DELTAA = X1
371. TC2 = TH1 - DELTAA
372. End If
373. '-----
374. 700 P = (TC2 - TC1) / (TH1 - TC1)
375. R = (TH1 - TH2) / (TC2 - TC1)
376. If R > 1 Then
377.     R1 = 1 / R
378.     P1 = P * R
379. Else
380.     P1 = P
381.     R1 = R
382. End If
383. A1 = (((R1) ^ 2 + 1) ^ 0.5) / (1 - R1)
384. A2 = Logn((1 - R1 * P1) / Abs(1 - P1))
385. A3 = 2 - P1 * (1 + R1 - (1 + (R1) ^ 2)) ^ 0.5 'up
386. A4 = Abs(2 - P1 * (1 + R1 + (1 + (R1) ^ 2)) ^ 0.5) 'down
387. A5 = Logn(A3 / A4)
388. FCORF = (A1 * A2) / A5
389. If Abs(FCORF) > 1 Then
390.     FCORF = 1
391. End If
392. If FLAG = 1 Then
393.     LMTD = Q / (U * AREAHEX * FCORF)
394.     CHOT = Q / (TH1 - TH2)
395.     HFR = CHOT * 24 * 3600 / SCHOT
396.     GoTo 800
397. End If
398. If FLAG = 2 Then
399.     LMTD = Q / (U * AREAHEX * FCORF)
400.     CCOLD = Q / (TH1 - TH2)
401.     HFR = CCOLD * 24 * 3600 / SCHOT
402. End If
403. 'EFFECTIVENESS
404. 800 If CCOLD > CHOT Then
405.     CMIN = CHOT
406.     C1 = CHOT
407.     EPS = (C1 * (TC2 - TC1)) / (CMIN * (TH1 - TC1))
408.     GoTo 900
409. Else
410.     CMIN = CCOLD
411.     C1 = CCOLD
412.     EPS = (C1 * (TH1 - TH2)) / (CMIN * (TH1 - TC1))
413. 900 End If
414. QEFF = EPS * CMIN * (TH1 - TC1)
415. 'Number of ELEMENT
416. NTU = U * AREAHEX / CMIN
417. If NTU <= 1 Then
418.     NTU = 1
419. Else
420. End If
421. End Sub
422.
423. Private Static Function OXYGENSPECIFICHEAT(O2TEMP) ' kJ/Kg.K T=oK

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424. A = 0.83001979: B = 0.00034795895: C = -0.00000088793629: D = -1.9960197E-11: E = 1.654545E-14: F = -3.2117954E-18: G = 2.0294416E-22
425. OXYGENSPECIFICHEAT = A + B * O2TEMP + C * O2TEMP ^ 2 + D * O2TEMP ^ 3 + E * O2TEMP ^ 4 + F * O2TEMP ^ 5 + G * O2TEMP ^ 6
426. End Function
427. Private Static Function NITROGENSPECIFICHEAT(TK) '(kJ/kg.K)
428. A1 = 1.100752: B1 = -0.00053474045: C1 = 0.0000013971884: D1 = -1.2555363E-09: E1 = 6.0109266E-13: F = -1.6836213E-16: G = 2.7735985E-20
429. H1 = -2.5125233E-24: I1 = 1.0066147E-28: J1 = -5.1950017E-34
430. NITROGENSPECIFICHEAT = A1 + B1 * TK + C1 * TK ^ 2 + D1 * TK ^ 3 + E1 * TK ^ 4 + F1 * TK ^ 5 + G1 * TK ^ 6 + H1 * TK ^ 7 + I1 * TK ^ 8 + J1 * TK
^ 9
431. End Function

```

EMS membrane

```

1. Sub Sheet6_Button1_Click()
2. '
3.
4. ' EMS:(Electrochemical Membrane System) act as scrubber
5. '
6. 'MASS
7. CH4FR1 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(22, 20) 'Mass of CH4 (Kg/day)
8. CO2FR1 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(23, 20) 'Mass of CO2 (Kg/day)
9. H2SFR1 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(24, 20) 'Mass of H2S (Kg/day)
10. NH3FR1 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(25, 20) 'Mass of H2) (Kg/day)
11. TGFR1 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(26, 20) 'TOTAL GAS FLOW RATE 'Mass of GAS (Kg/Day)
12. 'CONCENTRATION
13. CH4FC = ActiveWorkbook.Worksheets("DFB-ADB").Cells(29, 16) '% of CH4
14. CO2FC = ActiveWorkbook.Worksheets("DFB-ADB").Cells(30, 16) '% of CO2
15. H2SFC = ActiveWorkbook.Worksheets("DFB-ADB").Cells(31, 16) '% of H2S
16. NH3FC = ActiveWorkbook.Worksheets("DFB-ADB").Cells(32, 16) '% of NH3
17. TGASV = ActiveWorkbook.Worksheets("DFB-ADB").Cells(33, 20) 'Total gas volume (m^3/day)
18. 'Temperature
19. GTP = ActiveWorkbook.Worksheets("DFB-ADB").Cells(55, 4) 'Gas Temperature(oC)
20. GPR = ActiveWorkbook.Worksheets("DFB-ADB").Cells(56, 4) 'Gas Pressure (atm.)
21. N2TEMPIN = ActiveWorkbook.Worksheets("ITM").Cells(11, 4) 'N2 Temperature IN (oC)
22. N2FR = ActiveWorkbook.Worksheets("ITM").Cells(23, 4) 'N2 Flow Rate for EMS (Kg/Day)
23. STEAMTEMP = ActiveWorkbook.Worksheets("SOFC").Cells(31, 4) 'H2O Temperature IN (oC)
24. STEAMTEMPFD = ActiveWorkbook.Worksheets("ITM").Cells(29, 4) 'H2O Temperature IN (oC)
25. ' INPUT
26. N2FR = TGFR1
27. Cells(13, 4) = N2FR 'Mass of N2 (Kg /Day)
28. Cells(5, 4) = CH4FR1 'Mass of CH4 (Kg /Day)
29. Cells(6, 4) = CO2FR1 'Mass of CO2 (Kg /Day)
30. Cells(7, 4) = H2SFR1 'Mass of H2S (Kg /Day)
31. Cells(8, 4) = NH3FR1 'Mass of NH3 (Kg /Day)
32. Cells(9, 4) = TGFR1 'Mass of GAS (Kg /Day)
33. Cells(10, 4) = GTP 'Gas Temperature(oC)
34. Cells(11, 4) = GPR 'GAS Pressure (atm.)
35. 'Cell Properties
36. Cells(14, 4) = N2TEMPIN 'N2 Temperature(oC) IN
37. 1 MEMT1 = Cells(16, 4) 'Membrane Temperature(oC)
38. MEMP = Cells(17, 4) 'Membrane Pressure (atm.)
39. MEMTO = Cells(18, 4) 'Membrane Tortuosity
40. METH1 = Cells(19, 4) 'Membrane Thickness (mm)
41. MSFA = Cells(20, 4) 'Membrane Surface Area (cm^2)
42. MEPO1 = Cells(21, 4) 'Membrane Porosity (nm)
43. MATC = Cells(22, 4) 'Mass Transfer Coefficient [Km] (cm/sec.
44. ELDIF = Cells(23, 4) 'Electrolyte diffusivity (cm^2/sec)
45. EMAD = Cells(24, 4) 'Electrolyte Molar Density (mol/cm^3)
46. APPV = Cells(25, 4) 'Applied Voltage (Volt)
47. 2 PSEP1 = Cells(26, 4) '% Separation
48. 'Error Trapping
49. If PSEP1 > 99 Then
50. PSEP1 = 99
51. Cells(26, 4) = PSEP1
52. GoTo 2
53. Else

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54. End If
55. If MEMT1 > 650 Then
56. MEMT1 = 650
57. Cells(16, 4) = MEMT1
58. GoTo 1
59. Else
60. End If
61. '          CONSTANTS
62. PSEP = PSEP1 / 100
63. GASTK = GTP + 273 'GAS Temperature at Inlet (oK)
64. MEMT = MEMT1 + 273 'Cell Temperature in (oK)
65. S2MW = 64 / 1000 'S2 Molecular Weight
66. N2MW = 28 / 1000 'N2 Molecular Weight
67. CH4MW = 16 / 1000 'CH4 Molecular Weight
68. CO2MW = 44 / 1000 'CO2 Molecular Weight
69. H2SMW = 34 / 1000 'H2S Molecular Weight
70. NH3MW = 17 / 1000 'NH3 Molecular Weight
71. H2MW = 2 / 1000 'H2 Molecular Weight
72. S2MW = 64 / 1000 'S2 Molecular Weight
73. R = 8.3143 'Gas constant (J/mol.K)
74. R1 = 82.05746 'cm3 atm/mol.K
75. FA = 96485 'coulombs/mole
76. KM = 12 'Mass Transfer Coefficient (cm/sec)
77. METH = METH1 / 10 'Membrane Thickness (cm)
78. MEPO = MEPO1 / 100 'Membrane Porosity
79. STANDPOTEN = -0.239 'Volt at 650 oC
80. DELPHI = 5 * 10 ^ -5 'Potential drop across membrane (V)
81. EO = -0.239 '-0.761 'Standard state potential, V 1/2S2 +2e --> S2-at 923K (Volt) Ref:823016
82. ALA = 1
83. ALC = 1
84. SACTC = 0.992 'Activation of Sulfur at Cathode
85. SACTA = 0.136 'Activation of Sulfur at Cathode
86. '=====
87. '          Calculations
88. ' Mass Fraction of elements in Biogas
89. CH4FR = (CH4FR1 / 24) / 60 'Mass of CH4 in (Kg/min)
90. CO2FR = (CO2FR1 / 24) / 60 'Mass of CO2 in (Kg/min)
91. H2SFR = (H2SFR1 / 24) / 60 'Mass of H2S in (Kg/min)
92. NH3FR = (NH3FR1 / 24) / 60 'Mass of NH3 in (Kg/min)
93. TOTMGAS = CH4FR + CO2FR + H2SFR + NH3FR 'Total Mass of Gas in (Kg/min)
94. CH4PER = CH4FR / TOTMGAS ' % of CH4
95. CO2PER = CO2FR / TOTMGAS ' % of CO2
96. H2SPER = H2SFR / TOTMGAS ' % of H2S
97. NH3PER = NH3FR / TOTMGAS ' % of NH3
98. ' Kg and mols of H2 and S at INPUT from H2S
99. 'Mols
100. SMOL = (H2SFR * (32 / 2)) / H2SMW 'mols S in INPUT from H2S (mols/min)
101. H2MOL = H2SFR / H2SMW 'mols H2 in INPUT from H2S (mols/min)
102. TOTMOLH2S = H2MOL + SMOL 'Total mols of H2S(Mols/s)*****
103. 'Kg
104. H2KINH2S = H2SFR1 * H2MW / H2SMW 'H2 IN H2S at INPUT(Kg/min)
105. SKINH2S = H2SFR1 * (S2MW / 2) / H2SMW 'S IN H2S at INPUT(Kg/min)
106. 'Gas Removal (S2)
107. SMOLOUT = SMOL * PSEP 'S to be removed from H2S at INPUT (mol/min)
108. ' Total mols of Gas
109. CH4MOL = CH4FR / CH4MW 'mols of CH4/min
110. CO2MOL = CO2FR / CO2MW 'mols of CO2/min
111. H2SMOL = H2SFR / H2SMW 'mols of H2S/min
112. NH3MOL = NH3FR / NH3MW 'mols of NH3/min
113. GASMOW = TOTMGAS / (CH4MOL + CO2MOL + H2SMOL + NH3MOL) 'Gas Molecular Weight
114. GASDENSITY = (MEMP * GASMOW) / (R1 * MEMT)
115. GASMOLIN = (CH4MOL + CO2MOL + H2SMOL + SMOL + NH3MOL) 'mols of gas/min
116. H2SMOLC = H2SMOL / GASMOLIN '% H2S molar fraction at Input ***** Yin
117. H2MOLC = H2MOL / GASMOLIN '%H2 molar fraction
118. SMOLC = SMOL / GASMOLIN '%S molar fraction

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119. CH4MOLC = CH4MOL / GASMOLIN '%CH4 molar fraction
120. CO2MOLC = CO2MOL / GASMOLIN '%CO2 molar fraction
121. NH3MOLC = NH3MOL / GASMOLIN '%NH3 molar fraction
122. 'Component Partial Pressure
123. 'Partial Pressure of H2,S2,H2S at Cathode
124. H2SPPC = H2SMOLC * MEMP
125. H2PPC = H2MOLC * MEMP
126. S2PPC = SMOLC * MEMP
127. 'Gas Volume cm^3/sec
128. TGASVS = TGASV / 1440 'Total Gas (m^3/min)
129. TGASCS1 = TGASVS * 100 ^ 3 'Total VOLUME of Gas (cm^3/min)
130. TGASCS = (TGASCS1 * MEMT1) / 35 'Total VOLUME of Gas (cm^3/min) at menbrane temperature
131. '% H2S Out of the System
132. H2SMOLEOUT = (H2MOL + SMOL) - (H2MOL + SMOL) * PSEP 'H2S mols remaining
133. GASMOLOUT = (CH4MOL + CO2MOL + H2SMOLEOUT + NH3MOL) 'gmols of gas/sec
134. H2SMOLCOUT = H2SMOLEOUT / GASMOLOUT '% H2S molar fraction at OUTPUT ***** Yout
135. H2SREMOVED = (H2MOL + SMOL) * PSEP 'mols/min
136. ' Gas Density
137. GASDEN = GASDENSITY
138. 'N2 GAS and S2 at Exit
139. N2MOLE = ((N2FR / N2MW) / 24) / 60 'Mol/min
140. TOTMOLN2S2G = N2MOLE + SMOLOUT
141. S2PCOUT = SMOLOUT / TOTMOLN2S2G '% (Percent) S2 OUT kg/day
142. H2PCOUT = N2MOLE / TOTMOLN2S2G '% (Percent) N2 OUT kg/day
143. N2S2GASV = (TOTMOLN2S2G * R1 * MEMT) / MEMP 'cm^3 IN
144. 'Partial Pressure at Anode S2
145. S2PPA = S2PCOUT * MEMP
146. 'H2S Volume
147. H2SV = (H2SMOL * R1 * MEMT) / MEMP '(cm^3/min)
148. '% REMOVAL
149. PERCR = ((SMOL - (SMOL - SMOL * PSEP)) / SMOL) * 100
150. S2KGOUT = SMOL * S2MW * 60 * PSEP 'S2 kg/hr removed
151. GASANODOUT = N2FR + SKINH2S 'H2+N2 OUT at Anode (Kg/hr)
152. H2OUT = H2MOL * H2MW * 60 * PSEP 'H2 OUT at cathode (Kg/hr)
153. ' ===== Membrane Properties Calculations =====
154. 'Limited Sulfide Diffusion across the Membrane Molar Flux (maximum H2S removal flux)
155. MOLARFLUX = (ELDIF * MEPO * EMAD * SMOLC) / (MEMTO * METH) '...(REFERENCE:823016)(P24)(P23)
156. 'Limited Diffusive current
157. IDIFF = (MOLARFLUX * 2 * FA) 'Diffusive current (mA/cm^2)
158. '.....
159. 'Gas Mass Transfer Diffusion
160. FLUXL = KM * GASDEN * (H2SMOLC - H2SMOLEOUT) / (Logn(H2SMOLC / H2SMOLEOUT)) 'Limited Flux )
161. ' Mass Transfer Limited Current Density
162. IL = MOLARFLUX * 2 * FA 'Mass Transfer limited current Density (mA/cm^2)/Membrane...(REFERENCE:823016)(P24)
163. '.....
164. 'Stoichiometric current density... (REFERENCE:823016) (P24)
165. 'I-THEORETICAL must be equal to I-Stoichiometric
166. ITOIC = (2 * FA * MEMP * H2SV * H2SMOLCOUT) / (R * MSFA * MEMT) 'stoichiometric current density (mA/cm^2)
167. 'Constant for Over Potential
168. CNTA = (R * MEMT) / (ALA * FA)
169. CNTC = (R * MEMT) / (ALC * FA)
170. CNTC = (R * MEMT) / (2 * FA)
171. CNT = (R * MEMT) / FA
172. '=====
173. ' ..... Algorithm to find i => I1 and Tau-Concentration .....
174. II = IL
175. 4 TEST = (1 - II / IL)
176. If (TEST) = 0 Then
177. II = II + 0.00000001
178. End If
179. If (TEST) < 0 Then
180. II = II - 0.000010001
181. End If
182. If TEST < 1 And TEST > 0 Then
183. GoTo 5

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184. Else
185. GoTo 4
186. 5 End If
187. I1 = II
188. '.....
189. TAUCONC = -CNTC * Logn((1 - I1 / IL))
190. 'Electrode Area
191. EAREA = I1 / IL '(cm^2)
192. '=====
193. '..... Tafel Approximation Curve to find IO and Tau-Activation .....
194. 'IO = Y intercept
195. 6 ACTINTER = -CNT + CNT * Logn(II)
196. If ACTINTER >= 0 Then
197. IO = (II)
198. GoTo 7
199. Else
200. II = II + 0.01
201. GoTo 6
202. 7 End If
203. 'IO
204. IO = II
205. 'TAU-Activation
206. TAUACTI = -CNT * Logn(IO) + CNT * Logn(I1)
207. '===== PLOTS=====
208. '..... TAFEL and BUTLER-VOLMER EQUATION Plot .....
209. 'IO = Y intercept
210. ICOUNT = 0.01
211. For I = 1 To 14
212. ACT2 = -CNT + CNT * Logn(ICOUNT)
213. Cells(40 + I, 1) = ACT2
214. Cells(40 + I, 2) = Logn(ICOUNT)
215. ICOUNT = ICOUNT + 0.1
216. Next I
217. TACT1 = -CNT * Logn(IO)
218. RTF = R * MEMT / FA
219. 'ACT
220. ICOUNT1 = 1
221. For I = 1 To 20
222. ACT3 = -CNT * Logn(IO) + CNT * Logn(ICOUNT1)
223. Cells(57 + I, 1) = ACT3
224. Cells(57 + I, 2) = (ICOUNT1)
225. ICOUNT1 = ICOUNT1 + 1
226. Next I
227. TAUACT = -CNT * Logn(IO) + CNT * Logn(I1)
228. '===== Overpotentials =====
229. 'Concentration polarization at the cathode
230. LC = Logn((1 - I1) / IL)
231. NUC = (R * MEMT * LC) / (2 * FA) 'Volts
232. 'Concentration polarization at the anode
233. LA = Logn((1 - I1) / IDIFF)
234. NUA = (R * MEMT * LA) / (2 * FA) 'Volts
235. 'EQ Equilibrium Voltage
236. NUMER = SACTC * H2PPC * S2PPA ^ 0.5
237. DENUM = SACTA * H2SPPC
238. CLOG = NUMER / DENUM
239. EQ = EO - (R * MEMT) / (2 * FA) * Logn(CLOG)
240. '===== CELL AREA =====
241. 'I current Density from mA/m^2 to A/cm^2
242. ICD = I1 * 10 'Applied current Density(A/cm^2)
243. ' n-do S Flow Rate (g/sec)
244. H2SGS = ((H2SFR1 * 1000) / 24) / 3600 'Mass Flowrate of H2S (g/sec)
245. 'Cell Area m^2
246. CELLAREA = (2 * FA * H2SGS) / (0.99 * 2 * IL * 10) '(cm^2)
247. 'Number of Cell
248. NUBCELLS = CELLAREA / MSFA

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249.   If NUBCELLS < 1 Then
250.     NUBCELLS = 1
251.   End If
252. 'Total Applied Current
253.   TOTAPPLI = ICD * NUBCELLS * 1000 'Amp
254. '===== TOTAL CELL VOLTAGE =====
255. 'ECELL
256.   IA = I1 * NUBCELLS
257.   ECELL = Abs(EQ) + Abs(TAUCONC) + Abs(TAUACTI) + Abs(IA * 1.5)
258.   TOTALEV = ECELL * NUBCELLS
259. 'Conductivity
260.   T = MEMT1
261.   CONDUCTOT = CONDUCTIVITY(T)      'Conductivity (S/cm)
262.   RESISTOT = (METH / (CONDUCTOT * CELLAREA)) 'Total Resistance (Ohm)
263.   CURRENTS = TOTALEV / RESISTOT    'Total current (amps)'
264. 'Power
265.   CELLPPOWER = (TOTAPPLI * TOTALEV) / 1000 '(Watt)
266. '   OUTPUT
267.   Cells(4, 11) = SKINH2S      'S2 OUT Anode (Kg/day)
268.   Cells(5, 11) = GASANODOUT   'N2+S2 OUT (Kg/day)
269.   Cells(6, 11) = N2FR        'N2 OUT (Kg/day)
270.   Cells(8, 11) = CH4FR1      'Mass of CH4 (Kg /Day)
271.   Cells(9, 11) = CO2FR1      'Mass of CO2 (Kg /Day)
272.   Cells(10, 11) = H2KINH2S   'Mass of H2 (Kg /Day)
273.   Cells(11, 11) = NH3FR1     'Mass of NH3 (Kg /Day)
274.   Cells(12, 11) = MOLARFLUX  'H2S Flux (gmol/cm^2. sec)
275.   Cells(13, 11) = IL         'Limited Current Density(mA/cm^2)
276.   Cells(14, 11) = TOTAPPLI   'Total Applied Curren Current (mAmp)
277.   Cells(15, 11) = ECELL      'Cell Voltage
278.   Cells(16, 11) = TOTALEV    'Total Cells Voltage
279.   Cells(17, 11) = CELLAREA   'Cell Area m^2
280.   Cells(18, 11) = CELLPPOWER 'Required Work Power
281.   Cells(19, 11) = NUBCELLS   'Number of Cells
282.   Cells(29, 4) = -TAUACTI    'Activation (Volt)
283.   Cells(30, 4) = IO          'Avtivation current density (mA/cm^2)
284.   Cells(31, 4) = I1         'Applied current density (mA/cm^2)
285.   Cells(32, 4) = CONDUCTOT   'Conductivity (S/cm)
286.   Cells(33, 4) = RESISTOT    'Resistance (Ohm)
287. '=====
288. '===== HEAT EXCHANGER-2 =====
289.   TL = Cells(8, 16) 'Tube Length (m) <=====
290.   TOD = Cells(9, 16) 'Tube OD (m) <=====
291.   TH1 = N2TEMPIN + 273
292.   TH2 = MEMT1 + 273
293.   TC1 = GTP + 273
294.   'TC2 = ?
295. '.....
296.   SCN2 = NITROSPCHEAT(N2TEMPIN) 'N2 Specific Heat (kJ/kg.K)
297.   CN2 = ((N2FR / 24) / 3600) * CCN2 'N2 Heat Capacity kW/oK
298.   CH4SPCH = METHANESPEHEAT(GASTK) 'CH4 Specific Heat Capacity (kJ/kg.K)
299.   CO2SPCH = CARBODIOSPEHEAT(GASTK) 'CO2 Specific Heat Capacity (kJ/kg.K)
300.   NH3SPCH = 2.19 'NH3 Specific Heat Capacity (kJ/kg.K)
301.   H2SSPCH = 1 'H2S Specific Heat Capacity (kJ/kg.K)
302.   SCGAS = CH4PER * CH4SPCH + CO2PER * CO2SPCH + NH3PER * NH3SPCH + H2SPER * H2SSPCH 'Gas Specific Heat Capacity (kJ/kg.K)
303.   CGAS = (TGFR1 / 24) / 3600 * SCGAS 'BIOGAS HEAT CAPACITY kW/oK
304.   N2TEMPIN = TC1
305.   SCN2 = NITROSPCHEAT(N2TEMPIN)
306.   CN2 = ((N2FR / 24) / 3600) * SCN2
307.   QN2 = CN2 * (TH1 - TH2) 'Q-N2 (kW)
308.   TC2 = (QN2 / CGAS) + TC1 ' Temperature of Biogas out (K)
309.   QGAS = CGAS * (TC2 - TC1) 'Q-BIOGAS (KW)
310. 'FLAG = 1 'FOR HEATING, FLAG = 2 FOR COOLING, FLAG = 3 IF ALL TEMPERATURE ARE KNOWN
311.   FLAG = 3
312.   U = 0.02
313. '..... SUBROUTINE .....

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314. 'DATA IN
315.
316.    CCOLD = CGAS: CHOT = CN2: Q = QN2: SCHOT = SCN2: SCCOLD = SCGAS
317.    Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN
GER
318. '..... DATA OUT .....
319. 'DATA OUT
320.    Cells(4, 16) = TH1 - 273 'N2 Temperature IN (oC)
321.    Cells(5, 16) = TH2 - 273 'N2 Temperature OUT (oC)
322.    Cells(6, 16) = TC1 - 273 'BIOGAS Temperature IN (oC)
323.    Cells(7, 16) = TC2 - 273 'BIOGAS Temperature OUT (oC)
324.    Cells(10, 16) = NTU 'Number of Tubes No
325.    Cells(11, 16) = AREAHEX 'Shell Area (m2)
326.    Cells(12, 16) = QEFF 'Heat Transfer rate (W)
327. '=====
328. '===== HEAT EXCHANGER-3 =====
329.    TL = Cells(19, 16) 'Tube Length (m) <=====
330.    TOD = Cells(20, 16) 'Tube OD (m) <=====
331.    TC1 = TC2
332.    TC2 = MEMT
333.    TH1 = STEAMTEMP + 273
334.    'TH2=?
335. '-----
336.    GASTK = TC1
337.    CH4SPCH = METHANESPEAT(GASTK) 'CH4 Specific Heat Capacity (kJ/kg.K)
338.    CO2SPCH = CARBODIOSPEHEAT(GASTK) 'CO2 Specific Heat Capacity (kJ/kg.K)
339.    NH3SPCH = 2.19 'NH3 Specific Heat Capacity (kJ/kg.K)
340.    H2SSPCH = 1 'H2S Specific Heat Capacity (kJ/kg.K)
341.    SCGAS = CH4PER * CH4SPCH + CO2PER * CO2SPCH + NH3PER * NH3SPCH + H2SPER * H2SSPCH 'Gas Specific Heat Capacity (kJ/min.K)
342.    CGAS = (TGFR1 / 24) / 3600 * SCGAS 'BIOGAS HEAT CAPACITY kW/oK
343.    QGAS = CGAS * (TC2 - TC1)
344.    H2OTEMP = TH1
345.    SCH2O = WATERSPECIFICHEAT(H2OTEMP)
346. 'FLAG = 1 'FOR HEATING, FLAG = 2 FOR COOLING, FLAG = 3 IF ALL TEMPERTURE ARE KNOWN
347.    FLAG = 1
348.    U = 0.02
349. '
350.    CCOLD = CGAS: CHOT = CH2O: QFLUIDH = QGAS
351.    Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN
GER
352. '----- DATA OUT -----
353. 'DATA OUT
354.    H2OFR = HFR
355.    Cells(15, 16) = TC1 - 273 'BIOGAS Temperature IN (oC)
356.    Cells(16, 16) = TC2 - 273 'BIOGAS Temperature OUT (oC)
357.    Cells(17, 16) = TH1 - 273 'Steam Temperature IN (oC)
358.    Cells(18, 16) = TH2 - 273 'Steam Temperature OUT (oC)
359.    Cells(21, 16) = NTU 'Number of Tubes No
360.    Cells(22, 16) = AREAHEX 'Shell Area (m2)
361.    Cells(23, 16) = EPS * 100 'Effectiveness (%)
362.    Cells(24, 16) = QEFF 'Heat Transfer rate (W)
363.    Cells(25, 16) = H2OFR 'Water Flow Rate (Kg/hr)
364. '===== HEX COOLING No4=====
365. 'Finding the S2 Temperature of Condensation (Liquid)
366.    TCOND = MEMT
367. 40 S2PP = S2VAPORPRESSURE(TCOND)
368.    S2PPAntiLog10 = 10 ^ S2PP
369.    PTOTAL = S2PPAntiLog10
370.    If PTOTAL <= 1 Then
371.        GoTo 41
372.    Else
373.        TCOND = TCOND - 0.001
374.        GoTo 40
375. 41 End If
376.    TCONDK = TCOND - 273

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377. '=====
378. ' Gas Cp Mixture
379.   FRTOTAL = N2FR + SKINH2S   'Total Gas Flowrate (Kg/day)
380.   N2PRC = N2FR / FRTOTAL
381.   S2PERC = SKINH2S / FRTOTAL
382.   N2TEMPIN = MEMT1 + 273
383.   N2CP = NITROSPCHEAT(N2TEMPIN)
384.   S2CP = 0.71   'kJ/Kg.K
385.   TH1 = MEMT
386.   TH2 = TCOND
387. ' Condenser N01
388.   Cells(21, 11) = TH1 - 273
389.   Cells(22, 11) = TH2 - 273
390.   TC11 = Cells(23, 11)
391.   TC1 = TC11 + 273
392.   TL = Cells(25, 11) 'Tube Length (m) <=====
393.   TOD = Cells(26, 11) 'Tube OD (m) <=====
394.   SCGAS = N2CP * N2PRC + S2CP * S2PERC
395.   CGAS = (FRTOTAL / 24) / 3600 * SCGAS   'N2+S2 HEAT CAPACITY kW/K
396.   QGAS = CGAS * (TH1 - TH2)
397.   AIRINTK = TC1 + 273
398.   SCAIR = AIRSPECIFICHEAT(AIRINTK)
399. 'FLAG = 1 'FOR HEATING, FLAG = 2 FOR COOLING, FLAG = 3 IF ALL TEMPERATURE ARE KNOWN
400.   FLAG = 2
401.   U = 0.02
402. '
403.   CHOT = CGAS: Q = QGAS: SCHOT = SCGAS: SCCOLD = SCAIR
404.   Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN
GER
405. '
406.   AIRFR = HFR
407.   Cells(24, 11) = TC2 - 273   'Air Temperature out (oC)
408.   Cells(27, 11) = NTU
409.   Cells(28, 11) = AREAHEX
410.   Cells(29, 11) = EPS * 100
411.   Cells(30, 11) = QEFF
412.   Cells(31, 11) = SKINH2S
413.   Cells(32, 11) = AIRFR
414. '===== HEATING RECYCLED N2 =====
415. '===== HEAT EXCHANGER No =====
416. 'From Condenser
417.   N2TEMPIN = TCOND   'K
418.   CCN2COND = NITROSPCHEAT(N2TEMPIN)   'N2 Specific Heat (kJ/kg.K)
419.   CN2COND = ((N2FR / 24) / 3600) * CCN2COND
420. 'From ITM
421.   TITM = MEMT
422.   N2TEMPIN = MEMT   'K
423.   CCN2ITM = NITROSPCHEAT(N2TEMPIN)
424.   CN2ITM = ((N2FR / 24) / 3600) * CCN2ITM
425. 'HEX
426.   TL = Cells(38, 11) 'Tube Length (m) <=====
427.   TOD = Cells(39, 11) 'Tube OD (m) <=====
428. '
429.   TC1 = TCOND
430.   TC2 = MEMT1 + 273
431.   TH1 = STEAMTEMPFD + 273
432.   'TH2=?
433.   N2TEMPIN = TCOND 'TMIXK
434.   SCN2 = NITROSPCHEAT(N2TEMPIN)
435.   CN2 = ((N2FR / 24) / 3600) * SCN2
436.   QN2 = CN2 * (TC2 - TC1)
437.   H2OTEMP = TH1
438.   SCH2O = WATERSPECIFICHEAT(H2OTEMP)
439. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
440.   FLAG = 1

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441. U = 0.02
442. CCOLD = CN2: Q = QN2: SCHOT = SCH20: SCCOLD = SCN2
443. Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN
GER
444. 'DATA
445. H2OFR = HFR
446. Cells(34, 11) = TC1 - 273 'N2 Temperature IN oC
447. Cells(35, 11) = TC2 - 273 'N2 Temperature OUT oC
448. Cells(36, 11) = TH1 - 273 'Steam Temperature IN oC
449. Cells(37, 11) = TH2 - 273 'Steam Temperature IN oC
450. Cells(40, 11) = NTU 'No of Elements
451. Cells(41, 11) = AREAHEX 'Shell Area 'm
452. Cells(42, 11) = EPS * 100 'Effectiveness
453. Cells(43, 11) = QEFF 'Heat Transfer Rate kW
454. Cells(44, 11) = H2OFR 'Steam Flow Rate
455. '=====
456. ' CELL HEAT LOSSES
457. '=====
458. '-----INPUT HEAT
459. '...CH4
460. GASTK = TC2
461. CCH4 = METHANESPEAT(GASTK) 'CH4 SPECIFIC HEAT T= oK kJ/kg.K
462. QCH4IN = ((CH4FR1 / 24) / 3600) * CCH4 * GASTK 'Kj/sec = kW
463. '...CO2
464. CCO2 = CARBODIOSPEHEAT(GASTK) 'CO2 SPECIFIC HEAT T= oK kJ/kg.K
465. QCO2IN = ((CO2FR1 / 24) / 3600) * CCO2 * GASTK 'Kj/sec = kW
466. '...H2S
467. CH2S = H2SSPECIFICHEAT(GASTK) ' J/mol.K ' J/mol.K
468. 'H2S MoIs
469. H2SMOLS = ((H2SFR1 / 24) / 3600) / H2SMW 'kg-mol/sec
470. QH2SIN = H2SMOLS * CH2S * GASTK 'kW
471. '...N2
472. N2TEMPIN = GASTK
473. CN2 = NITROSPCHEAT(N2TEMPIN) 'kJ/kg.K
474. QN2IN = ((N2FR / 24) / 3600) * CN2 * N2TEMPIN 'kW
475. '...NH3
476. CNH3 = NH3SPECIFICHEAT(GASTK) 'kJ/kg.K T=K
477. QNH3IN = ((NH3FR1 / 24) / 3600) * CNH3 * GASTK 'kW
478. 'TOTAL Q IN
479. QTOTIN = QCH4IN + QCO2IN + QH2SIN + QN2IN + QNH3IN + CELLPWR 'kW
480. '
481. '-----OUTPUT HEAT
482. '...CH4
483. GASTK = TC2
484. CCH4 = METHANESPEAT(GASTK) 'CH4 SPECIFIC HEAT T= oK kJ/kg.K
485. QCH4OUT = ((CH4FR1 / 24) / 3600) * CCH4 * GASTK 'Kj/sec = kW
486. '...CO2
487. CCO2 = CARBODIOSPEHEAT(GASTK) 'CO2 SPECIFIC HEAT T= oK kJ/kg.K
488. QCO2OUT = ((CO2FR1 / 24) / 3600) * CCO2 * GASTK 'Kj/sec = kW
489. '...NH3
490. CNH3 = NH3SPECIFICHEAT(GASTK) 'kJ/kg.K T=K
491. QNH3OUT = ((NH3FR1 / 24) / 3600) * CNH3 * GASTK 'kW
492. '...H2
493. H2ITK = GASTK
494. CH2 = H2SPECHEAT(H2ITK) '(kJ/Kg K)
495. QH2OUT = ((H2KINH2S / 24) / 3600) * CH2 * GASTK 'Kj/sec = kW
496. '...N2
497. N2TEMPIN = GASTK
498. CN2 = NITROSPCHEAT(N2TEMPIN) 'kJ/kg.K
499. QN2OUT = ((N2FR / 24) / 3600) * CN2 * N2TEMPIN 'kW
500. '...S2
501. TK = GASTK
502. CS2 = S2PECIFICHEAT(TK) 'Sulfure Specific Heat TK=oK J/mol.K
503. 'MoIs of S2
504. S2MOLS = ((SKINH2S / 24) / 3600) / S2MW 'MoIs/sec

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505.   QS2 = S2MOLS * CS2 * TK 'kW
506. 'TOTAL Q OUT
507.   QTOTOUT = QCH4OUT + QC02OUT + QNH3OUT + QH2OUT + QN2OUT + QS2 'kW
508. 'Heat LOSS
509.   HEATLOSS = QTOTIN - QTOTOUT 'kW
510. 'Cell OUTPUT
511.   Cells(27, 16) = QTOTIN
512.   Cells(28, 16) = QTOTOUT
513.   Cells(29, 16) = HEATLOSS
514.   ss = ss
515.   End Sub
516. Static Function Logn(X)
517.   Logn = Log(X) / Log(2.718282)
518. End Function
519. Private Static Function S2VAPORPRESSURE(TCOND) ' T=oC
520.   A = 60.9106: B = -24971 / TCOND: C = 10870000# / (TCOND) ^ 2: D = -2206000000# / (TCOND) ^ 3: E = -14.4102 * (Log10((TCOND)))
521.   S2VAPORPRESSURE = A + B + C + D + E
522. End Function
523. Private Static Function NH3SPECIFICHEAT(GASTK) 'kJ/kg.K T=K
524.   A = 1.0948345: B = 0.002555016: C = 27119.844
525.   NH3SPECIFICHEAT = A + B * GASTK + C / (GASTK) ^ 2
526. End Function
527. Private Static Function METHANESPEAT(GASTK) 'CH4 SPECIFIC HEAT T= oK kJ/kg.K
528.   METHANESPEAT = -
529.   0.000016309634 + 0.034506522 * GASTK - 0.00023406789 * GASTK ^ 2 + 0.00000081665422 * GASTK ^ 3 - 0.00000001498062 * GASTK ^ 4 + 1.3742376E-
530.   12 * GASTK ^ 5 - 2.8910223E-16 * GASTK ^ 6 - 5.5762684E-19 * GASTK ^ 7 + 4.7619441E-22 * GASTK ^ 8 - 1.1825987E-25 * GASTK ^ 9
531. End Function
530. Private Static Function CARBODIOSPEHEAT(GASTK) 'CO2 SPECIFIC HEAT T= oK kJ/kg.K
531.   Z1 = 0.51476288
532.   Z2 = 5820.1918
533.   Z3 = 1.4877831
534.   Z4 = 1.404349
535.   CARBODIOSPEHEAT = (Z1 * Z2 + Z3 * GASTK ^ Z4) / (Z2 + GASTK ^ Z4)
536. End Function
537. Private Static Function H2SPECHEAT(H2ITK) '(kJ/Kg K)
538.   ZA = 8.3580785: ZB = 0.046774926: ZC = -0.00014346423: ZD = 0.00000023506381: ZE = -2.3076196E-10: ZF = 1.4608608E-13
539.   ZG = -6.1673082E-17: ZH = 1.7508367E-20: ZI = -3.2962768E-24: ZJ = 3.9405226E-28: ZK = -2.7046605E-32: ZL = 8.1083083E-37
540.   H2SPECHEAT = ZA + ZB * H2ITK + ZC * H2ITK ^ 2 + ZD * H2ITK ^ 3 + ZE * H2ITK ^ 4 + ZF * H2ITK ^ 5 + ZG * H2ITK ^ 6 + ZH * H2ITK ^ 7 + ZI * H2ITK
541.   ^ 8 + ZJ * H2ITK ^ 9 + ZK * H2ITK ^ 10 + ZL * H2ITK ^ 11
542. End Function
542. Private Static Function NITROSPCHEAT(N2TEMPIN) 'kJ/kg.K
543.   SA = 1.100752
544.   SB = -0.00053474045
545.   SC = 0.0000013971884
546.   SD = -1.2555363E-09
547.   se = 6.0109266E-13
548.   SF = -1.6836213E-16
549.   SG = 2.7735985E-20
550.   SH = -2.5125233E-24
551.   SI = 1.0066147E-28
552.   SJ = -5.1950017E-34
553.   NITROSPCHEAT = SA + SB * N2TEMPIN + SC * N2TEMPIN ^ 2 + SD * N2TEMPIN ^ 3 + se * N2TEMPIN ^ 4 + SF * N2TEMPIN ^ 5 + SG * N2TEMPIN ^ 6 + SH * N2
554.   TEMPIN ^ 7 + SI * N2TEMPIN ^ 8 + SJ * N2TEMPIN ^ 9
555. End Function
555. Private Static Function H2SSPECIFICHEAT(GASTK) ' J/mol.K
556.   A = 25.370955: B = 0.02716066: C = -0.0000072767698: D = 5.0872489E-10
557.   H2SSPECIFICHEAT = A + B * GASTK + C * (GASTK) ^ 2 + D * (GASTK) ^ 3
558. End Function
559. Private Static Function WATERSPECIFICHEAT(H2OTEMP) 'WATER SPECIFIC HEAT oK
560.   WATERSPECIFICHEAT = 1.224986 + 0.0014072339 * H2OTEMP - 0.00000039722778 * H2OTEMP ^ 2 + 5.3431749E-11 * H2OTEMP ^ 3 + -2.7473115E-
561.   15 * H2OTEMP ^ 4
562. End Function
562. Private Static Function AIRSPECIFICHEAT(AIRTK) 'AIRSPECIFICHEAT
563.   TA = 1.0828694: TB = -0.00063119116: TC = 0.0000016253087: TD = -1.3949526E-09: TE = 5.3826153E-13: TF = -7.9021928E-17
564.   AIRSPECIFICHEAT = TA + TB * AIRTK + TC * AIRTK ^ 2 + TD * AIRTK ^ 3 + TE * AIRTK ^ 4 + TF * AIRTK ^ 5

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565. End Function
566. Private Static Function S2PECIFICHEAT(TK) 'Sulfure Specific Heat SK=oK J/mol.K
567. A = 4253.0929: B = -44.893839: C = 0.20615426: D = -0.00052634833: E = 0.00000080409764: F = -7.3367121E-10: G = 3.6985582E-13: H = -
7.9436265E-17
568. S2PECIFICHEAT = A + B * TK + C * (TK) ^ 2 + D * (TK) ^ 3 + E * (TK) ^ 4 + F * (TK) ^ 5 + G * (TK) ^ 6 + H * (TK) ^ 7
569. End Function
570. Private Static Sub HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'H
EAT EXCHANGER
571. AREAHEX = 3.14 * TOD * TL
572. 'DELTAB = TH2 - TC1
573. LMTD = Q / (U * AREAHEX)
574. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
575. '----- HEATING -----
576. If FLAG = 1 Then
577. DELTAA = TH1 - TC2
578. 'DELTAB = TH2 - TC1
579. LMTD = Q / (U * AREAHEX)
580. X1 = 1
581. 300 S1 = DELTAA / (LMTD - Logn(DELTAA))
582. S2 = X1 / (LMTD - Logn(X1))
583. If S2 >= S1 Then
584. GoTo 400
585. Else
586. X1 = X1 + 0.1
587. GoTo 300
588. 400 End If
589. DELTAB = X1
590. TH2 = DELTAB + TC1
591. GoTo 700
592. End If
593. '-----
594. '----- COOLING -----
595. If FLAG = 2 Then
596. 'DELTAA = TH1 - TC2
597. DELTAB = TH2 - TC1
598. LMTD = Q / (U * AREAHEX)
599. X1 = 2
600. 500 S1 = Logn(X1) - X1 / LMTD
601. S2 = Logn(DELTAB) - DELTAB / LMTD
602. If S1 >= S2 Then
603. GoTo 600
604. Else
605. X1 = X1 + 0.1
606. GoTo 500
607. 600 End If
608. DELTAA = X1
609. TC2 = TH1 - DELTAA
610. End If
611. '-----
612. 700 P = (TC2 - TC1) / (TH1 - TC1)
613. R = (TH1 - TH2) / (TC2 - TC1)
614. If R > 1 Then
615. R1 = 1 / R
616. P1 = P * R
617. Else
618. P1 = P
619. R1 = R
620. End If
621. A1 = (((R1) ^ 2 + 1) ^ 0.5) / (1 - R1)
622. A2 = Logn((1 - R1 * P1) / Abs(1 - P1))
623. A3 = 2 - P1 * (1 + R1 - (1 + (R1) ^ 2)) ^ 0.5 'up
624. A4 = Abs(2 - P1 * (1 + R1 + (1 + (R1) ^ 2)) ^ 0.5) 'down
625. A5 = Logn(A3 / A4)
626. FCORF = (A1 * A2) / A5
627. If Abs(FCORF) > 1 Then

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628. FCORF = 1
629. End If
630. If FLAG = 1 Then
631. LMTD = Q / (U * AREAHEX * FCORF)
632. CHOT = Q / (TH1 - TH2)
633. HFR = CHOT * 24 * 3600 / SCHOT
634. GoTo 800
635. End If
636. If FLAG = 2 Then
637. LMTD = Q / (U * AREAHEX * FCORF)
638. CCOLD = Q / (TH1 - TH2)
639. HFR = CCOLD * 24 * 3600 / SCHOT
640. End If
641. 'EFFECTIVENESS
642. 800 If CCOLD > CHOT Then
643. CMIN = CHOT
644. C1 = CHOT
645. EPS = (C1 * (TC2 - TC1)) / (CMIN * (TH1 - TC1))
646. GoTo 900
647. Else
648. CMIN = CCOLD
649. C1 = CCOLD
650. EPS = (C1 * (TH1 - TH2)) / (CMIN * (TH1 - TC1))
651. 900 End If
652. QEFF = EPS * CMIN * (TH1 - TC1)
653. 'Number of ELEMENT
654. NTU = U * AREAHEX / CMIN
655. If NTU <= 1 Then
656. NTU = 1
657. Else
658. End If
659. End Sub
660.
661. Private Static Function CONCURRENT(CONC)
662. A = 596138.29: B = 19870526
663. CONCURRENT = (A * CONC) / (B + CONC)
664. End Function
665. Private Static Function CONCVOLTAGE(A, B, CONC)
666. CONCVOLTAGE = 1 / (A * CONC + B)
667. End Function
668. Private Static Function CONDUCTIVITY(T) ' T=oC S/cm
669. A = 47.708703: B = -0.042628774
670. CONDUCTIVITY = A + B * T
671. End Function
672.
673.
674.

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SOFEC

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1. Sub Sheet7_Button1_Click()
2. '
3. '
4. 'SOFEC
5. '
6. ' (Solid Oxide Fuel-assisted- steam Electrolyzer Cell)
7. 'Dim XCH4 As Single, CH4MOL As Single
8. '=====
9. ' INPUT DATA
10. WATER = ActiveWorkbook.Worksheets("DFB-ADB").Cells(5, 4) 'Dilution Water for waste ratio
11. CO2TEM2 = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(10, 4) 'CO2 TEMPERATURE oC
12. CO2FR2 = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(4, 11) 'CO2 Flowrate (Kg/day)
13. CO2FR1 = ActiveWorkbook.Worksheets("EMS").Cells(9, 11) 'CO2 Flowrate (Kg/day)
14. CH4FR = ActiveWorkbook.Worksheets("EMS").Cells(8, 11) 'CH4 Flowrate (Kg/day)
15. H2FR = ActiveWorkbook.Worksheets("EMS").Cells(10, 11) 'H2 Flowrate ((Kg/day)

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16. NH3FR = ActiveWorkbook.Worksheets("EMS").Cells(11, 11) 'NH3 Flowrate (Kg/day)
17. ST = ActiveWorkbook.Worksheets("SOFC").Cells(31, 4) 'STEAM TEMPERATURE oC
18. IT = ActiveWorkbook.Worksheets("EMS").Cells(16, 16) 'Gas TEMPERATURE oC
19. N2TC = ActiveWorkbook.Worksheets("ITM").Cells(31, 4) 'N2 TEMPERATURE oC
20. N2FR = ActiveWorkbook.Worksheets("ITM").Cells(8, 11) 'N2 Flow Rate (Kg/day)
21. '=====
22. BIOTOTFLR = CH4FR + CO2FR1 + H2FR + NH3FR 'Total BIOGAS Flow rate (Kg/day)
23. Cells(10, 4) = BIOTOTFLR 'Total BIOGAS Flow rate (Kg/day)
24. '' Steam & GAS Data
25. Cells(4, 4) = CH4FR 'CH4 Flowrate (Kg/day)
26. Cells(5, 4) = CO2FR1 'CO2 Flowrate (Kg/day)
27. Cells(6, 4) = H2FR 'H2 Flowrate (Kg/day)
28. Cells(7, 4) = NH3FR 'NH3 Flowrate (Kg/day)
29. Cells(8, 4) = IT 'Gas Inlet Temperature (oC)
30. IP = Cells(9, 4) 'Inlet Pressure (Atm)
31. 'Cells(12, 4) = H2OFR 'Steam Flow Rate(Kg/day)
32. Cells(13, 4) = ST 'Steam Temperature (oC)
33.
34. 'CT = ST
35. ' SOEFC Input DATA
36. CT = Cells(15, 4) 'Cell Temperature (oC)
37. PC = Cells(16, 4) 'Cell Pressure (Atm)
38. ICPT1 = Cells(17, 4) 'Ionic conductivity of Platine (S/m)
39. CELTH1 = Cells(18, 4) 'Cell Thickness (micm)
40. ODIA1 = Cells(19, 4) 'Outer Diameter (mm)
41. IDIA1 = Cells(20, 4) 'Inner Diameter (mm)
42. CLEN1 = Cells(21, 4) 'Channel Length (mm)
43. CELTH = CELTH1 / 10000 ' (cm) thickness'
44. '..... mm to cm .....
45. ODIA = ODIA1 / 10 '.....Outer Diameter (cm)
46. IDIA = IDIA1 / 10 '.....Inner Diameter (cm)
47. CLEN = CLEN1 / 10 '.....Channel Length (cm)
48. 'Catalyst Active Surface Area
49. CSA = 3.14 * CLEN 'Active surface Area (cm^2)
50. CSATUBE = CLEN * 3.14 * (IDIA1) * CELTH
51. Cells(22, 4) = CSA 'Catalyst Active Surface Area (cm^2)
52. '.....
53. CSA1 = WASTCATAL(WATER)
54. ' SCR =>Steam to Carbon Ratio of CH4FR:SCR=2, SCR=3 Extra for Heat Exchanger 'Ref: Thesis page 27 SCR=2 Here
55. '
56. ' REFERENCE:(F3029.Full) ->1-1-F3029.FullPage 3031: L=9cm. OD=12mm, ID=11.5mm
57. SCR = Cells(26, 4)
58. 'INPUT
59. ASR = 0.45 'Reference Thesis Sanders Page-37
60. ' Constant
61. ODIA = ODIA1 / 10 '.....Outer Diameter (cm)
62. IDIA = IDIA1 / 10 '.....Inner Diameter (cm)
63. CLEN = CLEN1 / 10 '.....Channel Length (cm)
64. ICPT = ICPT1 / 100 '.....Ionic Conductivity (1/cm.ohm)
65. CELTH = CELTH1 / 10000 '..Cell Thickness (cm)
66. R = 8.314 '.....J/(mol-K)
67. R1 = R / 1000 '.....kJ/(mol-K)
68. ITK = IT + 273 '.....Inlet Temperature Biogas in (oK)
69. STK = ST + 273 '.....Steam Temperature in oK
70. CTK = CT + 273 '.....Cell Temperature in oK
71. FARAD = 96485 '.....C/mole O2-
72. RHONI = 8.908 '.....Ni density (g/cm3)
73. CH4MW = 0.016 '.....CH4 Molecular Weight mole
74. CO2MW = 0.044 '.....CO2 Molecular Weight mole
75. H2MW = 0.002 '.....H2 Molecular Weight mole
76. NH3MW = 0.017 '.....NH3 Molecular Weight mole
77. H2OMW = 0.018 '.....H2O Molecular Weight mole
78. O2MW = 0.032 '.....O2 Molecular Weight mole
79. CMW = 0.012 '.....C Molecular Weight mole
80. COMW = 0.028 '.....CO Molecular Weight mole

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81. FA = 96485 '.....coulombs/mole
82. 'Cathode activation Energy= ECA = 120 kJ/mol
83. ECA1 = 120 'Cathode activation Energy (kJ/mol)ref Thesis sanders
84. ECA = ECA1 * 1000 'Cathode activation Energy (J/mol)ref Thesis sanders
85. BETACA1 = 0.12 'Cathode electrochemical kinetics parameter (1/ohm.m^2) ref Thesis sanders
86. BETACA = BETACA1 / 10000 'Cathode electrochemical kinetics parameter (1/ohm.cm^2) ref Thesis sanders
87. '
88. '===== CALCULATIONS =====
89. 'BIOGAS MASS %
90. CH4PER = CH4FR / BIOTOTFLR
91. CO2PER = CO2FR1 / BIOTOTFLR
92. NH3PER = NH3FR / BIOTOTFLR
93. '%MOLES
94. CH4MOL = CH4FR / CH4MW 'CH4(k-mol/day)
95. CO2MOL = CO2FR1 / CO2MW 'CO2(k-mol/day)
96. H2MOL1 = H2FR * H2MW 'H2 (Kg/day)
97. NH3MOL = NH3FR / NH3MW 'NH3(Kg/day)
98. GFRT = CH4MOL + CO2MOL + H2MOL + NH3MOL 'Gas Flow Rate (Kg mole/day)
99. '===== FUEL SOFEC CELL =====
100. '-----
101. 'Amount of Steam Input for the reaction: CH4 + 2H2O -> CO2 + 4H2
102. 'Steam Needed (H2O)
103. 'H2O steam needed for the REACTION
104. H2ONEEDEDREAC = (CH4FR * (2 * H2OMW)) / CH4MW 'H2O needed for the reaction (kg/day) for FULL REACTION
105. 'CO2 Produced from the Reaction
106. CO2FRCH2 = (CH4FR * CO2MW) / CH4MW 'CO2 from CH4 (kg/day)'CO2 from CH4 for FULL REACTION
107. 'H2 Produced from the Reaction
108. H2FRCH4 = (CH4FR * (H2MW * 4)) / CH4MW 'H2 from CH4 and H2O (kg/day)'H2 from CH4 for FULL REACTION
109. 'O2 transferred
110. O2STM = (CH4FR * (2 * O2MW)) / CH4MW 'O2 transfered (kg/day) from [Cathode] to [Anode]
111. ' SCR =>Steam to Carbon Ratio of CH4FR:SCR=2, SCR=3 Extra for Heat Exchanger 'Ref: Thesis page 27 SCR=2 Here
112. ' SCR = 1.2 given in input
113. If SCR < 3 Then
114. SCR = 3
115. 'Cells(22, 4) = SCR
116. Else
117. End If
118. CARB = CH4FR * CMW / CH4MW 'Kg/day C (carbon)
119. H2OTOCRAT = CARB * SCR 'Steam to Carbon ratio Needed(kg/day) [Anode] IN
120. 'TOTAL H2O NEEDED
121. H2ONEEDED = H2ONEEDEDREAC + H2OTOCRAT
122. Cells(12, 4) = H2ONEEDED
123. 'H2 left at cathode exit (Maximum Theoretical produced)
124. H2YOUT = H2FRCH4 'H2 Out at Cathode (kg/day)
125. 'Total Moles CATHODE
126. O2MOLCAT = O2STM / O2MW 'kg-Moles of O2 (kg-Moles/day)
127. H2MOLCAT = H2YOUT / H2MW 'kg-Molesof H2 (kg-Moles/day)
128. TOTCATMOL = O2MOLCAT + H2MOLCAT 'Total kg-Moles
129. O2PERCAT = O2MOLCAT / TOTCATMOL 'O2 %
130. H2PERCAT = H2MOLCAT / TOTCATMOL 'H2 %
131. 'Partial Pressure at Cathode
132. O2CATPP = O2PERCAT * PC 'Partial Pressure of O2 at Cathode
133. H2CATPP = H2PERCAT * PC 'Partial Pressure of H2 at Cathode
134. '----- Partial Pressure at CATHODE -----
135. 'Moles of H2O (steam) IN
136. H2OMCA = H2ONEEDED / H2OMW 'H2O moles/day as steam IN cathode
137. H2MCA = H2YOUT / H2MW 'H2 moles/day Out at cathode
138. TOTMCA = H2OMCA + H2MCA 'Total moles of gas at cathode (kg-Moles/day)
139. H2OCON = H2OMCA / TOTMCA '% H2O
140. H2CON = H2MCA / TOTMCA '% H2
141. 'Partial Pleasure
142. H2OPP = H2OCON * PC 'Partial Pressure of H20 (atm)
143. H2PP = H2CON * PC 'Partial Pressure of H2 (atm)
144. 'O2 Pressure at Cathode ==> ((P'H2O(ca)/P'H2(ca)) *Exp(-Eca/RT))^2 Ref: Elementary Page-6
145. O2PPCA = ((H2OPP / H2PP) * Exp(-ECA / (R * CTK))) ^ 2 'O2 Pressure at Catode(atm)

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146. '-----
147. 'IONIC CONDUCTIVITY (ION) OF (SCSZ electrolyte) and YSZ Ref: Elementary Page-8 or Irvine Page-21
148. ICYSZ1 = (3.34 * (10) ^ 4) * Exp(-10300 / CTK) 'Ionic Conductivity (S/m)= "1/ohm.m)"
149. ICYSZ = ICYSZ1 / 100 'Ionic Conductivity (S/cm)= "1/ohm.cm)"
150. SCSZ1 = (3.34 * (10) ^ 4) * Exp(-9681 / CTK) 'Ionic Conductivity (S/m)= "1/ohm.m)"
151. SCSZ = SCSZ1 / 100 'Ionic Conductivity (S/cm)= "1/ohm.cm)"
152. 'ELECTRONIC Equivalent ionic conductivity of electrolyte (Sigma-el)
153. LSMEC = 4.2 * (10) ^ 7 * Exp(-1150 / CTK) / 100 'LSM Ionic Conductivity (S/cm)= "1/ohm.cm)" Cathode
154. NIEC = (3.27 * (10) ^ 6 - 1065.3 * CTK) / 100 'Nickel Ionic Conductivity (S/cm)= "1/ohm.cm)" Anode
155. 'SUM of IONIC + ELECTRONIC
156. SUMIONCON1 = (((5.5075 * (10) ^ -6 * (CTK) ^ (2))) - (6.1989 * (10) ^ -3) * CTK + 1.499) / 100
157. SUMIONCON2 = SCSZ
158. SUMIONCON = SUMIONCON1
159. RESISTOT = (CELTH) / (CSA * SUMIONCON)
160. '----- Current Density -----
161. 'Cathode Exchange Current Density io (amp/m^3 Ref: Elementary. Page6
162. IOC = (((BETACA * R * CTK * (10) ^ 7.79) / (3 * FA)) * Exp(-
ECA / (R * CTK))) * (O2PPCA) ^ 0.133) * CELTH 'Cathode Exchange Current Density(Amp/cm^3)
163. 'Reference Thesis Page-8
164. 'Cathode Exchange Current Density io for H2O
165. IOH2O = BETACA * (H2OPP / PC) * (H2PP / PC) * Exp(-ECA / (R * STK)) ' io Cathode Exchange current density (Amp/cm^2)
166. 'Cathode Exchange Current Density io for CO2
167. IOCO2 = (IOH2O / 2.2) 'Cathode Exchange Current Density io for CO2
168. '-----
169. '-----
170. '.....O2 Partial Pressure at CATHODE and ANODE Ref: IRVINE Page-7 .....
171. '---Cathode
172. DELTAHC = 967.2 * 1000 'J/mol
173. DELTASC = 177.7 'J/K
174. DELTAGC = DELTAHC - DELTASC * CTK
175. '---ANODE ==> Ref:FKB_Wijers_Final_THESIS Page 37
176. 'Delta H
177. STDELTAH = 206000 'Steam Reform 'J/mol
178. WSDDELTAH = -41200 'Water Shift 'J/mol
179. H2XDELTAH = -967200 'H2 Oxidation 'J/mol
180. H2ELECTRO = 967200
181. ADELTAH = STDELTAH + WSDDELTAH + H2XDELTAH + H2ELECTRO
182. 'Delta S
183. STDELTA S = 214.7 'J/K
184. WSDDELTA S = -30.7 'J/K
185. H2SDELTA S = -177.7 'J/K
186. DFGTYS = 177.7 'J/K
187. ADELTA S = STDELTA S + WSDDELTA S + H2SDELTA S + DFGTYS
188. 'DELTAG
189. ADELTA G = ADELTAH - (CTK * ADELTA S)
190. '=== CO and CO2 formed at Anode
191. '
192. 'CO formed from CH4
193. COFR = CH4FR * COMW / CH4MW 'kg/day
194. 'CO2 formed from CO
195. CO2FR3 = COFR * CO2MW / COMW 'Kg/day
196. 'TOTAL CO2 OUT
197. CO2TOTAOUT = CO2FR1 + CO2FR3
198. 'O2 Partial Pressure at Anode
199. O2PPA = (CO2FR3 / COFR) * Exp((ADELTAG / (R * CTK))) ^ 2
200. '===== Complete Reaction =====
201. 'CO2 Produced from the Reaction
202. CO2FRCH2 = (CH4FR * CO2MW) / CH4MW 'CO2 from CH4 (kg/day)'CO2 from CH4 for FULL REACTION)
203. 'CO2 Total
204. CO2TOTAOUT = CO2FRCH2 + CO2FR1
205. 'H2 Produced from the Reaction
206. H2FRCH4 = (CH4FR * (H2MW * 4)) / CH4MW 'H2 from CH4 and H2O (kg/day)'H2 from CH4 for FULL REACTION
207. 'O2 Transferred
208. O2STM = (CH4FR * O2MW) / CH4MW 'O2 transfered (kg/day)from [Cathod] to [Anode]
209. '

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210. '***** OPEN CIRCUIT VOLTAGE *****'
211. 'Open Circuit Voltage (Reversible-Voltage): Ref: Irvine Page-7
212.   EOCV = ((R * CTK) / (2 * FA)) * Logn(O2PPCA / O2PPA)
213. 'Nerst Potential Equilibrium Potential (Eq):Ref: Irvine Page-7
214.   ENERST = ((R * CTK) / (4 * FA)) * Logn(O2PPA / O2PPCA) '=Eq
215.   Cells(32, 4) = ENERST
216.
217. '*****'
218. '           FLUX - AREA - Number of Cells
219.   H2MOLGENE = H2RATE * H2MW * (24) * (3600) '* CSA   'H2 produced per Cell (kg/cm^2.Day)
220.
221. '+++++ IONIC CURRENT DENSITY +++++'
222. 'With Applied Voltage ref.CACHE ALL
223.   RINT = CELTH / (SCSZ * CSA)           'Internal Resistance
224.   CURDEN = ICELL / CSA                 'Current Density (A/cm^2)
225. 'POWER BALANCE
226.   POWBAL = POWERIN - POWERTOT
227. '+++++
228. 'Plot of Butler-Volmer equation to find IO
229.   II1 = 0.1
230.   For I = 1 To 10
231.     TACT1 = ((R * CTK) / (0.5 * FA)) * Logn(II1)
232.     II1 = II1 + 0.1
233.     Cells(53 + I, 1) = TACT1
234.     Cells(53 + I, 2) = II1
235.   Next I
236. 'Plot of Activation Overpotential Versus i
237.   II2 = 0.1
238.   For I = 1 To 30
239.     TACT2 = ((R * CTK) / (0.5 * FA)) * Logn(II2)
240.     II2 = II2 + 0.1
241.     Cells(53 + I, 3) = TACT2
242.     Cells(53 + I, 4) = II2
243.   Next I
244. '=====
245. '           'O2 FLUX'
246. '=====
247.
248. VAPP = Cells(30, 4) 'Applied voltage (volt)'
249. ICELLST = ((ENERST - VAPP) / RESISTOT) / CSA 'Amp/CM2'
250. Cells(34, 4) = ICELLST * 10000 'Amp/m2'
251. ECELLS1 = EOCV - (ICELLST * RESISTOT * CSA)
252. O2FLUX1 = -((EOCV) * SUMIONCON) / (CELTH * 2 * FA)
253. TOTCURDEN1 = 2 * FA * O2FLUX1 * 10000 'Maximum Current density (Amp/m2)'
254. Cells(31, 4) = TOTCURDEN1
255. CVOLT = (ENERST + TACT1 + TACT2 + (RESISTOT * TOTCURDEN1 * (CSA / 10000))) 'Applied volatge (V)'
256. EOPERAT = -CVOLT + EOCV 'Operating voltage (V)'
257. O2FLUX = ((EOCV - EOPERAT) * SUMIONCON) / (CELTH * 2 * FA)
258. TOTCURDEN = 2 * FA * O2FLUX * 10000 'Current density (Amp/m2)'
259. TOTICELL = TOTCURDEN * CSA / 10000 'Current (Amp)'
260. Cells(16, 11) = TOTCURDEN
261. LOOP9 = O2FLUX * CSA 'FLOW RATE FROM ONE TUBE (mol/s)'
262. H2OUSED = H2ONEEDEDREAC '(H2KPR * H2OMW) / H2MW   'H2O USED (Kg/day)
263. 'Steam Remaining out of CATHODE
264. H2OCATOUT = H2ONEEDED - H2OUSED   'H2O out of CATHODE (Kg/day)
265. 'Steam Formed out of Anode
266. O2MOLE = O2FLUX * CSA 'mol/s'
267. O2TOTALYOU = (H2ONEEDEDREAC * O2MW) / H2OMW
268. H2OANODEOUTX = (O2MOLE * H2OMW / (O2MW / 2)) * (86400) 'H2O Aout at Anode (mol/d)
269. H2OANODEOUT = H2OANODEOUTX * 0.018 'kg/d'
270. 'Steam Total OUT
271. H2TOTTAOUT = H2OCATOUT - H2OANODEOUT
272. GHT54YOU = (O2TOTALYOU / O2MW)
273. GHT54YOU7 = GHT54YOU / 3600
274. GHT54YOU8 = GHT54YOU7 / 24

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275. GHT54YOU10U = GHT54YOU8 / O2FLUX
276. NUMCEL = GHT54YOU10U / CSA
277. GHT54YOU09 = GHT54YOU / O2FLUX
278. ICD = (CVOLT / (RESISTOT * CSA)) * 10000 'Current density (AMP)'
279. Cells(24, 4) = ICD
280. Cells(23, 4) = CVOLT
281. IHG = EOCV / ((RESISTOT * CSA) / 10000)
282. EOPERAT = -CVOLT + EOCV 'Operating voltage (V)'
283. EAPP = Cells(30, 4)
284. '=====
285. POWERTOT = (ECELLS1 * ICELLST * CSA * NUMCEL) / 1000
286. FT2 = VAPP + (ICELLST * CSA * RESISTOT)
287. POWERIN = (FT2 * ICELLST * CSA * NUMCEL) / 1000
288.
289. '===== INPUT POWER =====
290. Cells(25, 4) = POWERTOT
291. POWERTOTINX = (-POWERTOT) - POWERIN
292. '===== CELL OUTPUT =====
293. Cells(17, 4) = SUMIONCON 'Ionic conductivity (S/m)
294. Cells(5, 11) = H2YOUT + H2FR 'H2 produced [Cathode](kg/day)
295. Cells(6, 11) = CO2TOTAOUT 'CO2 produced [Anode](Kg/day)
296. Cells(7, 11) = H2OANODEOUT 'H2O produced [Anode](Kg/day)
297. Cells(8, 11) = H2ONEEDEDREAC 'H2OCATOUT 'H2O produced [CATHODE](Kg/day)
298. Cells(9, 11) = H2OTOTAOUT 'H2O Total A out(Kg/day)
299. Cells(11, 11) = NIEC 'Ionic conductiviti of Nickel (S/cm)
300. Cells(12, 11) = LSMEC 'Ionic conductiviti of LSM(S/cm)
301. Cells(13, 11) = SCSZ 'Ionic conductiviti of SCSZ (S/cm)
302. Cells(14, 11) = ICYSZ 'Ionic conductiviti of YSZ (S/cm)
303. Cells(15, 11) = O2FLUX 'Oxygen Flux 'mole O^2-/cm^2.sec
304. Cells(16, 11) = TOTCURDEN 'Current Density Amp/cm^2
305. Cells(17, 11) = CSA 'Membrane Surface Area Required (m^2)
306. Cells(18, 11) = NUMCEL 'Number of Cells
307. Cells(19, 11) = RESISTOT 'Resistance (Ohm)
308. ION45 = (ENERST / RESISTOT) / CSA 'Amp/cm2'
309. Cells(33, 4) = ION45 * 10000
310. Cells(20, 11) = -EOCV '-EOCVTOT 'Open circuit Voltage
311. Cells(21, 11) = SUMIONCON 'Total Conductivity ((S/cm)= "1/ohm.cm")
312. Cells(22, 11) = -EOPERAT 'Total Voltage
313. Cells(23, 11) = TOTICELL 'Total current (amps)
314. Cells(24, 11) = POWERIN 'Total Power (kW)
315. Cells(25, 11) = POWERTOTINX 'Total Power (kW)
316. '=====
317. '===== HEAT EXCHANGER No4 =====
318. TL = Cells(8, 16) 'Tube Length (m)
319. TOD = Cells(9, 16) 'Tube Outside Diameter (m)
320. TH1 = ST + 273 'H2O Temperature Steam Temperature IN oK
321. TC1 = IT + 273 'Biogas IN Temperature Biogas(oK)
322. TC2 = CT + 273 'Biogas OUT Temperature Biogas(oK)
323. '.... BIOGAS
324. GASTK = TC1
325. CH4SPCH = METHANESPEHEAT(GASTK) 'CH4 Specific Heat Capacity (kJ/kg.K)
326. CO2SPCH = CARBODIOSPEHEAT(GASTK) 'CO2 Specific Heat Capacity (kJ/kg.K)
327. NH3SPCH = 2.19 'NH3 Specific Heat Capacity (kJ/kg.K)
328. SCGAS = CH4PER * CH4SPCH + CO2PER * CO2SPCH + NH3PER * NH3SPCH 'Gas Specific Heat Capacity (kJ/kg.K)
329. CGAS = ((BIOTOTFLR / 24) / 3600) * SCGAS
330. QGAS = CGAS * (TC2 - TC1) 'Q-BIOGAS (KW)
331. H2OTEMP = TH1
332. SCH2O = WATERSPECIFICHEAT(H2OTEMP) 'H2O Specific Heat (kJ/kg.K)
333. 'FLAG=1 for HEATING and FLAG=0 for COOLING
334. FLAG = 1
335. U = 0.02
336. '..... SUB HEX .....
337. CCOLD = CGAS: CHOT = CH2O: Q = QGAS: SCCOLD = SCGAS: SCHOT = SCH2O
338. Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHANG
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339. H2OTOTAOUT = HFR
340. '----- DATA OUTPUT -----
341. Cells(4, 16) = ST 'H2O Temperature Steam Temperature IN (oC)
342. Cells(5, 16) = (TH2 - 273) 'H2O Temperature Steam Temperature OUT (oC)
343. Cells(6, 16) = IT 'Biogas Temperature IN (oC)
344. Cells(7, 16) = CT 'Biogas Temperature OUT (oC)
345. Cells(10, 16) = NTU 'Number of Tubes
346. Cells(11, 16) = AREAHEX 'Shell Area(m^2)
347. Cells(12, 16) = EPS * 100 'Effectiveness
348. Cells(13, 16) = QEFF 'Heat Out (kW)
349. Cells(14, 16) = H2OTOTAOUT 'Water to SOFEC (Kg/day)
350. '
351. '===== HEAT EXCHANGER No5 =====
352. 'Steam to HEAT the Extra H2O needed for the Reaction
353. TL = Cells(21, 16) 'Tube Length (m)
354. TOD = Cells(22, 16) 'Tube Diameter (m)
355. TH1 = ST + 273 'Steam Temperature IN oK
356. 'TH2 =? 'Steam Temperature OUT oK
357. TC1 = 25 + 273 'Inlet Temperature of Needed Water oK
358. TC2 = CT + 273 'Outlet Temperature of Needed Water oK
359. 'H2O Cold Side
360. H2OTEMP = TC1
361. SCH2O = WATERSPECIFICHEAT(H2OTEMP) 'H2O Specific Heat (kJ/kg.K)
362. CH2O = ((H2ONEEDED / 24) / 3600) * SCH2O 'Water Heat Capacity (kJ/kg.K)
363. QH2O = CH2O * (TC2 - TC1) 'Q-Water (KW)
364. 'Steam Hot Side
365. STEAM = TH1
366. SCSTEAM = WATERSPECIFICHEAT(H2OTEMP) 'H2O Specific Heat (kJ/kg.K)
367. FLAG = 1
368. U = 0.0425
369. CCOLD = CH2O: Q = QH2O: SCHOT = SCSTEAM: SCCOLD = SCH2O
370. Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHA
NGER
371. '----- DATA OUTPUT -----
372. AREAHEX = HFR
373. Cells(17, 16) = TH1 - 273 'Water for SOEFC (HOT SIDE IN) (oC)
374. Cells(18, 16) = TH2 - 273 'Water for SOEFC (COLD SIDE OUT)(oC)
375. Cells(19, 16) = TC1 - 273 'AIR (CoId SIDE IN) (oC)
376. Cells(20, 16) = TC2 - 273 'AIR (HOT SIDE OUT) (oC)
377. Cells(23, 16) = NTU 'Number of Tube
378. Cells(24, 16) = AREAHEX 'Shell Area (m^2)
379. Cells(25, 16) = EPS * 100 'Effectiveness
380. Cells(26, 16) = QEFF 'Q Effective (kW)
381. Cells(27, 16) = AREAHEX 'Air Flow rate needed (Kg/hr)
382. '=====
383. '===== HEAT EXCHANGER No8 From SYSTEM Heat Balance =====
384. '...CO2 Mixed Temperature
385. CO2T1 = CT + 273
386. GASTK = CO2T1
387. CO2SPCH1 = CARBODIOSPEHEAT(GASTK) 'CO2 Specific Heat Capacity (kJ/kg.K)
388. CO2T2 = CO2TEM2 + 273
389. GASTK = CO2T2
390. CO2SPCH2 = CARBODIOSPEHEAT(GASTK) 'CO2 Specific Heat Capacity (kJ/kg.K)
391. CO2TEMPMIXK = (CO2MASS * CO2SPCH1 * CO2T1 + CO2FR2 * CO2SPCH2 * CO2T2) / (CO2MASS * CO2SPCH1 + CO2FR2 * CO2SPCH2) 'T=oK of CO2 Mixture
392. CO2MIXCTEMPC = CO2TEMPMIXK - 273 'CO2 MixTemperature 192 oC To Urea
393. '===== HEAT LOSSES =====
394. '----- Heat IN
395. '...CH4
396. GASTK = CTK
397. CCH4 = METHANESPEHEAT(GASTK) 'CH4 SPECIFIC HEAT ('CH4 Specific Heat Capacity (kJ/kg.K))
398. QCH4IN = ((CH4FR / 24) / 3600) * CCH4 * GASTK '(kW)
399. '...CO2
400. CO2 = CARBODIOSPEHEAT(GASTK) 'CO2 SPECIFIC HEAT (kJ/kg.K))
401. QCO2IN = ((CO2FR1 / 24) / 3600) * CCO2 * GASTK '(kW)
402. '...NH3

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403. CNH3 = NH3SPECIFICHEAT(GASTK) 'kJ/kg.K T=K
404. QNH3IN = ((NH3FR / 24) / 3600) * CNH3 * GASTK '(kW)NH3FR
405. '...H2O
406. H2OTEMP = GASTK
407. CH2O = WATERSPECIFICHEAT(H2OTEMP)
408. QH2OIN = ((H2ONEEDED / 24) / 3600) * CH2O * GASTK '(kW)
409. 'HEAT TOTAL IN
410. QTOTALIN = QCH4IN + QCO2IN + QNH3IN + QH2OIN + POWERIN
411. '----- Heat OUT
412. '...CO2
413. CCO2 = CARBODIOSPEHEAT(GASTK) 'CO2 SPECIFIC HEAT (kJ/kg.K)
414. QCO2OUT = ((CO2TOTAOUT / 24) / 3600) * CCO2 * GASTK '(kW)
415. '...NH3
416. CNH3 = NH3SPECIFICHEAT(GASTK) 'kJ/kg.K T=K
417. QNH3OUT = ((NH3FR / 24) / 3600) * CNH3 * GASTK '(kW)NH3FR
418. '...H2O
419. H2OTEMP = GASTK
420. CH2O = WATERSPECIFICHEAT(H2OTEMP)
421. QH2OOUT = ((H2OTOTAOUT / 24) / 3600) * CH2O * GASTK '(kW)
422. '...H2
423. H2TOTAL = H2YOUT + H2FR
424. H2TK = CTK
425. CH2 = HYDROGENSPEHEAT(H2TK) 'T=K kJ/kg.K
426. QH2OUT = ((H2TOTAL / 24) / 3600) * CH2 * CTK '(kW)
427. 'HEAT TOTAL OUT
428. QTOTALOUT = QCO2OUT + QNH3OUT + QH2OOUT + QH2OUT + POWERTOT
429. '----- HEAT LOSSES
430. QLOSSES = QTOTALIN - QTOTALOUT
431. 'OUTPUT OF HEAT LOSSES
432. Cells(27, 11) = QTOTALIN
433. Cells(28, 11) = QTOTALOUT
434. Cells(29, 11) = QLOSSES
435. '===== PLOT GRAPH =====
436. 'Waste Water Dilution Versus Catalyst active surface area/cell
437. WATER = 1
438. For I = 1 To 10
439. CSA2 = WASTACATAL(WATER)
440. Cells(54 + I, 6) = WATER
441. Cells(54 + I, 7) = CSA2
442. WATER = WATER + 4
443. Next I
444. End Sub
445. Static Function Logn(X)
446. Logn = Log(X) / Log(2.718282)
447. End Function
448. Private Static Function EQC(A, B, STK) 'EQUILIBRIUM CONSTANT
449. EQC = Exp(A + B / STK)
450. End Function
451. Private Static Function ARRH(C, D, R, STK) 'Arrhenius Constant ki
452. ARRH = C * Exp(D / (R * STK))
453. End Function
454. Private Static Function VAPRESSURE(A, B, C, CT)
455. VAPRESSURE = 10 ^ ((A - B) / (C + CT))
456. End Function
457. Private Static Function ENTHALPY(TCK, R) 'H2O Enthalpy of Steam T=K, J/mol
458. A1 = 2.717633: A2 = 2.9451374 * 10 ^ -3: A3 = -8.0224374 * 10 ^ -7: A4 = 1.0226682 * 10 ^ -10
459. A5 = -4.8472145 * 10 ^ -15: A6 = -2.9905826 * 10 ^ 4
460. ENTHALPY = (A1 + (A2 / 2) * TCK + (A3 / 3) * TCK ^ 2 + (A4 / 4) * TCK ^ 3 + (A5 / 5) * TCK ^ 4 + A6 / TCK) * R * TCK
461. End Function
462. Private Static Function ENTROPY (TCK, R) 'H2O Entropy of Steam T=K, J/mol
463. A1 = 2.717633: A2 = 2.9451374 * 10 ^ -3: A3 = -8.0224374 * 10 ^ -7: A4 = 1.0226682 * 10 ^ -10
464. A5 = -4.8472145 * 10 ^ -15: A7 = 6.6305671
465. ENTROPY = (A1 * Logn(TCK) + A2 * TCK + (A3 / 2) * TCK ^ 2 + (A4 / 3) * TCK ^ 3 + (A5 / 4) * TCK ^ 4 + A7) * R
466. End Function
467. Private Static Function METHANESPEHEAT(GASTK) 'CH4 SPECIFIC HEAT ('CH4 Specific Heat Capacity (kJ/kg.K))

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468. METHANESPEAT = -
    0.000016309634 + 0.034506522 * GASTK - 0.00023406789 * GASTK ^ 2 + 0.00000081665422 * GASTK ^ 3 - 0.000000001498062 * GASTK ^ 4 + 1.3742376E-
    12 * GASTK ^ 5 - 2.8910223E-16 * GASTK ^ 6 - 5.5762684E-19 * GASTK ^ 7 + 4.7619441E-22 * GASTK ^ 8 - 1.1825987E-25 * GASTK ^ 9
469. End Function
470. Private Static Function CARBODIOSPEHEAT(GASTK) 'CO2 SPECIFIC HEAT (kJ/kg.K)
471. Z1 = 0.51476288
472. Z2 = 5820.1918
473. Z3 = 1.4877831
474. Z4 = 1.404349
475. CARBODIOSPEHEAT = (Z1 * Z2 + Z3 * GASTK ^ Z4) / (Z2 + GASTK ^ Z4)
476. End Function
477. Private Static Function NH3SPECIFICHEAT(GASTK) 'kJ/kg.K T=K
478. A = 1.0948345: B = 0.002555016: C = 27119.844
479. NH3SPECIFICHEAT = A + B * GASTK + C / (GASTK) ^ 2
480. End Function
481. Private Static Function HYDROGENSPEHEAT(H2TK) 'T=oK kJ/kg.K
482. ZA = 8.3580785: ZB = 0.046774926: ZC = -0.00014346423: ZD = 0.00000023506381: ZE = -2.3076196E-10: ZF = 1.4608608E-13
483. ZG = -6.1673082E-17: ZH = 1.7508367E-20: ZI = -3.2962768E-24: ZJ = 3.9405226E-28: ZK = -2.7046605E-32: ZL = 8.1083083E-37
484. HYDROGENSPEHEAT = ZA + ZB * H2TK + ZC * H2TK ^ 2 + ZD * H2TK ^ 3 + ZE * H2TK ^ 4 + ZF * H2TK ^ 5 + ZG * H2TK ^ 6 + ZH * H2TK ^ 7 + ZI * H2TK ^
    8 + ZJ * H2TK ^ 9 + ZK * H2TK ^ 10 + ZL * H2TK ^ 11
485. End Function
486. Private Static Function WATERSPECIFICHEAT(H2OTEMP) 'WATER SPECIFIC HEAT (H2O Specific Heat (kJ/kg.K))_
487. WATERSPECIFICHEAT = 1.224986 + 0.0014072339 * H2OTEMP - 0.00000039722778 * H2OTEMP ^ 2 + 5.3431749E-11 * H2OTEMP ^ 3 + -2.7473115E-
    15 * H2OTEMP ^ 4
488. End Function
489. Private Static Function AIRSPECIFICHEAT(AIRTK) 'AIRSPECIFICHEAT (kJ/kg.K)
490. TA = 1.0828694: TB = -0.00063119116: TC = 0.0000016253087: TD = -1.3949526E-09: TE = 5.3826153E-13: TF = -7.9021928E-17
491. AIRSPECIFICHEAT = TA + TB * AIRTK + TC * AIRTK ^ 2 + TD * AIRTK ^ 3 + TE * AIRTK ^ 4 + TF * AIRTK ^ 5
492. End Function
493. Private Static Function NITROGENSPECIFICHEAT(TK) '(kJ/kg.K)
494. A1 = 1.100752: B1 = -0.00053474045: C1 = 0.0000013971884: D1 = -1.2555363E-09: E1 = 6.0109266E-13: F = -1.6836213E-16: G = 2.7735985E-20
495. H1 = -2.5125233E-24: I1 = 1.0066147E-28: J1 = -5.1950017E-34
496. NITROGENSPECIFICHEAT = A1 + B1 * TK + C1 * TK ^ 2 + D1 * TK ^ 3 + E1 * TK ^ 4 + F1 * TK ^ 5 + G1 * TK ^ 6 + H1 * TK ^ 7 + I1 * TK ^ 8 + J1 * TK
    ^ 9
497. End Function
498. Private Static Sub HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'H
    EAT EXCHANGER
499. AREAHEX = 3.14 * TOD * TL
500. DELTAB = TH2 - TC1
501. LMTD = Q / (U * AREAHEX)
502. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
503. '----- HEATING -----
504. If FLAG = 1 Then
505. DELTAA = TH1 - TC2
506. 'DELTAB = TH2 - TC1
507. LMTD = Q / (U * AREAHEX)
508. X1 = 1
509. S1 = DELTAA / (LMTD - Logn(DELTAA))
510. S2 = X1 / (LMTD - Logn(X1))
511. If S2 >= S1 Then
512. GoTo 400
513. Else
514. X1 = X1 + 0.1
515. GoTo 300
516. 400 End If
517. DELTAB = X1
518. TH2 = DELTAB + TC1
519. GoTo 700
520. End If
521. '----- COOLING -----
522. '----- COOLING -----
523. If FLAG = 2 Then
524. 'DELTAA = TH1 - TC2
525. DELTAB = TH2 - TC1
526. LMTD = Q / (U * AREAHEX)

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527. X1 = 2
528. 500 S1 = Logn(X1) - X1 / LMTD
529. S2 = Logn(DELTAB) - DELTAB / LMTD
530. If S1 >= S2 Then
531. GoTo 600
532. Else
533. X1 = X1 + 0.1
534. GoTo 500
535. 600 End If
536. DELTAA = X1
537. TC2 = TH1 - DELTAA
538. End If
539. '-----
540. 700 P = (TC2 - TC1) / (TH1 - TC1)
541. R = (TH1 - TH2) / (TC2 - TC1)
542. If R > 1 Then
543. R1 = 1 / R
544. P1 = P * R
545. Else
546. P1 = P
547. R1 = R
548. End If
549. A1 = (((R1) ^ 2 + 1) ^ 0.5) / (1 - R1)
550. A2 = Logn((1 - R1 * P1) / Abs(1 - P1))
551. A3 = 2 - P1 * (1 + R1 - (1 + (R1) ^ 2)) ^ 0.5 'up
552. A4 = Abs(2 - P1 * (1 + R1 + (1 + (R1) ^ 2)) ^ 0.5) 'down
553. A5 = Logn(A3 / A4)
554. FCORF = (A1 * A2) / A5
555. If Abs(FCORF) > 1 Then
556. FCORF = 1
557. End If
558. If FLAG = 1 Then
559. LMTD = Q / (U * AREAHEX * FCORF)
560. CHOT = Q / (TH1 - TH2)
561. HFR = CHOT * 24 * 3600 / SCHOT
562. GoTo 800
563. End If
564. If FLAG = 2 Then
565. LMTD = Q / (U * AREAHEX * FCORF)
566. CCOLD = Q / (TH1 - TH2)
567. HFR = CCOLD * 24 * 3600 / SCHOT
568. End If
569. 'EFFECTIVENESS
570. 800 If CCOLD > CHOT Then
571. CMIN = CHOT
572. C1 = CHOT
573. EPS = (C1 * (TC2 - TC1)) / (CMIN * (TH1 - TC1))
574. GoTo 900
575. Else
576. CMIN = CCOLD
577. C1 = CCOLD
578. EPS = (C1 * (TH1 - TH2)) / (CMIN * (TH1 - TC1))
579. 900 End If
580. QEFF = EPS * CMIN * (TH1 - TC1)
581. 'Number of ELEMENT
582. NTU = U * AREAHEX / CMIN
583. If NTU <= 1 Then
584. NTU = 1
585. Else
586. End If
587. End Sub
588.
589. Private Static Function WASTCATAL(WATER) 'Water dilution in waste versus Catalyst surface. ratio to cm^2/cell
590. A = 0.61179479: B = -1.0756981: C = 1.0199136
591. WASTCATAL = A * (WATER - B) ^ C

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SSAS

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1. Sub Sheet8_Button1_Click()
2. ' SSAS
3. 'N2
4. N2FRK = ActiveWorkbook.Worksheets("ITM").Cells(10, 11) 'N2 Total Available from (ITM) (Kg/Day)
5. N2EMS = ActiveWorkbook.Worksheets("ITM").Cells(23, 4) 'N2 Needed for EMS (Kg/day)
6. N2ITMTEMP = ActiveWorkbook.Worksheets("ITM").Cells(11, 4) 'N2 Temperature from (ITM)(oC)
7. N2ITMTPRE = ActiveWorkbook.Worksheets("ITM").Cells(12, 4) 'N2 Pressure from (ITM)(oC)
8. 'CO2
9. CO2MFI = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(4, 11) 'CO2 From Dark(Kg/Day)
10. CO2SOFEC = ActiveWorkbook.Worksheets("SOFEC").Cells(6, 11) 'CO2 From SOFEC(kg/hr)
11. CO2MFITEMP = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(10, 4) 'CO2 TEMPERATURE From Dark oC
12. CO2SOFECTEMP = ActiveWorkbook.Worksheets("SOFEC").Cells(15, 4) 'CO2 TEMPERATURE From Dark oC
13. 'H2
14. H2MFI = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(6, 11) 'H2 From MFI(ZM) (Kg/Day)
15. H2FRKSOFEC = ActiveWorkbook.Worksheets("SOFEC").Cells(5, 11) 'H2 IN From SOFEC(kg/hr)
16. H2FRKSOFC = ActiveWorkbook.Worksheets("SOFC").Cells(5, 11) 'H2 IN From SOFC(kg/hr)
17. 'TEMPERATURE
18. H2MFITEMP = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(10, 4) 'H2 Temperature From MFI(ZM) (oC)
19. H2SOFECTEMP = ActiveWorkbook.Worksheets("SOFEC").Cells(15, 4) 'H2 Temperature From SOFEC(ZM) (oC)
20. H2SOFCTEMP = ActiveWorkbook.Worksheets("SOFC").Cells(13, 4) 'H2 Temperature From SOFC(ZM) (oC)
21. '
22. ' INPUT
23. ' N2 Total Available
24. N2TOTAVAILABLE = (N2FRK) - (N2EMS) '+ (N2SOFC) 'N2 TOTAL AVAILABLE (Kg/day)
25. ' H2 Total Available
26. H2TOTAVAILABLE = H2MFI + H2FRKSOFEC + H2FRKSOFC
27. ' N2
28. Cells(5, 4) = N2TOTAVAILABLE 'N2 Total Available from (ITM) (Kg/Day)
29. Cells(6, 4) = N2ITMTEMP 'N2 Mixed Inlet Temperature (oC)
30. Cells(7, 4) = N2ITMTPRE 'N2 Inlet Pressure (atm)
31. ' H2
32. ' Cells(9, 4) = H2FRK 'H2 Flow Rate (kg/hr)
33. Cells(10, 4) = H2TOTAVAILABLE 'H2 Flow Rate (kg/hr)
34. 'H2IT = Cells(11, 4) 'H2 Inlet Temperature (oC)
35. HIP = Cells(12, 4) 'H2 Inlet Pressure (atm)
36. ' Cell
37. CIT = Cells(15, 4) 'Cell Temperature (oC)
38. CIP = Cells(16, 4) 'Cell Pressure (atm)
39. MC = Cells(17, 4) 'Membrane Conductivity (1/cm.ohm)
40. MSA1 = Cells(18, 4) 'Membrane Surface Area (m^2)
41. MTH = Cells(19, 4) 'Membrane Thickness (cm)
42. APC = Cells(20, 4) 'Applied Current(mA)
43. APV = Cells(21, 4) 'Applied Voltage
44. FU1 = Cells(47, 2)
45. 'N2 Mixed Temperature
46. 'Temperature of Mixed N2 gas
47. 'N2ITMTEMP of N2HIGHTEM (Temperature of N2 not used)
48. 'N2ITSOFEC of N2FREXCHANGER (Temperature of N2 out of the Heat Exchanger from SOFEC
49. N2HIGHTEM = N2TOTAVAILABLE - N2FREXCHANGER 'N2 Flow rate from (ITM) not used at T= 900 (oC)
50. N2FREXCHANGER = N2FREXCHANGER 'N2 Flow rate from (ITM)Used for the Heat Exchanger at T=305.65 (oC)
51. '<===== Input Data =====
52. ' Constant
53. MSA = MSA1 * 10000
54. N2ITK = N2ITMTEMP + 273
55. H2TK = H2IT + 273
56. CITK = CIT + 273
57. TSTPK = 25 + 273
58. FU = FU1 / 100
59. ECD = 3.5 ' Electrical Current Density Mole/cm^2.sec
60. FA = 96485 ' coulombs/mole
61. R = 8.314 'J/K.mol

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62.    RG = 82.05746 'cm3 atm/mol.K
63.    DELH0 = 91.88 'kJ/mole
64.    AWN2 = 14 'Weight of one N2 atom
65.    N2MW = 28
66.    H2MW = 2
67.    NH3MW = 17
68.    UREAMW = 60.6
69.    CO2MW = 44
70.    THPLUS = 1.11 'Proton transport number
71.    '=====  

72.    '***** Needed Components for Urea *****  

73.    ' CO2 TOTAL PRODUCED  

74.    CO2TOTAL = CO2MFI + CO2SOFEC '(Kg/Day)  

75.    'Urea Needed to consume all the CO2  

76.    UREA = (CO2TOTAL * UREAMW) / CO2MW 'Urea Prduced'Total CO2 produced is Used For Urea (according to the UREA production ratio)(KG/day)  

77.    'NH3 Needed for this Urea production  

78.    NH3TOTUREA = (UREA * (2 * NH3MW)) / UREAMW 'Total NH3 NEEDED FOR UREA PRODUCTION (Kg/day)  

79.    'H2 Needed for this NH3 production for Urea  

80.    H2TOTUREA = (NH3TOTUREA * (H2MW * 3)) / (2 * NH3MW) 'H2 Needed for NH3 To UREA (kg/day)  

81.    'N2 Needed for this NH3 production for Urea  

82.    N2TOTUREA = (NH3TOTUREA * N2MW) / (NH3MW * 2) 'N2 Needed for NH3 To UREA (Kg/day)  

83.    '***** Component Availability *****  

84.    'H2 Available  

85.    H2AVAILABLE = H2TOTAVAILABLE - H2TOTUREA 'H2 Available (Kg/day)  

86.    'N2 Available  

87.    N2AVAILABLE = N2TOTAVAILABLE - N2TOTUREA 'N2 Available (Kg/day)  

88.    '.....  

89.    'Ratio of Available H2 for Extra NH3 and SOFC  

90.    NR = Cells(32, 3)  

91.    If NR <= 0 Then  

92.    Cells(22, 6) = "ERROR N=0"  

93.    End  

94.    Else  

95.    Cells(22, 6) = ""  

96.    End If  

97.    'H2 For NH3  

98.    H2NH3EXTRA = H2AVAILABLE / NR 'H2 for Extra NH3 (Kg/day)  

99.    'H2 For SOFC  

100.    H2SOFEC = H2AVAILABLE - H2NH3EXTRA 'H2 for SOFC (Kg/day)  

101.    If H2SOFEC < 0 Then  

102.    Cells(31, 3) = H2SOFEC  

103.    Cells(22, 6) = "ERROR H2 is NEGATIVE"  

104.    End  

105.    Else  

106.    Cells(22, 6) = "H/N OK for SOFC"  

107.    End If  

108.    'H2 Needed For Membrane  

109.    H2MEMBRANE = H2TOTUREA + H2NH3EXTRA 'H2 Total For SSAS Membrane (Kg/day)  

110.    '.....Extra NH3 .....  

111.    NH3EXTRA = (H2NH3EXTRA * (NH3MW * 2)) / (H2MW * 3) 'Extra NH3 (Kg/day)  

112.    'N2 Needed For Extra NH3  

113.    N2NH3EXTRA = (NH3EXTRA * N2MW) / (NH3MW * 2) 'N2 Used for Extra NH3 (Kg/day)  

114.    'N2 Remaining  

115.    N2REMAIN = N2FRK - N2EMS - N2TOTUREA - N2NH3EXTRA  

116.    '  

117.    '***** TOTAL NH3 *****  

118.    '.....TOTAL H2 and N2 Needed For A TOTAL of NH3.....  

119.    'N2 Needed for a Total of NH3  

120.    N2TOTNH3 = N2TOTUREA + N2NH3EXTRA 'N2 Needed for a Total of NH3 (Kg/day)  

121.    'H2 Needed for a Total of NH3  

122.    H2TOTNH3 = H2TOTUREA + H2NH3EXTRA  

123.    'Total NH3 Needed  

124.    NH3TOTALNEEDED = NH3TOTUREA + NH3EXTRA  

125.    '*****  

126.    '=====  


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192. H2TOTALIN = H2MEMBRANE
193. NH3TOTAL = NH3TOTUREA + NH3EXTRA
194. ' TOTAL Moles
195. N2MOLTOT = N2FRKUSED / N2MW 'N2 Moles/day
196. H2MOLTOT = H2TOTALIN / H2MW 'H2 Moles/day
197. NH3MOLTOT = NH3TOTAL / NH3MW 'NH3 Moles/day
198. 'AT Cathode
199. H2PERCTOT = H2MOLTOT / TOTMOLTOT 'H2 %
200. 'AT Anode
201. TOTMOLTOT = N2MOLTOT + NH3MOLTOT 'Total Moles
202. N2PERCTOT = N2MOLTOT / TOTMOLTOT 'N2 %
203. NH3PERCTOT = NH3MOLTOT / TOTMOLTOT 'NH3 %
204. 'Partial Pressure
205. PPN2TOT = N2PERCTOT * CIP
206. PPH2TOT = H2PERCTOT * CIP
207. PPNH3TOT = NH3PERCTOT * CIP
208. '=====
209. PPN2 = PPN2TOT
210. PPH2 = PPH2TOT
211. PPNH3 = PPNH3TOT
212. '=====
213. ' Thermodynamics - DELTA : C,H, S, G in function of T
214. A = TSTPK
215. B = 573 'CITK
216. N = 263
217. ' DELTA(H)with TK
218. Call DELTAH(A, B, N, INTEGRALH) 'Simpson integrator for DELTA(H)263
219. DELH = INTEGRALH - 91.88 'DELTA(H) (kJ/mole)
220. ' DELTA(S)with TK
221. N = 108
222. Call DELTAH(A, B, N, INTEGRALS) 'Simpson integrator for DELTA(S)108
223. DELS = (-198.091 + INTEGRALS) / 1000 'DELTA(S) (J/mole)
224. ' DELTA(G)with TK
225. DELTAGKJ = DELH - CITK * DELS 'DELTA (G)(kJ/mole)
226. DELTAG = DELTAGKJ * 1000 'DELTA (G)(J/mole)
227. ' Reversible Voltage E0
228. E0 = (DELTAG / (6 * FA)) ' * 1000 'Gibbs Free Energy in (Volt)Ref:75969 Page-11 or Electrochemical_Synthesis_of_Ammonia_in_Solid_Elec Page-7
229. ENERST = E0 + ((R * CITK) / (6 * FA)) * Logn(((PPN2) * (PPH2) ^ 1 / 3) / (PPNH3) ^ 1 / 2) 'Nerst Voltage Ref: Fogler Reactor design SOFC
230. 'Area Specific Resistance
231. ASR = (MTH / MC)
232. 'RATE OF NH3 at MEMBRANE(FLUX)
233. RNH3 = -((ENERST - APV) / (ASR * 6 * FA)) * 2 / 3 'Rate of NH3 'At MEMBRANE(FLUX) RATE OF Reaction of NH3 moles/cm^2.s
234. 'Maximum RATE OF NH3 at Working Electrode
235. RNH3MAX = 1.13 * (10) ^ -8 'Maximum Rate of NH3 moles/cm^2.sec Ref:XU209 Page-4 or 75969 Page-12
236. 'Exchange Current Density io
237. IO = RNH3 * 3 * FA * MSA1 'mAmp/cm^2
238. 'Faradaic Efficiency
239. FE = ((3 * FA * RNH3MAX * (MSA1) * 100) / (APC * 1.07))
240. 'Current il Needed for maximum fuel efficiency of this RNH3MAX => ICUR = 0.005972+>Limited current desity
241. ' or-Electrochemical_Synthesis_of_Ammonia_in_Solid_Elec Page-7
242. ICURL = (6 * FA * MSA * RNH3MAX) / THPLUS '(0.904 * TH) 'AMP Ref:XU209 Page-4 or 75969 Page-12
243. 'Limited Current Density
244. IL = ICURL / MSA 'mAmp/cm^2
245. 'Current Density
246. II = APC / MSA
247. 'Moles of NH3 Required
248. NH3MOLNEED = (NH3TOTAL * 1000) / NH3MW 'Moles/day
249. NH3MOLSEC = (NH3MOLNEED / 24) / 3600 'Moles /sec
250. 'AREA
251. AREANEED = NH3MOLSEC / RNH3
252. 'Number Of Electrode
253. NUMBCELLS = AREANEED / MSA
254. 'Activation Energy
255. ETAACT = ((R * CITK) / (0.5 * FA)) * Logn(II / IO)

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256. 'Concentration Energy
257.   ETACONT = ((R * CITK) / (6 * FA)) * Logn(1 - II / IL)
258. 'Ohmic Energy
259.   IOHM = II * (MTH / MC)
260. 'TOTAL VOLTAGE
261.   TOTVOLT = -((ENERST) + (APV) + (ETAAct) + (ETACONT) + (IOHM)) * NUMBCELLS
262. '===== PLOT =====
263. 'Plot of Butler-Volmer equation to find II
264.   II1 = 0.1
265.   For I = 1 To 10
266.     TACT1 = ((R * CITK) / (0.5 * FA)) * Logn(II1)
267.     II1 = II1 + 0.1
268.     Cells(64 + I, 1) = -TACT1
269.     Cells(64 + I, 2) = II1
270.   Next I
271. 'Resistance R
272.   RES = 1 / 0.051
273. '***** COMPONENT OUT *****
274. 'N2 Out at Cathode
275.   N2OUT = N2REMAIN
276.   Cells(5, 11) = N2OUT      'N2 OUT UNUSED (kg/hr)
277.   If N2OUT <= 0 Then
278.     Cells(4, 7) = "ERROR"
279.     Cells(5, 7) = "N2 OUT LOW"
280.     Cells(6, 7) = "First Check H/N"
281.     Cells(7, 7) = "AGAIN, if N2<0"
282.     Cells(8, 7) = "RUN ITM"
283.     Cells(9, 7) = "AGAIN"
284.   End
285.   Else
286.     Cells(5, 11) = N2OUT      'N2 OUT UNUSED (kg/hr)
287.     Cells(4, 7) = " "
288.     Cells(5, 7) = " "
289.     Cells(6, 7) = " "
290.     Cells(7, 7) = " "
291.     Cells(8, 7) = " "
292.     Cells(9, 7) = " "
293.   End If
294. '----- CELL POWER IN              CELLPPOWER = (TOTAPPLI * TOTALEV) / 1000
295.   IVMC = 1 / MC      '(Ohm.cm) Inverse of conductivity
296.   RESISTANCE = IVMC / MTH '(Ohm)
297.   TOTALCURRENT = (TOTVOLT / RESISTANCE) 'Total Current (Amp)
298.   CELLPPOWER = (TOTALCURRENT * TOTVOLT * NUMBCELLS) / 1000 '(kW)
299.   Cells(49, 3) = CELLPPOWER
300.   Cells(50, 3) = RESISTANCE
301.   Cells(51, 3) = FE      'Faradaic Efficiency
302. 'OUTPUT
303.   Cells(13, 4) = H2SOFC
304.   Cells(4, 11) = NH3TOTAL      'NH3(kg/Day)Formed
305.   Cells(5, 11) = N2OUT      'N2 OUT UNUSED (kg/hr)
306.   Cells(6, 11) = RNH3MAX      'Maximum Reaction Rate
307.   Cells(7, 11) = RNH3      'Actual Reaction Rate
308.   Cells(8, 11) = AREANEEDED      'Required Area from Reaction
309.   Cells(9, 11) = NUMBCELLS      'Number of Cells
310.   Cells(10, 11) = APC      'Current Imposed (Amp)
311.   Cells(11, 11) = TOTALCURRENT      'Total Current (Amp)
312.   Cells(12, 11) = TOTVOLT      'Voltage (Volt)
313.   Cells(13, 11) = H2SOFC      'H2 Out(kg/Day)
314.   Cells(14, 11) = NH3TOTUREA      'NH3 for Urea (kg/hr)
315.   Cells(15, 11) = NH3EXTRA      'Extra NH3 produced (kg/hr)
316.   Cells(16, 11) = CO2TOTAL      'Total CO2 For Urea (kg/hr)
317.   Cells(17, 11) = UREA      'Amount of Urea (kg/day) for complete CO2 Elimination
318. '
319. '===== END OF CELL CALCULATIONS =====
320. '

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321. '===== HEAT EXCHANGER-6 CALCULATION =====
322. 'H2 Temperature Mixed
323. H2TEMPMIXED1 = (H2FRKSOFEC * H2SOFECTEMP + H2MFI * H2MFITEMP) / (H2FRKSOFEC + H2MFI)
324. If H2TEMPMIXED1 < CIT Then
325. H2TEMPMIXED2 = CIT - H2TEMPMIXED1
326. H2TEMPMIXED = H2TEMPMIXED2 + H2TEMPMIXED1 + H2TEMPMIXED2 * 0.16
327. GoTo 5
328. Else
329. H2TEMPMIXED1 = (H2FRKSOFEC * H2SOFECTEMP + H2MFI * H2MFITEMP) / (H2FRKSOFEC + H2MFI)
330. H2TEMPMIXED = H2TEMPMIXED1
331. 5 End If
332. Cells(11, 4) = H2TEMPMIXED
333. TL = Cells(8, 16)
334. TOD = Cells(9, 16)
335. '=====
336. '..... Heat Exchanger No6 for H2 cooling .....
337. '=====
338. TL = Cells(8, 16)
339. TOD = Cells(9, 16)
340. ' Hydrogen
341. H2TK = H2TEMPMIXED + 273
342. SCH2 = HYDROGENSPECHEAT(H2TK) 'H2 Specific Heat (kJ/kg.K)
343. CH2 = ((H2TOTAVAILABLE / 24) / 3600) * SCH2 'H2 Heat capacity (KW/oK)
344. TH1 = (H2TEMPMIXED) + 273 'H2 Hot Side (oK)
345. TH2 = CIT + 273 'Cell Temperature in Kelvin 'H2 Cold Side (oK)
346. QH2 = CH2 * (TH1 - TH2)
347. 'Air
348. TC1 = 25 + 273
349. 'TC2=?
350. AIRINTK = TC1
351. SCAIR = AIRSPECIFICHEAT(AIRINTK)
352. 'Air Flow rate needed to Cool H2
353. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
354. FLAG = 2
355. U = 0.02
356. CCOLD = CH2: CHOT = CH2: Q = QH2: SCHOT = SCH2: SCCOLD = SCAIR
357. Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN
GER
358. '----- OUTPUT DATA FOR HEAT-EXCHANGER No-6 -----
359. AIRFLR = HFR
360. Cells(4, 16) = TH1 - 273 'H2 Temperature IN (oC)
361. Cells(5, 16) = TH2 - 273 'H2 Temperature OUT (oC)
362. Cells(6, 16) = TC1 - 273 'AIR Temperature In (oC)
363. Cells(7, 16) = TC2 - 273 'AIR Temperature OUT (oC)
364. Cells(10, 16) = NTU 'Number of Elements (No)
365. Cells(11, 16) = AREAHEX 'Shell Area (m^2)
366. Cells(12, 16) = EPS * 100 'Effectiveness (%)
367. Cells(13, 16) = QEFF 'Heat Transfer Rate (KW)
368. Cells(14, 16) = AIRFLR 'N2 Flow Rate (Kg/hr)
369. '-----
370. '===== HEAT EXCHANGER-7 CALCULATION =====
371. 'Cooling remaining of N2 with air
372. TL = Cells(21, 16)
373. TOD = Cells(22, 16)
374. 'NITROGEN
375. N2FRREM = N2TOTAVAILABLE - N2FLR 'N2 remaining to be cooled (kg/day)
376. TH1 = N2ITMTEMP + 273 'N2 Temperature IN
377. TH2 = CIT + 273
378. N2ITK = TH2
379. SCN2 = NITROSPCHEAT(N2ITK) 'N2 Specific Heat (kJ/kg.K)
380. CN2 = ((N2FRREM / 24) / 3600) * SCN2 'N2 Heat capacity (KW/oK)
381. QN2 = CN2 * (TH1 - TH2) 'Q-N2 (kw)
382. 'Air Flow rate needed to Cool N2
383. Cells(19, 16) = AIRTEMIN
384. TC1 = 25 + 273

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385. AIRINTK1 = 25 + 273
386. SCAIR = AIRSPECIFICHEAT(AIRINTK1)
387. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
388. FLAG = 2
389. U = 0.02
390. CHOT = CN2: Q = QN2: SCHOT = SCN2: SCCOLD = SCAIR
391. Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN
GER
392. 'DATA
393. AIRFR = HFR
394. Cells(17, 16) = N2ITMTEMP 'N2 Temperature IN (oC)
395. Cells(18, 16) = TH2 - 273 'N2 Temperature OUT (oC)
396. Cells(19, 16) = 25 'AIR Temperature IN (oC)
397. Cells(20, 16) = TC2 - 273 'AIR Temperature OUT(oC)
398. Cells(23, 16) = NTU 'Number of Elements (No)
399. Cells(24, 16) = AREAHEX 'Shell Area (m^2)
400. Cells(25, 16) = EPS * 100 'Effectiveness (%)
401. Cells(26, 16) = QEFF 'Heat Transfer Rate (KW)
402. Cells(27, 16) = AIRFR 'Air Flow Rate (Kg/hr)
403. Cells(28, 16) = COMPOP 'Condenser inside Pressure (Atm.)
404. '===== COMPRESSOR-3 ===== NH3TOTAL
405. '...INPUT
406. COMPIP = Cells(21, 11) 'Compressor Inlet Pressure (atm.)
407. COMPOP = Cells(22, 11) 'Compressor Outlet Pressure (atm.)
408. Cells(23, 11) = CIT 'Gas Temperature (oC)
409. COMETREFF = Cells(24, 11) 'Compressor Entropy Efficiency (%)
410. SPHASVOL = Cells(25, 11) 'Single Phase Voltage (Volts)
411. MOTOREFF1 = Cells(26, 11) 'Single Phase Motor Efficiency (%)
412. THREPASEVOL = Cells(27, 11) '3 Phase Voltage (Volts)
413. MOTOREFF3 = Cells(28, 11) '3 Phase Motor Efficiency (%)
414. '...Chemical Calculation
415. TK = CIT + 273 'Inlet Gas Temperature (oK)
416. NH3SPCHEAT = NH3SPECHEAT(TK) 'NH3 Specific Heat (kJ/Kg.K)kJ/kg.K (>1atm)
417. NH3TEMPC = CIT
418. GAMMA = 1.289 'NH3GAMMA(NH3TEMPC) 'GAMMA=Cp/Cv
419. RHONH3 = NH3DENSITY(NH3TEMPC) 'NH3 Density (Kg/m^3)
420. NH3KG = NH3TOTUREA 'NH3 Rquired for Urea(Kg/day)
421. NH3VOLD = NH3KG / RHONH3 'NH3 Volume m^3/day
422. NH3VOLM = (NH3VOLD / 24) / 60 'NH3 Volume m^3/min
423. NH3VOLIT = NH3VOLM * 1000 'NH3 Volume L/min
424. Cells(20, 11) = NH3VOLIT 'NH3 Volume L/min,<=====
425. NH3MOL = NH3KG / NH3MW 'NH3 Mols
426. ENTCC = NH3MOL * R * Logn(COMPOP / COMPIP)
427. GASTEMPC = NH3TEMPC: GASVOL = NH3VOLIT
428. MASSMIXCP = 2.22 '1.13
429. STGE = 5
430. ISENEFF = 0.75
431. MECHANICEFF = 0.95
432. OUTADIATEMP = ((GASTEMPC + 273) * ((COMPOP / COMPIP) ^ ((GAMMA - 1) / GAMMA))) - 273 ' OUTLET ADIABATIC TEMPERATURE
433. DRMOTWATT = ((OUTADIATEMP + 273) - (GASTEMPC + 273)) * 2.22 * (NH3KG / 86400) / ISENEFF 'KW
434. Call COMPRESSOR(GASTEMPC, COMPOP, COMPIP, GAMMA, GASVOL, OUTADIATEMP, COMETREFF, WATT, ENTCC, DRMOTWATT, DRMOTHP, MOTOREFF1, M
OTOREFF3, SPHASVOL, THREPASEVOL, CURRENT1, CURRENT3)
435. Cells(30, 11) = OUTADIATEMP
436. Cells(31, 11) = DRMOTWATT
437. Cells(32, 11) = DRMOTHP
438. Cells(33, 11) = CURRENT1
439. Cells(34, 11) = CURRENT3
440. '===== CONDENSER-2 (EXCHANGER) CALCULATION =====
441. TL1 = Cells(34, 16)
442. TOD1 = Cells(35, 16)
443. TH1C = OUTADIATEMP
444. Cells(30, 11) = TH1C
445. TH1 = TH1C + 273
446. TH2C = Cells(31, 16)
447. TH2 = TH2C + 273

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448. '...NH3
449.   TK = TH1
450.   SCNH3 = NH3SPECHEAT(TK)
451.   CNH3 = ((NH3TOTUREA / 24) / 3600) * SCNH3
452.   QNH3 = CNH3 * (TH1 - TH2)
453. '...AIR
454.   TC1 = 25 + 273
455.   AIRINTK1 = TC1
456.   SCAIR2 = AIRSPECIFICHEAT(AIRINTK1)
457. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
458.   FLAG = 2 'COOLING
459.   U = 0.02
460.   CHOT = CNH3: Q = QNH3: SCHOT = SCNH3: SCCOLD = SCAIR2
461.   Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN
GER
462. '...DATA OUT
463.   AIRFR2 = HFR
464.   Cells(30, 16) = OUTADIATEMP
465.   Cells(33, 16) = TC2 - 273 'Air Temperature OUT (oC)
466.   Cells(36, 16) = NTU 'Number of Elements (No)
467.   Cells(37, 16) = AREAHEX 'Shell Area (m^2)
468.   Cells(38, 16) = EPS * 100 'Effectiveness (%)
469.   Cells(39, 16) = QEFF 'Heat Transfer Rate (KW)
470.   Cells(40, 16) = AIRFR2 'Air Flow Rate (Kg/hr)
471.   Cells(41, 16) = COMPOP 'Condenser inside Pressure (Atm.)
472.   Cells(13, 4) = H2SOFC
473. '-----
474. '           NH3 --> POWER
475. '-----
476.   NH3HHV = NH3EXTRA * 2.604 'High Heating Value (kw)
477.   NH3LHV = NH3EXTRA * 2.15 'Low Heating Value (kw)
478.   Cells(53, 3) = NH3HHV 'High Heating Value (kw)
479.   Cells(54, 3) = NH3LHV 'High Heating Value (kw)
480. '-----
481. '           Cell Heat Losses
482. '-----
483. '----- HEAT IN -----
484. '...N2
485.   N2ITK = CITK
486.   CN2 = NITROSPCHEAT(N2ITK) 'kJ/kg.K
487.   QN2IN = ((N2TOTAVAILABLE / 24) / 3600) * CN2 * N2ITK '(kw)
488. '...H2
489.   H2TK = CITK
490.   CH2 = HYDROGENSPECHEAT(H2TK) 'kJ/kg.K (T=K)
491.   QH2IN = ((H2TOTAVAILABLE / 24) / 3600) * CH2 * H2TK '(kw)
492. 'Total Heat IN
493.   QTOTIN = QN2IN + QH2IN + CELLPPOWER '(kw)
494. '----- HEAT OUT -----
495. '...NH3
496.   TK = CITK
497.   CNH3 = NH3SPECIFICHEAT(TK) 'kJ/kg.K (1atm)
498.   QNH3OUT = ((NH3TOTAL / 24) / 3600) * CNH3 * TK '(kw)
499. '...H2
500.   H2TK = CITK
501.   CH2 = HYDROGENSPECHEAT(H2TK) 'kJ/kg.K (T=K)
502.   QH2IN = ((H2SOFC / 24) / 3600) * CH2 * H2TK '(kw)
503. 'Total Heat OUT
504.   QTOTOUT = QNH3OUT + QH2IN '(kw)
505. '----- HEAT LOSSES -----
506.   QLOSSES = QTOTIN - QTOTOUT
507. 'Cells OUTPUT
508.   Cells(36, 11) = QTOTIN
509.   Cells(37, 11) = QTOTOUT
510.   Cells(38, 11) = QLOSSES
511. '----- COMPRESSOR-4 ----- NH3 EXTRA

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512. '...INPUT
513.   COMPIP = Cells(42, 11)   'Compressor Inlet Pressure (atm.)
514.   COMPOP = Cells(43, 11)   'Compressor Outlet Pressure (atm.)
515.   Cells(44, 11) = CIT       'Gas Temperature (oC)
516.   COMETREFF = Cells(45, 11) 'Compressor Entropy Efficiency (%)
517.   SPHASVOL = Cells(46, 11)  'Single Phase Voltage (Volts)
518.   MOTOREFF1 = Cells(47, 11) 'Single Phase Motor Efficiency (%)
519.   THREPASEVOL = Cells(48, 11) '3 Phase Voltage (Volts)
520.   MOTOREFF3 = Cells(49, 11) '3 Phase Motor Efficiency (%)
521. '...Chemical Calculation
522.   TK = CIT + 273           'Inlet Gas Temperature (oK)
523.   NH3SPECHEAT = NH3SPECHEAT(TK) 'NH3 Specific Heat (kJ/Kg.K)kJ/kg.K (>1atm)
524.   NH3TEMPC = CIT
525.   GAMMA = NH3GAMMA(NH3TEMPC) 'GAMMA=Cp/Cv
526.   RHONH3 = NH3DENSITY(NH3TEMPC) 'NH3 Density (Kg/m^3)
527.   NH3KGX = NH3EXTRA        'NH3 Rquired for Urea (Kg/day)
528.   NH3VOLD = NH3KGX / RHONH3 'NH3 Volume m^3/day
529.   NH3VOLM = (NH3VOLD / 24) / 60 'NH3 Volume m^3/min
530.   NH3VOLIT = NH3VOLM * 1000    'NH3 Volume L/min
531.   Cells(41, 11) = NH3VOLIT    'NH3 Volume L/min,<=====
532.   NH3MOL = NH3KG / NH3MW      'NH3 MoIs
533.   ENTCC = NH3MOL * R * Logn(COMPOP / COMPIP)
534.   GASTEMPC = NH3TEMPC: GASVOL = NH3VOLIT
535.   OUTADIATEMP = ((GASTEMPC + 273) * ((COMPOP / COMPIP) ^ ((GAMMA - 1) / GAMMA))) - 273 ' OUTLET ADIABATIC TEMPERATURE
536.   DRMOTWATT = ((OUTADIATEMP + 273) - (GASTEMPC + 273)) * 2.22 * (NH3KGX / 86400) / ISENEFF 'KW
537.
538.   Call COMPRESSOR(GASTEMPC, COMPOP, COMPIP, GAMMA, GASVOL, OUTADIATEMP, COMETREFF, WATT, ENTCC, DRMOTWATT, DRMOTHP, MOTOREFF1, MOTOREFF3, SPH
ASVOL, THREPASEVOL, CURRENT1, CURRENT3)
539.   Cells(51, 11) = OUTADIATEMP
540.   Cells(52, 11) = DRMOTWATT
541.   Cells(53, 11) = DRMOTHP
542.   Cells(54, 11) = CURRENT1
543.   Cells(55, 11) = CURRENT3
544. '===== CONDENSER-3 (EXCHANGER) CALCULATION =====
545.   COMPIP = COMPOP
546.   TL1 = Cells(49, 16)   'TUBE LENGTH (m)
547.   TOD1 = Cells(50, 16)  'TUBE DIAMETER (m)
548.   TH1 = OUTADIATEMP + 273 'NH3 TEMPERATURE IN (K)
549.   TH2 = CIT + 273
550. '...NH3
551.   TK = TH1
552.   SCNH3 = NH3SPECHEAT(TK)
553.   CNH3 = ((NH3EXTRA / 24) / 3600) * SCNH3
554.   QNH3 = CNH3 * (TH1 - TH2)
555. '...AIR
556.   TC1 = 25 + 273
557.   AIRINTK1 = TC1
558.   SCAIR2 = AIRSPECIFICHEAT(AIRINTK1)
559. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
560.   FLAG = 2
561.   U = 0.02
562.   CHOT = CNH3: Q = QNH3: SCHOT = SCNH3: SCCOLD = SCAIR2
563.   Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN
GER
564. '...DATA OUT
565.   AIRFR2 = HFR
566.   Cells(44, 16) = COMPIP    'Condenser inlet Pressure (atm)
567.   Cells(45, 16) = OUTADIATEMP 'Inlet NH3 Temperature (oC)
568.   Cells(46, 16) = TH2 - 273 'Outlet NH3 Temperature (oC)
569.   Cells(47, 16) = 25       'Inlet Air Temperature (oC)
570.   Cells(48, 16) = TC2 - 273 'Outlet Air Temperature (oC)
571.   Cells(51, 16) = NTU       'Number of Elements (No)
572.   Cells(52, 16) = AREAHEX   'Shell Area (m^2)
573.   Cells(53, 16) = EPS * 100 'Effectiveness (%)
574.   Cells(54, 16) = QEFF      'Heat Transfer Rate (KW)

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575. Cells(55, 16) = AIRFR2 'Air Flow Rate (Kg/hr)
576. ss = ss
577. '----- CO2 -----
578.
579. 70 End Sub
580. Static Function Logn(X)
581. Logn = Log(X) / Log(2.718282)
582. End Function
583. Private Static Sub DELTAH(A, B, N, INTEGRALH)
584. H = (B - A) / N
585. T = A
586. SUMM = DELCP(T): C = 2
587. For K = 1 To N - 1
588. C = 6 - C ' Rem GENERATES COEFFICIENTS 4,2,4,2, ...
589. T = A + K * H
590. SUMM = SUMM + C * DELCP(T)
591. Next K
592. SUMM = Sum + DELCP(T)
593. INTEGRALH = (H / 3) * SUMM
594. End Sub
595. Private Static Function DELCP(T)
596. DELCP = -55.169 + 49.856 * 10 ^ -3 * T - 4.05 * 10 ^ 5 * T ^ -2 - 1.976 * 10 ^ -6 * T ^ 2
597. End Function
598. Private Static Function DELCPT(T)
599. DELCPT = (-55.169 + 49.856 * 10 ^ -3 * T - 4.05 * 10 ^ 5 * T ^ -2 - 1.976 * 10 ^ -6 * T ^ 2) ' / T
600. End Function
601. Private Static Function NH3SPECIFICHEAT(TK) 'kJ/kg.K (1atm)
602. A = 1.0948345: B = 0.002555016: C = 27119.844
603. NH3SPECIFICHEAT = A + B * GASTK + C / (TK) ^ 2
604. End Function
605. Private Static Function NH3SPECHEAT(TK) 'kJ/kg.K (>1atm)
606. A = 2.200434: B = -0.001750475: C = 0.000026445871: D = -0.000000741651: E = 7.330493E-11
607. NH3SPECHEAT = A + B * TK + C * TK ^ 2 + D * TK ^ 3 + E * TK ^ 4
608. End Function
609. Private Static Function HYDROGENSPECHEAT(H2TK) 'T=oK kJ/kg.K
610. ZA = 8.3580785: ZB = 0.046774926: ZC = -0.00014346423: ZD = 0.0000023506381: ZE = -2.3076196E-10: ZF = 1.4608608E-13
611. ZG = -6.1673082E-17: ZH = 1.7508367E-20: ZI = -3.2962768E-24: ZJ = 3.9405226E-28: ZK = -2.7046605E-32: ZL = 8.1083083E-37
612. HYDROGENSPECHEAT = ZA + ZB * H2TK + ZC * H2TK ^ 2 + ZD * H2TK ^ 3 + ZE * H2TK ^ 4 + ZF * H2TK ^ 5 + ZG * H2TK ^ 6 + ZH * H2TK ^ 7 + ZI * H2TK ^
8 + ZJ * H2TK ^ 9 + ZK * H2TK ^ 10 + ZL * H2TK ^ 11
613. End Function
614. Private Static Function NITROSPCHEAT(N2ITK) 'kJ/kg.K
615. SA = 1.100752
616. SB = -0.00053474045
617. SC = 0.0000013971884
618. SD = -1.2555363E-09
619. se = 6.0109266E-13
620. SF = -1.6836213E-16
621. SG = 2.7735985E-20
622. SH = -2.5125233E-24
623. SI = 1.0066147E-28
624. SJ = -5.1950017E-34
625. NITROSPCHEAT = SA + SB * N2ITK + SC * N2ITK ^ 2 + SD * N2ITK ^ 3 + se * N2ITK ^ 4 + SF * N2ITK ^ 5 + SG * N2ITK ^ 6 + SH * N2ITK ^ 7 + SI * N2I
TK ^ 8 + SJ * N2ITK ^ 9
626. End Function
627. Private Static Function AIRSPECIFICHEAT(AIRINTK) 'T=oK
628. TA = 1.0828694: TB = -0.00063119116: TC = 0.000016253087: TD = -1.3949526E-09: TE = 5.3826153E-13: TF = -7.9021928E-17
629. AIRSPECIFICHEAT = TA + TB * AIRINTK + TC * AIRINTK ^ 2 + TD * AIRINTK ^ 3 + TE * AIRINTK ^ 4 + TF * AIRINTK ^ 5
630. End Function
631. Private Static Sub HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'H
EAT EXCHANGER
632. AREAHEX = 3.14 * TOD * TL
633. 'DELTAB = TH2 - TC1
634. LMTD = Q / (U * AREAHEX)
635. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
636. '----- HEATING -----

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637.   If FLAG = 1 Then
638.     DELTAA = TH1 - TC2
639.     'DELTAB = TH2 - TC1
640.     LMTD = Q / (U * AREAHEX)
641.     X1 = 1
642. 300 S1 = DELTAA / (LMTD - Logn(DELTAA))
643.     S2 = X1 / (LMTD - Logn(X1))
644.     If S2 >= S1 Then
645.       GoTo 400
646.     Else
647.       X1 = X1 + 0.1
648.       GoTo 300
649. 400 End If
650.     DELTAB = X1
651.     TH2 = DELTAB + TC1
652.     GoTo 700
653.   End If
654. '-----
655. '----- COOLING -----
656.   If FLAG = 2 Then
657.     'DELTAA = TH1 - TC2
658.     DELTAB = TH2 - TC1
659.     LMTD = Q / (U * AREAHEX)
660.     X1 = 2
661. 500 S1 = Logn(X1) - X1 / LMTD
662.     S2 = Logn(DELTAB) - DELTAB / LMTD
663.     If S1 >= S2 Then
664.       GoTo 600
665.     Else
666.       X1 = X1 + 0.1
667.       GoTo 500
668. 600 End If
669.     DELTAA = X1
670.     TC2 = TH1 - DELTAA
671.   End If
672. '-----
673. 700 P = (TC2 - TC1) / (TH1 - TC1)
674.     R = (TH1 - TH2) / (TC2 - TC1)
675.     If R > 1 Then
676.       R1 = 1 / R
677.       P1 = P * R
678.     Else
679.       P1 = P
680.       R1 = R
681.     End If
682.     A1 = (((R1) ^ 2 + 1) ^ 0.5) / (1 - R1)
683.     A2 = Logn((1 - R1 * P1) / Abs(1 - P1))
684.     A3 = 2 - P1 * (1 + R1 - (1 + (R1) ^ 2)) ^ 0.5 'up
685.     A4 = Abs(2 - P1 * (1 + R1 + (1 + (R1) ^ 2)) ^ 0.5) 'down
686.     A5 = Logn(A3 / A4)
687.     FCORF = (A1 * A2) / A5
688.     If Abs(FCORF) > 1 Then
689.       FCORF = 1
690.     End If
691.     If FLAG = 1 Then
692.       LMTD = Q / (U * AREAHEX * FCORF)
693.       CHOT = Q / (TH1 - TH2)
694.       HFR = CHOT * 24 * 3600 / SCHOT
695.       GoTo 800
696.     End If
697.     If FLAG = 2 Then
698.       LMTD = Q / (U * AREAHEX * FCORF)
699.       CCOLD = Q / (TH1 - TH2)
700.       HFR = CCOLD * 24 * 3600 / SCHOT
701.     End If

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702. 'EFFECTIVENESS
703. 800 If CCOLD > CHOT Then
704.     CMIN = CHOT
705.     C1 = CHOT
706.     EPS = (C1 * (TC2 - TC1)) / (CMIN * (TH1 - TC1))
707.     GoTo 900
708. Else
709.     CMIN = CCOLD
710.     C1 = CCOLD
711.     EPS = (C1 * (TH1 - TH2)) / (CMIN * (TH1 - TC1))
712. 900 End If
713. QEFF = EPS * CMIN * (TH1 - TC1)
714. 'Number of ELEMENT
715. NTU = U * AREAHEX / CMIN
716. If NTU <= 1 Then
717.     NTU = 1
718. Else
719.     End If
720. End Sub
721. Private Static Function FCORF1(P, R)
722. S1 = (2 - P * (1 + R - (1 + R ^ 2) ^ 0.5)) / (2 - P * (1 + R + (1 + R ^ 2) ^ 0.5))
723.     S2 = (1 - R * P) / (1 - P)
724.     S3 = ((1 + R ^ 2) ^ 0.5) / (1 - R)
725.     FCORF1 = S3 * Logn(S2) * (Logn(S1)) ^ -1
726. End Function
727. Private Static Function NH3DENSITY(NH3TEMPC) ' T=oC
728. Dim F As Double
729. A = 0.76249107: B = -0.0030065503: C = 0.000012095274: D = -0.000000038570889: E = 7.2102508E-11: F = -5.5332429E-14
730. NH3DENSITY = A + B * NH3TEMPC + C * NH3TEMPC ^ 2 + D * NH3TEMPC ^ 3 + E * NH3TEMPC ^ 4 + F * NH3TEMPC ^ 5
731. End Function
732. Private Static Function NH3GAMMA(NH3TEMPC) ' T=oC
733. A = 1.3320734: B = -0.00049999747: C = 0.0000010911546: D = -0.000000002975822: E = 3.4313946E-12
734. NH3GAMMA = A + B * NH3TEMPC + C * NH3TEMPC ^ 2 + D * NH3TEMPC ^ 3 + E * NH3TEMPC ^ 4
735. End Function
736. Private Static Sub COMPRESSOR(GASTEMPC, COMPPOP, COMPPIP, GAMMA, GASVOL, OUTADIATEMP, COMETREFF, WATT, ENTCC, DRMOTWATT, DRMOTHP, MOTOREFF1, MOTO
    REFF3, SPHASVOL, THREPASEVOL, CURRENT1, CURRENT3)
737.     A1 = 1000
738.     A2 = 60
739. End Sub

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UREA

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1. Sub Sheet9_Button1_Click()
2. '----- UREA PRODUCTION -----
3.
4. '
5.     UREACTU = ActiveWorkbook.Worksheets("SSAS").Cells(14, 11) 'NH3 Total Available from SSAS (Kg/Day)
6.     NH3TEMPERATURE = ActiveWorkbook.Worksheets("SSAS").Cells(15, 4) 'NH3 Temperature SSAS(ITM) (Kg/Day)
7.     CO2AVFR = ActiveWorkbook.Worksheets("SSAS").Cells(16, 11) 'CO2 Total Available from SSAS(ITM) (Kg/Day)
8. )
9.     WTRBAL = ActiveWorkbook.Worksheets("DFB-ADB").Cells(6, 4) 'WTRBAL (Kg/Day)
10.    UREACTUX4 = ActiveWorkbook.Worksheets("SSAS").Cells(41, 6) 'NH3 Total Available from SSAS (Kg/Day)
11.    Dim TOTALAH2OVAOUTVE As Double, XR As Double, XRES As Double, AAT As Double, BBT As Double, Z As Double
12.    Dim REACPERF1 As Double
13.    Dim K1(10), K2(10), K3(10), K4(10), X As Double, Y As Double, CST As Double, choice As Integer
14.    Dim X0 As Double, XMAX As Double, N As Long, Y0 As Double, H As Double, S As Integer, XUR As Double
15.    '=====
16.    PRESSURE = Cells(3, 4) 'Pressure
17.    TEMPREACT = Cells(4, 4) 'Temperature
18.    PERCPURITY = Cells(5, 4) '% UREA OUT
19.    PERCONV1 = Cells(11, 4) '% PERCPURITYSION
20.    '----- DATA OUT -----
21.    Cells(6, 4) = UREACTUX4

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21. UREAOUT = UREACTUX4 * (PERCPURITY / 100)
22. Cells(7, 4) = UREAOUT
23. '----- MOLECULAR MASS -----'
24. MMUREA = 60
25. MMCO2 = 44
26. MMNH3 = 17
27. MMH2O = 18
28. MMBIURE = 103
29. MMCARBAMATE = 78
30. MMCARBH2O = 103
31. '-----'
32. FT45 = UREACTUX4 - UREAOUT 'urea converted to NH3 & Biuret'
33. PERCB1 = FT45 / 2 'Biuret%'
34. PERCH201 = FT45 / 2 'Water%'
35. Cells(17, 4) = PERCB1 'Biuret'
36. Cells(18, 4) = PERCH201 'Water'
37. RETORPER = Cells(3, 10) '% UREA AT REACTOR EXIT REACTOR PERFORMANCE'
38. MPSPERF1 = Cells(3, 18) '% Urea out from Medium pressure separator'
39. PERUREAOUTEV1 = Cells(17, 13) '% UREA OUT from EVAPORATOR-1'
40. PERUREAOUTEV2 = Cells(17, 18) '% Urea out from EVAPORATOR-2'
41. PERURAOUTPTW = Cells(29, 10) '% Urea out from prilling tower'
42. PERCENTPURITY = PERCPURITY / 100
43. PERCB = PERCB1 / 100
44. PERCH20 = PERCH201 / 100
45. PERCONV = PERCONV1 / 100
46. REACTPERF = RETORPER / 100
47. MPSPERF = MPSPERF1 / 100
48. PERUREAOUTEV1 = PERUREAOUTEV1 / 100
49. PERUREAOUTEV2 = PERUREAOUTEV2 / 100
50. PERURAOUTPTW = PERURAOUTPTW / 100
51. KGH2O = UREACTUX4 * PERCH20
52. KGBIURET = UREACTUX4 * PERCB
53. KGBU = ((2 * MMUREA) / MMCARBH2O) * PERCB1 'BIURET PRODUCED BY REACTION-4 (side reaction) OK'
54. KGUREAR2 = UREAOUT + KGBU 'UREA PRODUCED FROM REACTION-2 OK'
55. KGC02RQ = (MMCO2 / MMUREA) * KGUREAR2 'CO2 REQUIRED FOR REACTION-1 OK'
56. CO2CONV = KGC02RQ / PERCENTPURITY 'Assuming 98.9% conversion CO2 ACTUALLY REQUIRED OK'
57. Cells(13, 4) = CO2CONV
58. KGNH3RQ = ((MMNH3 * 2) / MMUREA) * KGUREAR2 'NH3 required from reaction-1 ok'
59. NH3CONV = KGNH3RQ / PERCENTPURITY 'NH3 Assuming 98.9% conversion ACTUALLY REQUIRED) OK'
60. Cells(12, 4) = NH3CONV
61. RT45 = ((NH3CONV * 1000) / MMCO2) / ((CO2CONV * 1000) / MMNH3)
62. Cells(14, 4) = RT45
63. KGUREAR3 = (MMUREA / MMCO2) * CO2CONV 'UREA PRODUCED TOTAL if the cnversion is 100%' OK'
64. KGUREAPR = KGUREAR3 * PERCENTPURITY 'UREA PRUDUCED AT % COVERSION 98.9 OK'
65. UREATOBIURET = KGUREAPR - UREAOUT 'UREA CONVERTED TO BIURET AND NH3' OK'
66. BIURETPROD = (MMCARBH2O / (2 * MMUREA)) * UREATOBIURET 'BIURET PRODUCED OK'
67. Cells(24, 4) = BIURETPROD
68. H2OPROD = (MMH2O / MMUREA) * KGUREAR2 'H2O IN REACTOR IN REACTION-2 OK'
69. TOTWAT1 = (WTRBAL - H2OPROD)
70. TOTWAT = TOTWAT1 + H2OPROD
71. ' MASS BALANCE
72. '----- REACTOR BALANCE -----'
73. REACTOTFL = UREAOUT / REACTPERF 'AT REACTOR'S EXIT FLOW RATE'
74. KGUREAR4 = (MMNH3 / (MMUREA * 2)) * UREATOBIURET 'NH3 PRODUCED IN REACTION-4
75. KGUREATRE = ((MMNH3 * 2) / MMUREA) * KGUREAPR 'NH3 REACTED IN REACTION-1'
76. UNREACNH3 = NH3CONV - KGUREATRE + KGUREAR4 'NH3 UNREACTED'
77. Cells(6, 9) = UNREACNH3
78. Cells(9, 9) = UREAOUT
79. KGUREATREXC = ((MMCO2) / MMUREA) * KGUREAPR 'CO2 REACTED IN REACTION-1'
80. UNREACTCO2X = CO2CONV - KGUREATREXC 'UNREACTED CO2'
81. BGTR = PERCPURITY * CO2CONV / 100 'CO2 required based on the conversion rate'
82. CO2OUTREACT = CO2CONV - BGTR 'UNREACTED CO2 OUT OF REACTOR'
83. Cells(7, 9) = UNREACTCO2X
84. CARBREATOUT = REACTOTFL - (UREAOUT + UNREACTCO2X + UNREACNH3 + H2OPROD + BIURETPROD) ' CARBAMATE FLOW RATE OUT'

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85. Cells(8, 7) = CARBREATOUT
86. Cells(8, 9) = CARBREATOUT
87. Cells(10, 9) = H2OPROD
88. Cells(11, 9) = BIURETPROD 'BIURET PRODUCED
89. '----- STRIPPER ----- NO REACTION (SEPARATION ONLY BY EXCEL) -----
-----
90. '----- MEDIUM PRESSURE SEPARATOR --- NO REACTION (% SEPARATION OF NH3 & CO2) --
-
91. NH3OUTMPS = UNREACNH3 * MPSPERF
92. CO2OUTMPS = CO2OUTREACT * MPSPERF
93. Cells(6, 17) = NH3OUTMPS
94. Cells(7, 17) = CO2OUTMPS
95. MPSRECYNH3 = NH3CONV + NH3INTMPS 'NH3 RECYCLED IN MPS
96. MPSRECYCO2 = CO2CONV + CO2INTMPS 'CO2 RECYCLED IM MPS
97. NH3INTMPS = UNREACNH3 - NH3OUTMPS 'NH3 REMAINING IN MPS
98. CO2INTMPS = CO2OUTREACT - CO2OUTMPS 'CO2 REMAINING IN MPS
99. Cells(6, 18) = NH3INTMPS
100. Cells(7, 18) = CO2INTMPS
101. '----- LOW PRESSURE SEPARATOR ----NO REACTION (% SEPARATION OF NH3 & CO2) --
-
102. NHREXTLPS = NH3INTMPS
103. CO2EXTLPS = CO2INTMPS
104. NH3TOTRECY = MPSRECYNH3 + NHREXTLPS 'TOTAL NH3 RECYCLED
105. CO2TOTRECY = MPSRECYCO2 + CO2EXTLPS 'TOTAL CO2 RECYCLED
106. Cells(20, 9) = NHREXTLPS
107. Cells(21, 9) = CO2EXTLPS
108. RATIONH3CO2 = (NH3TOTRECY / 17) / (CO2TOTRECY / 44)
109. TOTALNH3INREACT = NHREXTLPS + UNREACNH3
110. TOTALCO2INREACT = CO2INTMPS + CO2OUTREACT
111. '----- Evaporator-----
112. TOTALINVE1 = UREAOUT + PERCB1 + H2OPROD 'TOTAL FLOW IN VACUUM EVAPORATOR-1 Kg/day
113. FSDR32 = (PERUREAOUTEV1 / PERUREAOUTEV2) * TOTALINVE1
114. HGYT67 = TOTALINVE1 - FSDR32 'evaporated 'loss
115. TOTGASOUTVE1 = HGYT67 / 2
116. KH2OLIQOUTVE2 = H2OPROD - HGYT67
117. Cells(23, 18) = KH2OLIQOUTVE2
118. TOTALINVE2 = UREAOUT + PERCB1 + KH2OLIQOUTVE2
119. FSDR32C = (PERUREAOUTEV2 / PERUREAOUTPTW) * TOTALINVE2
120. TOTALH2OLIQ = TOTALINVE2 - FSDR32C
121. TOTALH2OLIQX = KH2OLIQOUTVE2 - TOTALH2OLIQ
122. Cells(33, 10) = TOTALH2OLIQX
123. ' TOTALH2OVAOUTPT
124. Cells(33, 9) = TOTALH2OVAOUTPT
125. H2OOUT = H2OPROD
126. Cells(23, 11) = H2OOUT
127.
128. PCUREAEV1 = UREAOUT / TOTALINVE1 '%UREA IN OUT OF EVAPORATOR-1
129. TOTLIQUIDOUTVE1 = (TOTALINVE1 * PCUREAEV1) / PERUREAOUTEV1 'TOTAL LIQUID OUT
130. OUT
131. Cells(25, 13) = TOTGASOUTVE1 'RECYCLED
132. KH2OLIQOUTVE1 = (H2OOUT - KH2OLIQOUTVE2) / 2 'AMOUNT OF H2O (Kg/day) OUT of VACUUM EVAPORATOR-1
133. Cells(23, 15) = KH2OLIQOUTVE1
134. KH2OLIQINVE2 = KH2OLIQOUTVE1
135. Cells(23, 13) = KH2OLIQINVE2
136. Cells(26, 15) = TOTLIQUIDOUTVE1
137. '----- VACUUM EVAPORATOR-2 -----
138. TOTALINVE2 = UREAOUT + KH2OLIQOUTVE1 + BIURETPROD 'TOTAL FLOW IN VACUUM EVAPORATOR-2 Kg/day
139. PCUREAEV2 = UREAOUT / TOTALINVE2 '%UREA IN OUT OF EVAPORATOR-2
140. TOTLIQUIDOUTVE2 = TOTALINVE2 * PCUREAEV2 / PERUREAOUTEV2 'TOTAL LIQUID OUT
141. TOTGASOUTVE2 = TOTALINVE2 - TOTLIQUIDOUTVE2 ' AMOUNT OF H2O VAPOR OUT
142. Cells(25, 17) = HGYT67 / 2
143. KH2OLIQOUTVE2 = KH2OLIQOUTVE1 - TOTGASOUTVE2 'AMOUNT OF H2O (Kg/day) OUT of VACUUM EVAPORATOR-2
144. '
145. ' PRILLING TOWER
146. TOTALLIQUIDINPTW = TOTLIQUIDOUTVE2

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210. ' HEAT OUTPUT (M)x(CP)x(DELT)
211. TDELHROUT = TOTALMROUT * TCPROUT * 180 'HEAT OUT of REACTOR KJ/day
212. Cells(5, 23) = TDELHROUT 'Kj/d'
213. ' HEAT IN + HEAT of REACTION - HEAT OUT = H RATE OF ACCUMULATION
214. HACCR = REACHEATIN + DELTHREAC - TDELHROUT 'ACCUMULATED HEAT KJ/day
215. 'Assumption: Cooling water at 25oC is used to remove heat from the reactor. The outlet is
216. 'steam at an absolute pressure of 4.5 bar (Ts = 147.9 oC).
217. 'So, heat gained by cooling water:
218. LAMDAH2OR = 2120.6 'Landa H2) KJ/Kg
219. LAMDH2OR = 4.187 'Landa H2O KJ/Kg.oC
220. MH2OCWR = HACCR / (LAMDH2OR * (147.9 - 25) + LAMDAH2OR) ' Heat Given OUT to water used for Cooling Water Kg/day
221. '
222. 'ssssssssssssssssssssssssssssssssssssssssssssssssss STRIPPER sssssssssssssssss
223. '
224. ' HEAT OUT
225. ' Moles
226. MNH3SOUT = NH3INTMPS / MMNH3
227. MCO2SOUT = CO2OUTREACT / MMCO2
228. MUREASOUT = UREAOUT / MMUREA
229. MH2OSOUT = H2OPROD / MMH2O
230. MBIURESOUT = BIURETPROD / MMBIURE
231. TOTALMSOUT = MNH3SOUT + MCO2SOUT + MUREASOUT + MH2OSOUT + MBIURESOUT ' Total Mole Out
232. ' MOLE FRACTION
233. MFNH3SOUT = MNH3SOUT / TOTALMSOUT
234. MFCO2SOUT = MCO2SOUT / TOTALMSOUT
235. MFUREASOUT = MUREASOUT / TOTALMSOUT
236. MFH2OSOUT = MH2OSOUT / TOTALMSOUT
237. MFBIURESOUT = MBIURESOUT / TOTALMSOUT
238. SSST = MFNH3SOUT + MFCO2SOUT + MFUREASOUT + MFH2OSOUT + MFBIURESOUT
239. ' CP at 185 oC
240. CPNH3SOUT = 41.31
241. CPCO2SOUT = 44.22
242. CPCARBMSOUT = 202.49
243. CPUREASOUT = 135.3
244. CPH2OSOUT = 75.37
245. CPBIURETSOUT = 183.8
246. TCPSOUT = CPNH3SOUT * MFNH3SOUT + CPCO2SOUT * MFCO2SOUT + MFUREASOUT * CPUREASOUT + MFH2OSOUT * CPH2OSOUT + MFB
IURESOUT * CPBIURETSOUT
247. ' HEAT OUT OF STRIPPER
248. TDELHSOUT = TOTALMSOUT * TCPSOUT * 185
249. Cells(5, 24) = TDELHSOUT
250. CARBAMTX = CARBREATOUT / MMCARBAMATE
251. ' CARBAMATE VAPOR OUT
252. LAMDACARBM = 210 'LAMDA CARBAMATE= 210KJ/kg
253. HEATCARBOUT = CARBAMTX * CPCARBMSOUT * 185 + CARBREATOUT * LAMDACARBM ' KJ/day
254. 'Heat required from steam
255. HREQSST = TDELHSOUT + HEATCARBOUT - TDELHROUT
256. LAMDAH2OS = 1855.3
257. MH2OSS = HREQSST / LAMDAH2OS 'Heat supplied by steam Kg/day
258. '
259. 'CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC CARBAMATE CONDENSER CCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
260. KSTEAMCOND = (CARBREATOUT * 210) / (4.187 * (147.9 - 25) + 2120.6) 'Kg/day
261. 'msmsmsmsmsmsmsmsmsmsmsmsmsmsmsmsmsmsms MEDIUM PRESSURE SEPARATOR msmsmsmsmsmsmsmsmsmsmsmsmsms
262. '
263. ' HEATCARBOUT HEAT IN
264. TDELHPSIN = TDELHSOUT
265. ' LIQUID STREAM OUT AT 140 oC
266. ' TOTAL MOLES
267. MNH3MPS = NH3OUTMPS / MMNH3
268. MCO2MPS = CO2OUTMPS / MMCO2
269.
270. TOTALMPSOUT = MNH3MPS + MCO2MPS + MUREASOUT + MH2OSOUT + MBIURESOUT
271. '

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466. '*****
467. DFMFCARBROUT = MFCARBROUT
468. DFMFUREAOUT = MFNH3ROUT
469. DFMFCO2ROUT = MFCO2ROUT
470. FCARB = VOLFCARREA
471. FUREA = VOLFUREA
472. FCO2 = VOLFCO2REA
473. FNH3 = VOLFNH3REA
474. FH2O = VOLH2OREA
475. EPS1 = (FCARB + FUREA) / (FCARB + FUREA + FCO2)
476. EPS2 = FUREA / (FCARB + FUREA)
477. EPS = FUREA / (FCARB + FUREA + FCO2)
478. AR = FNH3 / (FCARB + FUREA + FCO2)
479. BR = FH2O / (FCARB + FUREA + FCO2)
480. FNR = (1 + AR + BR - 2 * EPS1 + EPS)
481. XCARB = (EPS1 - EPS / FNR)
482. XUREA = MFUREASOUT
483. XNH3 = MFNH3ROUT
484. XH2O = MFH2OSOUT
485. XBIURE = MFBIURESOUT
486. TR = TEMPREACT
487. TK = TR + 273
488. TT = TK / 100
489. TOTALGAS = (VOLFUREA + VOLFCO2REA) * 1440 ' H2O negligible
490. YGASMFNH3 = (VOLFUREA * 1440) / TOTALGAS
491. YGASMFCO2 = (VOLFCO2REA * 1440) / TOTALGAS
492.
493. ' EPSILON STAR
494. EPSSTAR = -3.4792 + AR * (8.2677 * 1010 ^ -1) - ((1.8998 * 10 ^ -2) * AR ^ 2) - ((2.3155 * 10 ^ -
1) * BR) - ((1.144 * 10 ^ -1) * TT / 100) + ((2.9879 * 10 ^ -2) * AR * BR) - ((1.3294 * 10 ^ -
1) * AR * TT) + ((4.5348 * 10 ^ -1) * (TT ^ 2)) - ((5.5339 * 10 ^ -2) * TT ^ 3)
495. NUR = EPS / EPSSTAR
496. ' GAMMA
497. GAMNH3 = 0.396 - (2.88447 * 10 ^ -
3) * TT + 0.6111 * AR - 0.274 * AR * NUR + 0.88 * NUR + 0.068 * AR ^ 2 - (0.24894 * 10 ^ -4) * TT * AR ^ 2
498. GAMMACO2 = 0.6082 + (3.5532 * 10 ^ -4) * TT - 0.3681 * AR + 0.111 * BR + (3.7508 * 10 ^ -
4) * TT * AR * NUR - 0.10245 * AR * NUR - (4.8257 * 10 ^ -2) * AR ^ 2
499. GAMMAH2O = 22.6745 - (1.5546 * 10 ^ -2) * TT - 4.0697 * AR + 2.0369 * NUR ^ 2 - 15.8744 * NUR + 4 * AR * NUR
500. ' VAPOR EQUILIBRIUM
501. P1SNH3 = -25.07 / TK + 56.321 * Logn(TK) - 0.2625 * TK + 1.753 * 10 ^ -4 / TK ^ -2 - 258.139
502. PSNH3 = Logn(P1SNH3)
503. P1SCO2 = -2370.26 / TK + 0.5911 * Logn(TK) - (1.178 * 10 ^ -2) * TK + 1.598 * 10 ^ -5 / TK ^ -2 + 15.272
504. PSCO2 = Logn(P1SCO2)
505. P1SH2O = -5231.82 / TK - (6.167 * 10 ^ -2) * Logn(TK) - (3.291 * 10 ^ -3) * TK + (1.222 * 10 ^ -6) / (TK ^ -
2) + 13.183
506. PSH2O = Logn(P1SH2O)
507. ' PHYSICAL PROPERTIES
508. ' Critical Pressure (Atm)
509. CPNH3 = 113.3
510. CPH2O = 217.7
511. CPCO2 = 72.8
512. ' Critical Temperature K
513. CTNH3 = 405.5
514. CTH2O = 647.096
515. CTCO2 = 304.19
516. ' Reduced Pressure
517. RPNH3 = PRESSURE / CPNH3
518. RPH2O = PRESSURE / CPH2O
519. RPCO2 = PRESSURE / CPCO2
520. ' Reduced Temperature
521. RTNH3 = TK / CTNH3
522. RTH2O = TK / CTH2O
523. RTCO2 = TK / CTCO2
524. ' Redlich-Kwong quation
525. ANH3 = 0.42748 * (RPNH3 / RTNH3 ^ 2.5)

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526. AH20 = 0.42748 * (RPH20 / RTH20 ^ 2.5)
527. ACO2 = 0.42748 * (RPCO2 / RTCO2 ^ 2.5)
528. '
529. BNH3 = 0.08664 * (RPNH3 / RTNH3)
530. BH20 = 0.08664 * (RPH20 / RTH20)
531. BCO2 = 0.08664 * (RPCO2 / RTCO2)
532. '
533. AAT = (YGASMFNH3 * (ANH3) ^ 1 / 2 + YGASMFCO2 * (ACO2) ^ 1 / 2) ^ 2
534. BBT = YGASMFNH3 * BNH3 + YGASMFCO2 * BH20
535. Z = 0
536. For I = 1 To 1000
537. ZZ1 = ZZ(AAT, BBT, Z)
538. Z = Z + 1
539. If ZZ1 >= 0 Then
540. GoTo 2
541. End If
542. Next I
543. 2 TTT = TTT
544. PHI1NH3 = (BNH3 / BBT) * (ZZ1 - 1) - Logn(ZZ1 - BBT) + (AAT / BBT) * (BNH3 / BBT - ZZ1 * (ANH3 / AAT) ^ 1 / 2)
* Logn(1 + BBT / ZZ1)
545. PHI1CO2 = (BCO2 / BBT) * (ZZ1 - 1) - Logn(ZZ1 - BBT) + (AAT / BBT) * (BCO2 / BBT - ZZ1 * (ACO2 / AAT) ^ 1 / 2)
* Logn(1 + BBT / ZZ1)
546. PHI1H2O = (BH20 / BBT) * (ZZ1 - 1) - Logn(ZZ1 - BBT) + (AAT / BBT) * (BH20 / BBT - ZZ1 * (AH20 / AAT) ^ 1 / 2)
* Logn(1 + BBT / ZZ1)
547. PH1NH3 = Logn(PHI1NH3)
548. PH1CO2 = Logn(PHI1CO2)
549. PH1H2O = Logn(PHI1H2O)
550. ' ODE
551. ' Carbamate
552. '
553. '=====
554. 'Equipment design'
555. 'Reactor'
556. NH3DEN1 = 618 '(kg/m3) at liquid state'
557. CO2DEN1 = 277.38 '(kg/m3) at 40C gas'
558. CARBAMATEDEN1 = 1600 '(kg/m3)'
559. GHFT32 = NH3CONV / NH3DEN1 '(m3/day)NH3'
560. GHFT34 = CO2CONV / CO2DEN1 '(m3/day) CO2'
561. GHFT36 = CARBREATOUT / CARBAMATEDEN1 '(m3/day) carbamate'
562. TOTGH246 = GHFT32 + GHFT34 + GHFT36 '(m3/day) total flow in'
563. 'CO2 is the limiting reactant'
564. XBA = 0.65
565. TAW = 23.3 '(min) Calculated this based on Simpson's rule with the reaction rate equation based on CO2 being the li
miting reactant'
566. TAWHOU = TAW / (1440) 'Residence time (day)'
567. VOLREACTN = TOTGH246 * TAWHOU ' volume of reactor (m3)'
568. BETAX = Cells(27, 4)
569. DIAREATX = ((4 * VOLREACTN) / (BETAX * 3.14)) ^ (0.33333) ' reactor diamter (m)'
570. LENGTHREACTX = (DIAREATX * BETAX) 'length of reactor (m)'
571. DESIGNPRESS = 1.1 ' 10% extra design pressure'
572. Cells(28, 4) = DIAREATX
573. Cells(29, 4) = LENGTHREACTX
574. Cells(30, 4) = VOLREACTN
575.
576.
577. End Sub
578.
579. Private Function ODE(X0 As Double, XMAX As Double, N As Long, Y0 As Double, CST As Double, H As Double, choice As I
nteger, X As Double, Y As Double, S As Integer) As Double
580. 'Option Explicit 'forces strong typing
581. 'Numerical solution of dy/dx = f(x,y) x0 < x < xmax, y(x0) = y0
582. 'To use this code enter the following function call in the shreadsheet
583. 'cell where you want the final value of y to appear:
584. '=Euler( <initial x cell>, <final x cell>, <cell with number of steps>, <choice cell for derivative> )
585.

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586.             'x0 is the initial value of x
587.             'xmax is the final value of x
588.             'n is the number of steps in the solution
589.             'y0 is the initial value of y
590.             'choice allows different equations for f(x,y)
591.
592.     Dim deriv As Double 'value of derivative
593.     ' Dim H As Double   'step size
594.     Dim I As Long      'loop index for steps
595.     ' Dim CST As Double 'Constant of the derivative
596.
597.
598.     'Calculate step size and initial value of derivative
599.
600.     Y = Y0             'Initialize dependent variable
601.     H = (XMAX - X0) / N 'Define step size
602.     deriv = F(X0, Y0, CST, choice) 'See function f below
603.
604.     'Loop over all steps calculating the new x and y values
605.     For I = 0 To N
606.         X = X0 + I * H           'new x value
607.         Y = Y + deriv * H       'new y value
608.         deriv = F(X, Y, CST, choice) 'new derivative from function, f
609.         '----- POUR CE PROBL ( A EFASSER POUR D'AUTRE)
610.         If S = 1 Then
611.             Cells(73 + I, 1) = X
612.             Cells(73 + I, 2) = Y
613.             GoTo 1
614.         End If
615.         If S = 2 Then
616.             Cells(73 + I, 4) = X
617.             Cells(73 + I, 5) = Y
618.             GoTo 1
619.         End If
620.         If S = 3 Then
621.             Cells(73 + I, 7) = X
622.             Cells(73 + I, 8) = Y
623.             GoTo 1
624.         End If
625.         If S = 4 Then
626.             Cells(73 + I, 10) = X
627.             Cells(73 + I, 11) = Y / 29.5
628.             GoTo 1
629.         End If
630.     1   S = S
631.         '----- Z -----
632.     Next I
633.         'Return final y value and end function
634.         ' Euler = Y / 10
635.     End Function
636. Private Function F(X As Double, Y As Double, CST As Double, choice As Integer) As Double
637.     Select Case choice
638.
639.         Case 1
640.             F = X * CST + Y           'First example problem
641.         Case 2
642.             F = 0.023 - CST * Y       'Second example problem
643.         Case 3
644.             F = 0.0049366322 + 0.92342793 * X + -0.35614229 * X ^ CST
645.         Case 4
646.             F = -X / Y                 'No solution about x = y0
647.         Case Else
648.             F = 0                       'Default is zero derivative
649.     End Select
650. End Function

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651. Private Function MLRYIE(XR As Double)
652. A = 84.27319
653. B = 0.46672546
654. MLRYIE = A * (1 - Exp(-B * XR))
655. End Function
656. Private Function Logn(X)
657. Logn = Log(X) / Log(2.718282)
658. End Function
659. Private Function ZZ(AAT As Double, BBT As Double, Z As Double)
660. ZZ = Z ^ 3 - Z ^ 2 + (AAT - BBT - BBT ^ 2) * Z - AAT * BBT
661. End Function
662. Private Function RUNKUTEXCEL(XUR As Double, K1 As Double, K2 As Double, K3 As Double, K4 As Double, K5 As Double)
663. RUNKUTEXCEL = ((K1 + K2 * XUR) / (1 + K3 * XUR + K4 * XUR ^ 2)) * K5
664. End Function

```

SOFC

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1. Sub Sheet10_Button1_Click()
2. '
3. ' SOFC
4. '
5. '===== H2 =====
6. 'Temperature
7. TH2T = ActiveWorkbook.Worksheets("SSAS").Cells(11, 4) 'H2 Temperature (oC)
8. 'Total Flow Rate Available
9. H2FRSSAS = ActiveWorkbook.Worksheets("SSAS").Cells(31, 3) 'H2 Flowrate from SSAS Available (Kg/day)
10. H2TOTALFR = H2FRSSAS 'Total H2 Flow Rate Available (kg/day)
11. '===== O2 =====
12. O2FRITM = ActiveWorkbook.Worksheets("ITM").Cells(11, 11) 'O2 Flowrate from ITM (Kg/day)
13. TO2 = ActiveWorkbook.Worksheets("ITM").Cells(11, 4) 'O2 Temperature (oC)
14. '
15. '===== H2O FROM HEAT EXCHANGER =====
16. H2OHXITM = ActiveWorkbook.Worksheets("ITM").Cells(26, 4) 'H2O flow rate from ITM Heat Exchanger (kg/hr)
17. H2OHXEMS = ActiveWorkbook.Worksheets("EMS").Cells(25, 16) 'H2O flow rate from EMS Heat Exchanger (kg/hr)
18. H2OHXSOFEC = ActiveWorkbook.Worksheets("SOFEC").Cells(14, 16) 'H2O flow rate from SOFEC Heat Exchanger 4 (kg/hr)
19. H2OHXSOFEC1 = ActiveWorkbook.Worksheets("SOFEC").Cells(27, 16) 'H2O flow rate from SOFEC Heat Exchanger 10 (kg/hr)
20. '
21. '===== Water Produced Total =====
22. 'SOFEC
23. H2OSOFEFCROUT = ActiveWorkbook.Worksheets("SOFEC").Cells(9, 11) 'WATER FLOW RATE OUT of [SOFEC] at CATHODE Kg/day)
24. H2OSOFECTEMP = ActiveWorkbook.Worksheets("SOFEC").Cells(15, 4) 'WATER Temperature [SOFEC] (oC)
25. H2OSOFEFCFRIN = ActiveWorkbook.Worksheets("SOFEC").Cells(8, 11) 'WATER FLOW RATE IN of [SOFEC] at CATHODE Kg/day)
26. H2OSOFEFCFRIN56 = ActiveWorkbook.Worksheets("SOFEC").Cells(12, 4) 'WATER FLOW RATE IN of [SOFEC] at CATHODE Kg/day)
27. 'UREA
28. H2OUREAFR = ActiveWorkbook.Worksheets("UREA").Cells(23, 4) 'WATER FLOW RATE(From UREA)Kg/day)
29. H2OUREATEMP = ActiveWorkbook.Worksheets("UREA").Cells(25, 4) 'WATER Temperature UREA(oC)
30. '
31. '===== Water Used in HEAT EXCHANGERS =====
32. 'MIXING TANK DFB
33. HXH2OMIXTANK = ActiveWorkbook.Worksheets("DFB-ADB").Cells(98, 4) 'Heat HEX-Water Flow Rate (Kg/day)
34. HXH2OMIXTTEM = ActiveWorkbook.Worksheets("DFB-ADB").Cells(89, 4) 'Heat HEX-Water Temperature OUT (oC)
35. HXH2OMIXTTEMH2O = ActiveWorkbook.Worksheets("DFB-ADB").Cells(6, 4) 'Heat HEX-Water Temperature OUT (oC)'Water DF and ADB NEEDED'
36. 'ITM
37. H2OITMFR = ActiveWorkbook.Worksheets("ITM").Cells(26, 4) 'WATER FLOW RATE{HEATING} [ITM] Kg/day)
38. H2OITMTEMP = ActiveWorkbook.Worksheets("ITM").Cells(30, 4) 'WATER Temperature [HEATING][ITM](oC)
39. 'EMS
40. H2OEMSFR = ActiveWorkbook.Worksheets("EMS").Cells(25, 16) 'WATER FLOW RATE(HEATING)[EMS](Kg/day)
41. H2OEMSTEMP = ActiveWorkbook.Worksheets("EMS").Cells(16, 4) 'WATER Temperature [HEATING][EMS](oC)
42. H2OEMSFRTEMPX1 = ActiveWorkbook.Worksheets("EMS").Cells(37, 11) 'WATER FLOW RATE(HEATING)[EMS](Kg/day)
43. H2OEMSFRXX = ActiveWorkbook.Worksheets("EMS").Cells(44, 11) 'WATER FLOW RATE(HEATING)[EMS](Kg/day)
44. 'SOFEC
45. H2OSOFEFCFR = ActiveWorkbook.Worksheets("SOFEC").Cells(14, 16) 'WATER FLOW RATE(HEATING BIOGAS)(Kg/day)
46. H2OSOFECTEMP = ActiveWorkbook.Worksheets("SOFEC").Cells(7, 16) 'WATER Temperature [HEATING][SOFEC](oC)
47. H2OHXSOFEFCR1 = ActiveWorkbook.Worksheets("SOFEC").Cells(27, 16) 'H2O flow rate from SOFEC Heat Exchanger 10 (kg/hr)
48. H2OSOFECTEMP1 = ActiveWorkbook.Worksheets("SOFEC").Cells(18, 16) 'WATER Temperature [HEATING][SOFEC](oC)

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49. '
50. '===== AIR FLOW RATE (Kg/say)  AND TEMPERATURE (oC) =====
51.   AIRSOFECFR = ActiveWorkbook.Worksheets("SOFEC").Cells(26, 16)  'AIR FLOW RATE From H-EXCHANGER [SOFEC](Kg/day)
52.   AIRSOFECTEMP = ActiveWorkbook.Worksheets("SOFEC").Cells(20, 16) 'AIR Temperature From H-EXCHANGER [SOFEC](oC)
53.   AIRSSASFR1 = ActiveWorkbook.Worksheets("SSAS").Cells(14, 16)  'AIR FLOW RATE From H-EXCHANGER-6 [SSAS](Kg/day)
54.   AIRSSASTEMP1 = ActiveWorkbook.Worksheets("SSAS").Cells(7, 16)  'AIR Temperature From H-EXCHANGER [SSAS](oC)
55.   AIRSSASFR2 = ActiveWorkbook.Worksheets("SSAS").Cells(27, 16)  'AIR FLOW RATE From H-EXCHANGER-7 [SSAS](Kg/day)
56.   AIRSSASTEMP2 = ActiveWorkbook.Worksheets("SSAS").Cells(20, 16) 'AIR Temperature From H-EXCHANGER [SSAS](oC)
57.   AIRSSASFR3 = ActiveWorkbook.Worksheets("SSAS").Cells(40, 16)  'AIR FLOW RATE From Condenser [SSAS](Kg/day)
58.   AIRSSASTEMP3 = ActiveWorkbook.Worksheets("SSAS").Cells(33, 16) 'AIR Temperature From Condenser [SSAS](oC)
59.   AIREMSFR4 = ActiveWorkbook.Worksheets("EMS").Cells(32, 11)    'AIR FLOW RATE From Condenser [EMS](Kg/day)
60.   AIREMSTEMP4 = ActiveWorkbook.Worksheets("EMS").Cells(24, 11)  'AIR Temperature From Condenser [EMS](oC)
61.   AIREMSTEMP4XC = ActiveWorkbook.Worksheets("ITM").Cells(11, 4)  'AIR Temperature From Condenser [EMS](oC)
62.   PRESSUREITM4XC = ActiveWorkbook.Worksheets("ITM").Cells(12, 4) 'AIR Temperature From Condenser [ITM](oC)
63.   SSOFEWCWAT1X = ActiveWorkbook.Worksheets("ITM").Cells(7, 11)   'AIR Temperature From Condenser [ITM](oC)
64.   SSOFEWCWAT1X445 = ActiveWorkbook.Worksheets("SOFEC").Cells(13, 4) 'AIR Temperature From Condenser [ITM](oC)
65. '
66. '=====
67.   Dim NC As Integer, NST As Integer
68.   H2FR = H2TOTALFR  'TOTAL H2 FLOW RATE AVAILABLE (kg/day)
69.   H2OUREATEMP = 25
70.   H2FR = H2TOTALFR  'H2 Flowrate (Kg/day)
71.   '
72.       INPUT DATA
73.   If H2FR <= 0 Then
74.       Cells(4, 7) = "<- Error"
75.       Cells(5, 7) = "Increase Ratio"
76.       Cells(6, 7) = "-> (N) In SSAS"
77.       Cells(7, 7) = "Cells(32,3)"
78.   End
79.   Else
80.       Cells(4, 7) = " "
81.       Cells(5, 7) = " "
82.       Cells(6, 7) = " "
83.       Cells(7, 7) = " "
84.   End If
85.   N2OUT = 0
86. 'Main Gases Side
87.   Cells(4, 4) = H2FR  'H2 Flowrate (Kg/day)
88.   Cells(5, 4) = O2FRITM 'O2 Flowrate (Kg/day)
89.   PIO = Cells(6, 4)  'Gas inlet Pressure (atm)
90.   Cells(7, 4) = TH2T  'H2 inlet Temperature (oC)
91.   Cells(8, 4) = T02  'O2 inlet Temperature (oC)
92. 'Cell Side
93.   O2TEMP = Cells(11, 4) 'AIR TEMPERATURE (oC)
94.   TC = Cells(13, 4)  'Cell Temperature (oC)
95.   PC = Cells(14, 4)  'Cell Pressure (atm)
96.   CICON1 = Cells(15, 4) 'Ionic conductivity (1/cm.ohm)
97.   ELECTH1 = Cells(16, 4) 'Electrolyte Thickness (mum)
98.   CCT = Cells(17, 4)  'Coefficient of Charge Transfer
99.   CAR = Cells(18, 4)  'Cell Area (cm^2)
100.  NCFST = Cells(19, 4) 'Number of Cells in series in Fuel Stack (N0)
101.  ECELLAPLV = Cells(20, 4) 'Applied Voltage (Volt)
102.  RCONV1 = Cells(21, 4)  'Required Conversion
103. '
104.  CONSTANT
105.  TCK = TC + 273
106.  O2TEMPK = T02 + 273
107.  TAIRK = O2TEMP + 273
108.  ELECTH = ELECTH1 / 10000 ' cm
109.  CICON = CICON1  'Ionic conductivity (1/m.ohm) meter
110.  RCONV = RCONV1 / 100
111.  FA = 96485 ' coulombs/mole
112.  R = 8.314 'J/(mol-K)
113.  H2MW = 2 'H2 Molecular Weight gm/mole
114.  O2MW = 32 'O2 Molecular Weight gm/mole
115.  H2OMW = 18 'H2O Molecular Weight gm/mole

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114. DELTAGO = 373740.7
115. PEF = 101.2 'Pre-exponential factor (kA/cm^2)
116. EACT = 120000 'Activation energy of electrochemical reaction (J/mol)
117. ' CELLS CONSTANT
118. AP = 101.2 'Pre-exponential factor (kA/cm2)
119. EACT = 120 * 10 ^ -3 'Activation energy of electrochemical reaction (J/mole)
120. BETA = 0.5 'Coefficient of charge transfer
121. NE = 2 'Number of electrons transferred
122. ALFA = -2870 'Temperature coefficient (K)
123. CT = 450 'Thermal capacity (kJ/K)
124. CT1 = 45
125. '=====
126. ' Chemical Calculations of FUEL CELL
127. '=====
128. 'Reaction Products -----> H2 + 1/2 O2 = H2O
129. H2USED = H2FR * RCONV
130. H2OUT = H2FR - H2USED 'H2 As INPUT (Kg/day)
131. ' O2 Needed FROM AIR
132. O2USED = (H2USED * O2MW) / (2 * H2MW) 'O2 Needed For the reaction
133. '..... Extra O2 Needed .....
134.
135. '<===== Cells(10, 4)
136. 'H2O OUT
137. H2SOFPCOUT = (H2USED * H2OMW) / H2MW 'H2O OUT (Kg/day)
138. 'Molar Flow Rate
139. H2MOLE = (H2USED * 1000) / (H2MW * 3600 * 24) 'H2 Molar Flow rate (mole H2/sec)
140. O2MOLE = (O2USED * 1000) / (O2MW * 3600 * 24) 'O2 Molar Flow rate (mole O2/sec)
141. H2OMOLE = (H2SOFPCOUT * 1000) / (H2MW * 3600 * 24) 'H2O Molar Flow rate (mole H2O/sec)
142. RAT = H2MOLE / O2MOLE
143. 'Partial Pressure at Anode
144. TOTMOLE = H2MOLE + H2OMOLE 'Total moles/sec at Anode
145. H2MOLFR = H2MOLE / TOTMOLE 'H2 mole fraction (%)
146. H2OMOLFR = H2OMOLE / TOTMOLE 'H2O mole fraction (%)
147. 'Partial Pressure at Cathode
148. O2MOLFR = O2MOLE / O2MOLE 'O2 mole fraction (%)
149. RAT = O2USED / H2FR
150. 'Partial Pressure
151. PPH2 = H2MOLFR * PC
152. PPO2 = O2MOLFR * PC
153. PPH2O = H2OMOLFR * PC
154. '..... Electrical Calculations .....
155. 'ENTHALPY DELTA-H
156. DELHH2O = ENTHALPY(TCK, R) '=====>H2O Enthalpy of Reaction (J/mole)
157. 'ENTROPY DELTA-S
158. DELSH2O = (ENTROPY(TCK, R)) '=>Entropy DELTA-S H2O OF Reaction (J/mole)
159. 'Gibbs Free Energy DELTA-G
160. DELGH2O = DELTAGO + DELHH2O - (TCK * DELSH2O) '=====>Gibbs Free Energy H2O OF Reaction (J/mole)
161. 'MAXIMUM Electrical Energy
162. ETAMAX = ((-DELGH2O / 1000) / (-DELHH2O / 1000)) * 100 ' Maximum (Efficiency) Electrical Enrgy available (ref:energies-06-05046/Page5052)
163. If ETAMAX > 100 Then
164. ETAMAX = 100
165. End If
166. 'Second Method of Calculation of E0 in function of Temperature
167. E01 = 1.2723 - 0.00027645 * TCK 'For Plotting
168. '-----
169. 'VOLTAGE.....REF ALL.FOGLER
170. E0 = -DELGH2O / (2 * FA) 'Reversible Maximum Voltage Generated (Volt) [OPEN CIRCUIT](ref:energies-06-05046/Page5052)
171. ' E01 = 1.2723 - (2.7645 * 10 ^ -4 ) * TCK 'Reference Voltage OPEN CIRCUIT (VOLT)at standard pressure(ref:energies-06-05046/Page5053)
172. ENERST = E0 + (R * TCK) / (2 * FA) * Logn(PPH2 * (PPO2) ^ 0.5 / PPH2O)
173. 'Area Surface Resistance
174. ASR = ELECTH / CICON 'ohms-cm^2
175. RINTB = (ELECTH) / (CAR * CICON) 'Ohm'
176. ICELLC = (ENERST - ECELLAPLV) / RINTB 'Amps'
177. 'Cell Current
178. ' ICELLC = (1.065 - ECELLAPLV) / RINTB 'Cell current amps

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179.   If ECELLAPLV >= 1.065 Then
180.     ECELLAPLV = 1
181.     Cells(20, 4) = ECELLAPLV
182.   End If
183. 'Cell Current Density
184.   ICELLCURDEN = ICELLC / CAR           'Cell current Density amp/cm^2
185. 'Loading Resistance
186.   RLOADB = ECELLAPLV / ICELLC
187. 'Ecell
188.   ECELL = ENERST - (RINTB * ICELLC)
189.   ICELLK = ENERST / (RLOADB + RINTB)
190.   POWRTY = (ICELLK * ECELLAPLV)
191. 'Reaction Rate
192. '..H2 and O2 Reaction Rates
193.   RH2 = ICELLC / (2 * FA)   'moles/s
194.   RO2 = ICELLC / (4 * FA)   'Moles/s
195. '..Flux of H2 and O2
196.   H2FLUX = RH2 / CAR   'H2 Flux moles/s.cm^2
197.   O2FLUX = RO2 / CAR   'O2 Flux moles/s.cm^2
198. 'Area Required
199.   AREARQ = H2MOLE / H2FLUX   'Required Cell AREA cm^2
200. 'Number of Cells
201.   NUMBCELL = AREARQ / CAR   'Number of Cells
202.   FUELTPOW = (POWRTY / (Abs(DELHH2O) * RH2)) * 100
203.   POWRTY = (ICELLK * ECELLAPLV * NUMBCELL) / (1000)
204.   Cells(41, 11) = POWRTY
205.   POWRTY = (ICELLK * ECELLAPLV * NUMBCELL) / (1000)
206.   POWRTYO = ((ICELLK * ECELLAPLV * NUMBCELL) - ((ICELLK) ^ (2) * RINUY * NUMBCELL)) / (100000)
207.   Cells(23, 11) = FUELTPOW
208. 'Total Current
209.   TOTICELLCUR = ICELLC   'Total Current (amps)
210. 'Total Current Density
211.   TOTCURDEN = ICELLCURDEN * NUMBCELL   'Total Current Density (amps/cm^2)
212. 'Number of Stack
213.   NST = NUMBCELL / NCFST
214.   If NST <= 0 Then
215.     NST = 1
216.   Else
217.     End If
218. ' Resistive Load
219.   RLOADB = ECELLAPLV / ICELLC 'ohms
220. ' Maximum Efficiency
221.   EFFMAX = DELGH2O / DELHH2O
222. 'Power Efficiency
223.   PEFF = ((ECELLAPLV / E0) * EFFMAX) * 100
224. '=====  

225. ' Ref: Energies 2013, 6, 5046-5068; doi:10.3390/en6105046
226. 'Maximum voltage that could be generated E
227.   EVMAX = -DELGH2O / (2 * FA) 'Maximum voltage that could be generated [E](Volt)
228. 'Exchange Current Density io [Ref: energies-06-05046-Page-8]
229.   IO1 = PEF * Exp(EACT / (R * TCK))           '[Exchange Current Density io (KA/cn^2)]: for A ->/ 1000=> Amp
230.   IO = (PEF * Exp(EACT / (R * TCK))) / 1000 '[Exchange Current Density io (A/cn^2)
231. 'Limiting Current Density
232.   IL = 2 * FA * H2FLUX   'Limiting Current Density (Amp/cm^2)
233. '.... Activation Energy ETA [Ref: energies-06-05046-Page-8] .....
234. ' ..... Algorithm to find i => II and Tau-ACTIVATION .....
235. 'Slope of 1/sinh(i/(2*i0)) to find the i=IC intercept at 1/sinh =0
236.   I2 = 0.1
237. 1 XX = I2 / (2 * IO)
238.   SINH1 = Logn(SINHINV(XX))
239.   TEST = SINH1
240.   If (TEST) >= 0.0001 Then
241.     GoTo 2
242.   Else
243.     I2 = I2 + 0.1

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244.   GoTo 1
245. 2   End If
246.   IC = I2           'Current Density A/m^2
247.   IC1 = IC * 1000  'Current Density mA/m^2
248.   IC2 = IC / 10000 'Current Density A/cm^2
249.   XX = IC2 / (2 * IO)
250.   SINH1 = SINHMV(XX)
251.   ETAACT = ((R * TCK) / (BETA * FA)) * SINH1
252. 'Concentration Energy ETACON [Ref: energies-06-05046-Page-8
253.   ETACON = ((R * TCK) / (2 * FA)) * Logn(1 - IC2 / IL)
254. 'Ohmic Energy
255.   TOHMIC = (ICELLK * CAR) * (RINTB + RLOADB) / (10000) 'IC ICCELLCDB
256. 'Total Voltage
257.   VTOT = (NUMBCELL * (Abs(ENERST) - (ETAACT) - Abs(ETACON)) - (TOHMIC))
258. 'SUM of IONIC + ELECTRONIC
259.   SUMIONCON = (ICVSZ)           'Summ of Conductivites (S/cm)= "1/ohm.cm"
260.   POWERTOT = ((TOTICELLCUR * VTOT) / (1000)) 'TOTAL POWER(KW)'
261. 'O2 OUT
262.   O2OUT = O2FRITM - O2USEDQ
263. '===== Error Trapping =====
264. 'Cell Area
265.   If AREARQ < CAR Then
266.     Cells(10, 7) = "Error ->"
267.     Cells(11, 7) = "Decrease"
268.     Cells(12, 7) = "Cell Area:"
269.     Cells(13, 7) = "Cell (18,D)"
270.     Cells(10, 11) = "Error"
271.   End
272.   Else
273.     Cells(10, 7) = ""
274.     Cells(11, 7) = ""
275.     Cells(12, 7) = ""
276.     Cells(13, 7) = ""
277.     Cells(10, 11) = ""
278.   End If
279. '=====
280. '..... DATA OUTPUT .....
281.   Cells(5, 11) = H2OUT           'H2 OUT (Kg/day)
282.   Cells(6, 11) = H2OSOFCOUT      'H2O OUT (Kg/day)
283.   Cells(7, 11) = O2USED          'O2 USED(Kg/day)
284.   Cells(8, 11) = O2OUT           'O2 OUT (Kg/day)
285.   Cells(10, 11) = AREARQ         'Total Cells Area (m^2)
286.   Cells(11, 11) = NUMBCELL       'Total Number of Cells
287.   Cells(12, 11) = EFFMAX * 100  'Maximum Efficiency %
288.   Cells(13, 11) = NST           'Number of Stacks
289.   Cells(14, 11) = TOTICELLCUR    'Total Current (A)
290.   Cells(15, 11) = O2FLUX         'Oxygen Flux (moles/s.cm^2)
291.   Cells(16, 11) = VTOT           'Total Voltage(Volt)
292.   Cells(17, 11) = TOTCURDEN      'Exchange Current Density (A/cm^2)
293.   Cells(18, 11) = ICELLCURDEN    'Cell Current(mA/cm^2)
294.   Cells(19, 11) = ENERST         'ENERST (Volt)
295.   Cells(20, 11) = E0             'Open Circuit Voltage (Volt)
296.   Cells(21, 11) = TC             'Steam Out at T
297.   Cells(22, 11) = POWERTOT       'TOTAL POWER OUT OF SOFC (KW)'
298.   'Cells(23, 11) = RESISTOT      'RESISTANCY OF THE SYSTEM (OHM)'
299.   Cells(40, 4) = SUMIONCON       'Conductivity S/m
300. '           Plot of Temperature VS Open Circuit
301.   TT = 10
302.   For I = 0 To 10
303.     TTK = TT + 273
304.     E01 = 1.2723 - (2.7645 * 10 ^ -4) * TTK
305.     Cells(100 + I, 1) = TT
306.     Cells(100 + I, 2) = E01
307.     TT = TT + 100
308.   Next I

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309. '=====  

310. '=====  

311. '=====  

312. '          WATER BALANCE  

313. '=====  

314. '-----TOTAL WATER PRODUCED  

315.   H2OFRTOT = H2OSOFECFRROUT + H2OSOFECOUT 'Total H2O Produced (Kg/day)  

316. '...Water Available  

317.   H2ONEEDED = H2OSOFECFRMB + H2OUREAFR - H2OFRTOT '***** H2O NEEDED for the system at Steady State(Kg/day)*****  

318. '...Water Balance of Heat Exchangers  

319. 'Mixing Tank  

320.   H2OMIXTFR = HXH2OMIXTANK 'WATER FLOW RATE needed FOR MIXING TANK (HEATING) (kg/day)  

321.   H2OMIXTANTEMP = HXH2OMIXTTEMP 'WATER Temperature [HEATING](oC)  

322. 'ITM  

323.   H2OITMFR = H2OITMFR 'WATER FLOW RATE needed FOR ITM(HEATING)(kg/day)  

324.   H2OITMTEMP = H2OITMTEMP 'WATER Temperature [HEATING](oC)  

325. 'EMS  

326.   H2OEMSFR = H2OEMSFR 'WATER FLOW RATE needed FOR EMS(HEATING)(kg/day)  

327.   H2OEMSTEMP = H2OEMSTEMP 'WATER Temperature [HEATING](oC)  

328. 'SOFEC  

329.   H2OSOFECFR = H2OSOFECFR 'WATER FLOW RATE needed FOR SOFEC(HEATING)(kg/day)  

330.   H2OSOFECTEMP = H2OSOFECTEMP 'WATER Temperature [HEATING](oC)  

331.   H2OSOFECFR1 = H2OSOFECFR1 'WATER FLOW RATE needed FOR SOFEC(HEATING)(kg/day)  

332.   H2OSOFECTEMP1 = H2OSOFECTEMP1 'WATER Temperature [HEATING](oC)  

333.   Cells(7, 16) = HXH2OMIXTTEMPH2O  

334. '=====  

335. '          H2O RECYCLING  

336. '=====  

337. 'Total Water needed for Heat Exchangers  

338.   H2OHEXRECY = H2OITMFR + H2OEMSFR + H2OSOFECFR + H2OSOFECFR1 + H2OEMSFRXX + H2OMIXTFR + (H2OSOFECFRIN56 - H2OSOFECFRROUT) 'H2O needed for rec  

   ycling ITM + EMS + SOFEC + Mixing Tank (Kg/day)  

339.   H2OFLOWX1 = H2OHEXRECY  

340. 'Temperature of this Mixed Water after Steady State  

341.   H2ORECYTEMP = (H2OITMFR * H2OITMTEMP + H2OEMSFR * H2OEMSTEMP + H2OSOFECFR * H2OSOFECTEMP + H2OEMSFRXX * H2OEMSFRTEMPX1 + H2OSOFECFR1 * H2OS  

   OFECTEMP1 + H2OMIXTFR * H2OMIXTANTEMP + (H2OSOFECFRIN56 - H2OSOFECFRROUT) * SSOFECHAT1X445) / H2OHEXRECY  

342. '=====  

343. ' HEAT EXCHANGER INSIDE OF THE HOT BOX FOR RECYCLING STEAM with EXTRA H2O from OUTSIDE  

344. '=====  

345.   H2OFLOWX1 = H2OHEXRECY  

346.   TL = Cells(29, 11) 'Tube Length (m)  

347.   TOD = Cells(30, 11) 'Tube Outside Diameter (m)  

348.   TH1 = TCK 'O2 Temperature IN (oK)  

349.   TC1 = H2ORECYTEMP + 273 'Recycling Temperature IN (oK)  

350.   TC2 = 920 + 273 'Recycling Temperature OUT (oK)  

351.   'H2OTEMP = TC1 'Recycling Temperature IN (oK)  

352. 'Recycled  

353.   SCRECYCLED = WATERSPECIFICHEAT(H2OTEMP) 'H2O Recycled Specific Heat (kJ/kg.K)  

354.   CRECYCLED = ((H2OHEXRECY / 24) / 3600) * SCRECYCLED 'H2O Recycled Heat (kJ/kg.K)  

355.   QRECYCLED = CRECYCLED * (TC2 - TC1) 'Q-Recycled Water (KW)  

356. 'Steam NEEDED  

357.   H2OTEMP = TH1  

358.   SCSTEAM = WATERSPECIFICHEAT(H2OTEMP) 'WATER SPECIFIC HEAT kJ/Kg.K in oK 'AIRSPECIFICHEAT(AIRTK) 'AIRSPECIFICHEAT kJ/Kg.K T=oK 'OXYGENSPECIFICHE  

   AT(O2TEMP)  

359. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.  

360.   FLAG = 1  

361.   U = 0.02  

362. '  

363.   CCOLD = CRECYCLED: Q = QRECYCLED: SCHOT = SCSTEAM: SCCOLD = SCRECYCLED  

364.   Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN  

   GER  

365. 'GAS Turbine  

366. 'Cells  

367.   STEAMFR = HFR  

368.   Cells(25, 11) = H2ORECYTEMP 'Recycling Temperature IN (oC)  

369.   Cells(26, 11) = TC2 - 273 'Recycling Temperature OUT (oC)

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370. Cells(27, 11) = TH1 - 273 'Steam Temperature IN (oC)
371. Cells(28, 11) = TH2 - 273 'Steam Temperature OUT (oC)
372. Cells(31, 11) = NTU 'Number of Tubes
373. Cells(32, 11) = AREAHEX 'Exchanger Area (m^2)
374. Cells(33, 11) = EPS * 100 'Effectiveness
375. Cells(34, 11) = QEFF 'EFFECTIVE Heat Transfer Rate Q (kW)
376. Cells(35, 11) = STEAMFR 'Steam Flow Rate Required(Kg/DAY)
377. '=====
378. '=====
379. 'WATER BALANCE OF THE WHOLE SYSTEM
380. 'Cells AOUT At Steady State
381. Cells(4, 16) = H2OSOFECFRMB 'WATER FLOW RATE IN(for SOFEC membrane)(Kg/day)
382. Cells(4, 17) = H2OSOFECFRIN - SSOFEWAT1X 'WATER FLOW RATE OUT(for SOFEC membrane)(Kg/day)
383. Cells(4, 18) = H2OSOFECTEMP 'WATER TEMPERATURE(for membrane)(oC)
384. Cells(5, 16) = H2OSOFECFRIN 'EXTRA WATER NEEDED FLOW RATE (for SOFEC membrane)(Kg/day)
385. Cells(5, 18) = H2OSOFECTEMP 'EXTRA H2O Needed Temperature SOFEC ((oC)
386. Cells(6, 17) = H2OSOFCOUT 'WATER FLOW RATE(from SOFC)(Kg/day)
387. Cells(6, 18) = TC 'WATER TEMPERATURE(from SOFC)(oC)
388. Cells(7, 17) = H2OUREAFR 'WATER FLOW RATE(from UREA)Kg/day)for DARK
389. Cells(7, 18) = H2OUREATEMP 'WATER TEMPERATURE(from UREA}(oC)
390. Cells(10, 16) = H2OMIXTFR 'WATER FLOW RATE IN for MIXING-TANK H-EXCHANGER (Kg/day)
391. Cells(10, 17) = H2OMIXTFR 'WATER FLOW RATE OUT for MIXING-TANK H-EXCHANGER (Kg/day)
392. Cells(10, 18) = H2OMIXTANTEMP 'WATER Temperature (MIXING-TANK) H-EXCHANGER (oC)
393. Cells(11, 16) = H2OITMFR 'WATER FLOW RATE IN for ITM H-EXCHANGER (Kg/day)
394. Cells(11, 17) = H2OITMFR 'WATER FLOW RATE OUT for ITM H-EXCHANGER (Kg/day)
395. Cells(11, 18) = H2OITMTEMP 'WATER Temperature (ITM) H-EXCHANGER (oC)
396. Cells(12, 16) = H2OEMSFR 'WATER FLOW RATE IN for EMS H-EXCHANGER (Kg/day)
397. Cells(12, 17) = H2OEMSFR 'WATER FLOW RATE OUT for EMS H-EXCHANGER (Kg/day)
398. Cells(12, 18) = H2OEMSTEMP 'WATER Temperature (EMS) H-EXCHANGER (oC)
399. Cells(13, 16) = H2OSOFECFR 'WATER FLOW RATE IN for SOFEC H-EXCHANGER (Kg/day)
400. Cells(13, 17) = H2OSOFECFR 'WATER FLOW RATE OUT for SOFEC H-EXCHANGER (Kg/day)
401. Cells(13, 18) = H2OSOFECTEMP 'WATER Temperature for SOFEC H-EXCHANGER ((oC)
402. Cells(14, 16) = H2OHSOFECFR1 'WATER Temperature for SOFEC H-EXCHANGER 10 ((oC)H2OHSOFECFR1
403. Cells(14, 17) = H2OHSOFECFR1 'WATER Temperature for SOFEC H-EXCHANGER 10 ((oC)H2OHSOFECFR1
404. Cells(14, 18) = H2OSOFECTEMP1 'WATER Temperature for SOFEC H-EXCHANGER 10 ((oC)H2OHSOFECFR1
405. Cells(15, 18) = H2OHEXRECY 'WATER FLOW RATE of MIXED IN (Kg/day)
406. Cells(15, 17) = H2OHEXRECY 'Total Recycled OUT(Kg/day)
407. Cells(15, 18) = H2ORECYTEMP 'WATER Recycled TEMPERATURE(from SOFC BOX)(oC)
408. '=====
409. ' STEAM COMPRESSOR FOR RECYCLING
410. '=====
411. 'DATA IN
412. RH20 = 461.52 'Steam Constant kJ/Kg.K
413. RHOH20 = 0.59 'Steam Density (Kg/m3)
414. COMPIP = 1 'Cells(26, 4) 'Compressor Inlet Pressure (Atm.)
415. COMPOP = 1.2 'Cells(27, 4) 'Compressor Outlet Pressure (Atm.)
416. COMIT = 920 'Cells(28, 4) 'Steam Temperature IN (oC)
417. COMETREFF = Cells(29, 4) 'Compressor Entropy Efficiency (%)
418. MOTOREFF1 = Cells(34, 4) 'Motor Efficiency Single Phase (%)
419. SPHASVOL = Cells(35, 4) 'Single Phase Voltage (Volt)
420. MOTOREFF3 = Cells(37, 4) 'Motor Efficiency 3-Phase (%)
421. THREPASEVOL = Cells(38, 4) '3-Phase Voltage (Volt)
422. 'Calculations
423. TOTALSTEAM = H2OHEXRECY + STEAMFR + FDR 'KG/day
424. MOLESTEAM = TOTALSTEAM / 18
425. TOTALSTEAMM = (TOTALSTEAM / 24) / 60 'KG/min
426. H2OTEMP = TC + 273
427. CCPSTEAM = WATERSPECIFICHEAT(H2OTEMP) 'kJ/Kg.K
428. CCVSTEAM = 1.822 'kJ/Kg.K
429. GAMMA = CCPSTEAM / CCVSTEAM
430. ENTCC = RH20 * RHOH20 'Entropy Change Constant (J/K.M^3)
431. H2OVOL = (TOTALSTEAMM / RHOH20) * 1000 'Steam Volume Lt/min
432. GASTEMPC = COMIT: GASVOL = H2OVOL
433. OUTADIATEMP = ((COMIT + 273) * ((COMPOP / COMPIP) ^ ((1.327 - 1) / 1.327))) - 273 ' OUTLET ADIABATIC TEMPERATURE
434. OUTADIATEMPX = OUTADIATEMP + 273

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435.   DRMOTWATT = (OUTADIATEMPX - (GASTEMPC + 273)) * CCPSTEAM * (TOTALSTEAM / 86400) / 0.75 'KW
436. 'COMPRESSOR OUTPUT
437.   Cells(24, 4) = TOTALSTEAM
438.   Cells(25, 4) = H2OVOL
439.   Cells(31, 4) = OUTADIATEMP
440.   Cells(32, 4) = DRMOTWATT
441.   Cells(33, 4) = DRMOTHP
442.   Cells(36, 4) = CURRENT1
443.   Cells(39, 4) = CURRENT3
444. '=====
445. '           HEAT_EXCHANGER IN THE HOT BOX FOR HEATING THE H2
446. '=====
447. 'Steam Side
448.   T1H = TCK + 0.01 'Steam Temperature IN (oK)
449.   'T2H=? 'Steam Temperature OUT (oK)
450.   H2OTEMP = T1H
451.   CCSTEAM = WATERSPECIFICHEAT(H2OTEMP) 'WATER SPECIFIC HEAT kJ/Kg.K in oK
452.   'CSTEAM=?
453. 'H2 Side
454.   Cells(42, 4) = TH2T 'H2 Temperature (oC)
455.   T1C = TH2T + 273 'H2 Temperature IN (K)
456.   T2C = TC + 273 'H2 Temperature OUT (K)
457.   H2TK = T1C
458.   CCH2 = HYDROGENSPECHEAT(H2TK) 'T=oK
459.   CH2 = ((H2TOTALFR / 24) / 3600) * CCH2 'H2 Recycled Heat (kJ/kg.K)
460.   QH2 = CH2 * (T2C - T1C) 'Q-H2 (KW)
461. 'Tubes Properties
462.   TL = Cells(46, 4) 'Tube Length (m)
463.   TOD = Cells(47, 4) 'Tube Outside Diameter (m)
464. 'Calculations
465.   STEAMOUT = 1
466. 30 CSTEAM = ((STEAMOUT / 24) / 3600) * CCSTEAM
467.   T2H = T1H - (QH2 / CSTEAM)
468.   If T2H >= T1C Then
469.     GoTo 40
470.   Else
471.     STEAMOUT = STEAMOUT + 0.1
472.     GoTo 30
473. 40 End If
474.   QSTEAM = CSTEAM * (T1H - T2H)
475.   DELTAA = T1H - T2C
476.   DELTAB = T2H - T1C
477.   LMTD = (DELTAA - DELTAB) / Logn(DELTAA / DELTAB) ' (K)
478.   U = 0.05
479.   K = 1
480.   CCOLD = CH2: CHOT = CSTEAM: QFLUID = QSTEAM
481. Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN
GER
482. 'DATA OUT
483.   Cells(42, 4) = T1C - 273 'H2 Temperature IN (oC)
484.   Cells(43, 4) = T1H - 273 'H2 Temperature OUT (oC)
485.   Cells(44, 4) = T2C - 273 'H2 Temperature OUT (oC)
486.   Cells(45, 4) = T2H - 273 'Steam Temperature OUT (oC)
487.   Cells(48, 4) = NELEM 'N0 of TUBES
488.   Cells(49, 4) = AEXCH 'Exchanger Area (m^2)
489.   Cells(50, 4) = EPS * 100 'Effectiveness (%)
490.   Cells(51, 4) = QEFF 'Heat Transfer (kW)
491.   H2ONOTREC = H2OSOFCOUT - STEAMOUT
492.   Cells(52, 4) = STEAMOUT 'Steam Recycled (kg/hr)
493.   Cells(53, 4) = H2ONOTREC 'Steam Recycled (kg/hr)
494.   FDR = STEAMOUT - H2ONOTREC
495. 'Steam MIXED TEMPERATURE FOR Steam TURBINE
496.   H2TOTALFLR = H2OSOFCOUT 'Total Oxygen
497.   H2OSTEAMTEMP = (H2ONOTREC * TC + STEAMOUT * (T2H - 273)) / H2OSOFCOUT
498. '=====

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499. ' STEAM COMPRESSOR-TURBINE
500. '-----
501. ' TOTAL WATER AVAILABLE FOR Steam Turbine
502. '...Steam
503. H2OSTEAM = H2OSOFCCOUT '+ H2OSOFCCOUT2 'Steam flow rate for Turbine (Kg/day)
504. H2OSTEAMTEMP = H2OSTEAMTEMP = (H2ONOTREC * TC + STEAMOUT * (T2H - 273)) / H2OSOFCCOUT 'Steam Temperature (oC)
505. 'In oK
506. H2OSTEAMTEMP = TC + 273 'Steam at Fuel Cell Temperature (oK)
507. '...Recycled Stream
508. H2ORECSS = H2OHEXRECY 'Total H2O recycled to SOFC (Kg/hr)
509. H2OITMFR = H2OITMFR 'Water used for ITM Heat-Exchanger (Kg/hr)
510. H2OTOTTURBINEFR = H2OSTEAM ' H2O Flow Rate for Turbine at STEADY STATE no recycling(Kg/day)
511. 'H2O TO COMPRESSOR and TURBINE SIDE
512. 'INPUT
513. RHOH2O = 0.59 'Steam Density (Kg/m3)
514. RH2O = 461.52 ' J/Kg.K
515. CPS = WATERSPECIFICHEAT(H2OTEMP) 'Steam specific Heat (kJ/Kg.K)
516. CVS = 1.822 'kJ/Kg.K
517. GAMMA = 1.22 'CPS / CVS
518. STEAMBN123 = STEAMFR + H2ONOTREC
519. STEAMBNXX = (STEAMFR * (H2ORECYTEMP)) + (H2OSOFCCOUT * TC)
520. STEAMBN = STEAMBNXX / STEAMBN123
521. STEAMFRSEC = STEAMBN123 / 24 / 3600 'Steam Flow Rate (KG/sec)
522. STEAMVOL = ((STEAMBN123 / 24 / 60) / RHOH2O) * 1000 'Steam Volume (Lt/min)
523. TC1 = H2OSTEAMTEMP + 273 'Steam Temperature IN (oC)
524. PC1 = PC 'Steam Pressure IN (atm) (Compressor)
525. ENTCC = RH2O * RHOH2O 'Entropy Change Constant (J/K.M^3)
526. 'DATA IN
527. Cells(18, 16) = STEAMBN123 'Compressor Steam Flow rate (Kg/day)
528. Cells(19, 16) = STEAMVOL 'Compressor Steam Volume (Lt/min)
529. Cells(20, 16) = TC 'Compressor Steam Temperature IN (oC)
530. Cells(21, 16) = PC1 'Compressor Steam Pressure IN (atm)(
531. PC2 = Cells(22, 16) 'Compressor Steam Pressure OUT(atm)
532. Cells(23, 16) = COMETREFF 'Compressor Entropy Efficiency (%)
533. MOTOREFF1 = Cells(24, 16) 'Motor Efficiency Single Phase (%)
534. SPHASVOL = Cells(25, 16) 'Single Phase Voltage (Volt)
535. MOTOREFF3 = Cells(26, 16) 'Motor Efficiency 3-Phase (%)
536. THREPASEVOL = Cells(27, 16) '3-Phase Voltage (Volt)
537. ENTCC = RH2O * RHOH2O 'Entropy Change Constant (J/K.M^3)
538. 'COMPRESSOR DATA OUT
539. GASTEMPC = TC + 273: COMPIP = PC1: COMPOP = PC2: GASVOL = STEAMVOL
540. OUTADIATEMP = ((STEAMBN + 273) * ((PC2 / COMPIP) ^ (0.2464))) - 273 ' OUTLET ADIABATIC TEMPERATURE
541. OUTADIATEMPX = OUTADIATEMP + 273
542. DRMOTWATT = ((OUTADIATEMPX - (TC + 273)) * CPS * (STEAMBN123 / 86400)) / 0.75 'KW
543. Call COMPRESSOR(GASTEMPC, COMPOP, COMPIP, GAMMA, GASVOL, OUTADIATEMP, COMETREFF, WATT, ENTCC, DRMOTWATT, DRMOTHP, MOTOREFF1, MOTOREFF3, SPH
ASVOL, THREPASEVOL, CURRENT1, CURRENT3)
544. Cells(28, 16) = DRMOTWATT 'KW
545. Cells(29, 16) = CURRENT3 'AMP
546. 'TURBINE DATA IN
547. TP2 = PC2
548. TTI1 = OUTADIATEMPX 'TURBINE TEMPERATUR IN TO TURBINE (oC)
549. PT1 = PC2 'TURBINE Steam Pressure IN(atm)
550. TT1 = TTI1 + 273 'TURBINE TEMPERATUR IN TO TURBINE (K)
551. Cells(31, 16) = OUTADIATEMP '- TC 'STEAM TEMPERATUR IN TO TURBINE (K)
552. ISENEFF = Cells(32, 16) 'ISENTROPIC EFFICIENCY (%)
553. Cells(33, 16) = TP2 'TURBINE Steam Pressure IN(atm)
554. PT2 = Cells(34, 16) 'TURBINE Steam Pressure OUT(atm)
555. 'CALCULATIONS
556. EG = (1 - GAMMA) / GAMMA
557. RP = PC2 / PC1
558. CYCLEFF = (RP) ^ EG 'Cycle Efficiency
559. EFFE = CYCLEFF * 100
560. TT2 = ((STEAMBN + 273) * ((RP) ^ -EG)) 'Exit TURBINR Temperature (K)
561. ACTEMPCHAN = (STEAMBN + 273) - TT2
562. POWET = STEAMFRSEC * CPS * ACTEMPCHAN

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563. POWER1X = POWET * CYCLEFF
564. Cells(35, 16) = TT2 - 273 'TEMPERATURE OUT of TURBINE (oC)
565. Cells(36, 16) = -POWER1X 'kw
566. '=====
567. ' O2 + Air COMPRESSOR-TURBINE
568. '=====
569. 'Total Gas kg/day
570. TOTGAS = O2FRITM - O2USED 'O2OUT 'Total Gas to Compressor (kg/day)
571. 'AIR Flow Rate
572. TC1 = AIREMSTEMP4XC 'TC - 100
573. RAIR = 0.287 'kJ/kg.K)
574. CVAIR = 0.718 '(kJ/kg.K)
575. TOTAIR = TOTGAS 'Air from Total O2 Nedded for the Cell= O2 Available
576. AIRTK = TC1 + 273
577. CPAIR = AIRSPECFICHEAT(AIRTK) 'AIRSPECFICHEAT kJ/Kg.K T=oK
578. AIRINFR = TOTAIR / 24 / 60 'Air Flow Rate IN (Kg/min)
579. AIRINFRSEC = TOTAIR / 24 / 3600 'Air Flow Rate IN (Kg/sec)
580. AIRTEMP = TC1
581. RHOAIR = AIRDENSITY(AIRTEMP) 'Air Density(Kg/m^3) oC
582. AIRVOLR = (AIRINFR * 1000) / RHOAIR 'Air Volumetric Flow Rate (L/min)
583. GASVOL = AIRVOLR
584. GAMMA = 1.4 'CPAIR / CVAIR
585. 'DATA IN
586. Cells(39, 16) = TOTAIR 'Gas Flow Rate IN (Kg/min)
587. Cells(40, 16) = AIRVOLR 'Gas Volumetric Flow Rate (L/min)
588. Cells(41, 16) = TC1 'Gas Temperature TC1 in (oC)
589. Cells(42, 16) = PC 'Gas Pressure in (atm)
590. GASPOUT = Cells(43, 16) 'Gas Pressure OUT (atm)
591. COMETREFF = Cells(44, 16) 'COMPRESSOR ENTROPY EFFICIENCY (%)
592. MOTOREFF1 = Cells(45, 16) 'Motor single phase Efficiency (%)
593. SPHASVOL = Cells(46, 16) 'Single Phase Voltage (Volt)
594. MOTOREFF3 = Cells(47, 16) 'Motor Efficiency 3-Phase (%)
595. THREPADEVOL = Cells(48, 16) '3-Phase Voltage (Volt)
596. ENTCC = RAIR * RHOAIR 'Entropy Change Constant (J/K.M^3)
597. 'COMPRESSOR DATA OUT
598. GASTEMPC = 1000 + 273: COMPIP = PC: COMPOP = GASPOUT
599. OUTADIATEMP = ((GASTEMPC) * ((GASPOUT / PRESSUREITM4XC) ^ (0.2464))) - 273 ' OUTLET ADIABATIC TEMPERATURE
600. OUTADIATEMPX = OUTADIATEMP + 273
601. DRMOTWATT = ((OUTADIATEMPX - (1000 + 273)) * CPAIR * (TOTAIR / 86400)) / 0.75 'KW
602. Call COMPRESSOR(GASTEMPC, COMPOP, COMPIP, GAMMA, GASVOL, OUTADIATEMP, COMETREFF, WATT, ENTCC, DRMOTWATT, DRMOTHP, MOTOREFF1, MOTOREFF3, SPH
ASVOL, THREPADEVOL, CURRENT1, CURRENT3)
603. Cells(49, 16) = DRMOTWATT 'KW
604. Cells(50, 16) = CURRENT3 'AMP
605. 'TURBINE DATA IN
606. Cells(52, 16) = OUTADIATEMP
607. 'Calculations
608. RP = 10
609. EG = (1 - GAMMA) / GAMMA
610. RP = GASPOUT
611. CYCLEFF = 1 - (RP) ^ EG 'Cycle Efficiency
612. EFFE = CYCLEFF * 100
613. TT2 = ((1000 + 273) * ((RP) ^ -EG)) 'Exit TURBINR Temperature (K)
614. ACTEMPCHAN = (1000 + 273) - TT2
615. POWET = (TOTGAS / 86400) * CPAIR * ACTEMPCHAN
616. POWER1 = POWET * CYCLEFF
617. Cells(57, 16) = -POWER1
618.
619. '=====
620. ' HEAT LOSS
621. '=====
622. 'INPUT HEAT
623. '...H2
624. H2TK = TCK
625. H2FRS = (H2FR / 24) / 3600 'H2 FLOW RATE (kg/sec)
626. CPH2 = HYDROGENSPECHEAT(H2TK) 'H2 Specific Heat (kJ/Kg.K T=oK)

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627. QH2IN = H2FRS * CPH2 * TCK 'Heat to H2 (kJ/sec)
628. '...O2
629. O2TEMP = T02 + 273
630. O2FRINS = (O2FRITM / 24) / 3600 'O2 FLOW RATE (kg/sec)
631. CPO2 = OXYGENSPECIFICHEAT(O2TEMP) 'O2 Specific Heat (kJ/Kg.K) T=oK
632. QO2IN = O2FRINS * CPO2 * O2TEMP 'Heat to O2 (kJ/sec)
633. '...Total Heat IN
634. QTOTIN = QH2IN + QO2IN 'Total Heat IN (kJ/sec)
635. 'OUTPUT HEAT
636. '...STEAM
637. H2OTEMP = TCK
638. H2OFRS = (H2OSOFOUT / 24) / 3600 'WATER FLOW RATE (kg/sec)
639. CPH2O = WATERSPECIFICHEAT(H2OTEMP) 'WATER SPECIFIC HEAT kJ/Kg.K in oK
640. QH2OOUT = H2OFRS * CPH2O * TCK 'Heat from Steam (kJ/sec)
641. '...O2
642. TCK = (O2TEMP + 25) / 2
643. O2FRS = (O2OUT / 24) / 3600 'O2 FLOW RATE (kg/sec)
644. CPO2 = OXYGENSPECIFICHEAT(O2TEMP) 'O2 Specific Heat (kJ/Kg.K) T=oK
645. QO2OUT = O2FRS * CPO2 * TCK 'Heat From O2 (kJ/sec)
646. '...Total Heat OUT
647. QTOTOUT = QH2OOUT + QO2OUT + POWRTY / 86400 'Total Heat Out (kJ/sec)
648. 'Heat Loss
649. QLOSS = QTOTIN - QTOTOUT 'Total Heat Loss (kJ/sec)or kW
650. 'Cell OUT
651. Cells(38, 11) = QTOTIN 'Total Heat IN (kW)
652. Cells(39, 11) = QO2OUT 'Total Heat Out (kW)
653. Cells(40, 11) = QLOSS 'Total Heat Loss (kW)
654. ss = ss
655. '=====
656. End Sub
657. Private Function Logn(X)
658. Logn = Log(X) / Log(2.718282)
659. End Function
660. Private Static Function SINHINV(XX)
661. SINHINV = Logn(XX + ((X ^ 2 + 1) ^ 0.5))
662. End Function
663. Private Static Function ENTHALPY(TCK, R) 'H2O Enthalpy of Steam T=K, J/mol
664. A1 = 2.717633: A2 = 2.9451374 * 10 ^ -3: A3 = -8.0224374 * 10 ^ -7: A4 = 1.0226682 * 10 ^ -10
665. A5 = -4.8472145 * 10 ^ -15: A6 = -2.9905826 * 10 ^ 4
666. ENTHALPY = ((A1 + (A2 / 2) * TCK + (A3 / 3) * TCK ^ 2 + (A4 / 4) * TCK ^ 3 + (A5 / 5) * TCK ^ 4 + A6 / TCK) * R * TCK) * 1.1849
667. End Function
668. Private Static Function ENTROPY(TCK, R) 'H2O Entropy of Steam T=K, J/mol
669. A1 = 2.717633: A2 = 2.9451374 * 10 ^ -3: A3 = -8.0224374 * 10 ^ -7: A4 = 1.0226682 * 10 ^ -10
670. A5 = -4.8472145 * 10 ^ -15: A7 = 6.6305671
671. ENTROPY = (((A1 * Logn(TCK) + A2 * TCK + (A3 / 2) * TCK ^ 2 + (A4 / 3) * TCK ^ 3 + (A5 / 4) * TCK ^ 4 + A7) * R))
672. End Function
673. Private Static Function WATERSPECIFICHEAT(H2OTEMP) 'WATER SPECIFIC HEAT kJ/Kg.K in oK
674. WATERSPECIFICHEAT = 1.224986 + 0.0014072339 * H2OTEMP - 0.00000039722778 * H2OTEMP ^ 2 + 5.3431749E-11 * H2OTEMP ^ 3 + -2.7473115E-
15 * H2OTEMP ^ 4
675. End Function
676. Private Static Function AIRSPECIFICHEAT(AIRTK) 'AIRSPECIFICHEAT kJ/Kg.K T=oK
677. TA = 1.0828694: TB = -0.00063119116: TC = 0.0000016253087: TD = -1.3949526E-09: TE = 5.3826153E-13: TF = -7.9021928E-17
678. AIRSPECIFICHEAT = TA + TB * AIRTK + TC * AIRTK ^ 2 + TD * AIRTK ^ 3 + TE * AIRTK ^ 4 + TF * AIRTK ^ 5
679. End Function
680. Private Static Function OXYGENSPECIFICHEAT(O2TEMP) ' kJ/Kg.K T=oK
681. A = 0.83001979: B = 0.00034795895: C = -0.00000088793629: D = -1.9960197E-11: E = 1.654545E-14: F = -3.2117954E-18: G = 2.0294416E-22
682. OXYGENSPECIFICHEAT = A + B * O2TEMP + C * O2TEMP ^ 2 + D * O2TEMP ^ 3 + E * O2TEMP ^ 4 + F * O2TEMP ^ 5 + G * O2TEMP ^ 6
683. End Function
684. Private Static Function NITROGENSPECIFICHEAT(TK) 'kJ/Kg.K T=oK
685. A1 = 1.100752: B1 = -0.00053474045: C1 = 0.0000013971884: D1 = -1.2555363E-09: E1 = 6.0109266E-13: F = -1.6836213E-16: G = 2.7735985E-20
686. H1 = -2.5125233E-24: I1 = 1.0066147E-28: J1 = -5.1950017E-34
687. NITROGENSPECIFICHEAT = A1 + B1 * TK + C1 * TK ^ 2 + D1 * TK ^ 3 + E1 * TK ^ 4 + F1 * TK ^ 5 + G1 * TK ^ 6 + H1 * TK ^ 7 + I1 * TK ^ 8 + J1 * TK
^ 9
688. End Function
689. Private Static Function HYDROGENSPECHEAT(H2TK) 'kJ/Kg.K T=oK

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690. ZA = 8.3580785: ZB = 0.046774926: ZC = -0.00014346423: ZD = 0.00000023506381: ZE = -2.3076196E-10: ZF = 1.4608608E-13
691. ZG = -6.1673082E-17: ZH = 1.7508367E-20: ZI = -3.2962768E-24: ZJ = 3.9405226E-28: ZK = -2.7046605E-32: ZL = 8.1083083E-37
692. HYDROGENSPECHEAT = ZA + ZB * H2TK + ZC * H2TK ^ 2 + ZD * H2TK ^ 3 + ZE * H2TK ^ 4 + ZF * H2TK ^ 5 + ZG * H2TK ^ 6 + ZH * H2TK ^ 7 + ZI * H2TK ^
      8 + ZJ * H2TK ^ 9 + ZK * H2TK ^ 10 + ZL * H2TK ^ 11
693. End Function
694. Private Static Sub HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'H
      EAT EXCHANGER
695. AREAHEX = 3.14 * TOD * TL
696. 'DELTAB = TH2 - TC1
697. LMTD = Q / (U * AREAHEX)
698. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
699. '----- HEATING -----
700. If FLAG = 1 Then
701. DELTAA = TH1 - TC2
702. 'DELTAB = TH2 - TC1
703. LMTD = Q / (U * AREAHEX)
704. X1 = 1
705. 300 S1 = DELTAA / (LMTD - Logn(DELTAA))
706. S2 = X1 / (LMTD - Logn(X1))
707. If S2 >= S1 Then
708. GoTo 400
709. Else
710. X1 = X1 + 0.1
711. GoTo 300
712. 400 End If
713. DELTAB = X1
714. TH2 = DELTAB + TC1
715. GoTo 700
716. End If
717. '----- COOLING -----
718. '----- COOLING -----
719. If FLAG = 2 Then
720. 'DELTAA = TH1 - TC2
721. DELTAB = TH2 - TC1
722. LMTD = Q / (U * AREAHEX)
723. X1 = 2
724. 500 S1 = Logn(X1) - X1 / LMTD
725. S2 = Logn(DELTAB) - DELTAB / LMTD
726. If S1 >= S2 Then
727. GoTo 600
728. Else
729. X1 = X1 + 0.1
730. GoTo 500
731. 600 End If
732. DELTAA = X1
733. TC2 = TH1 - DELTAA
734. End If
735. '-----
736. 700 P = (TC2 - TC1) / (TH1 - TC1)
737. R = (TH1 - TH2) / (TC2 - TC1)
738. If R > 1 Then
739. R1 = 1 / R
740. P1 = P * R
741. Else
742. P1 = P
743. R1 = R
744. End If
745. A1 = (((R1) ^ 2 + 1) ^ 0.5) / (1 - R1)
746. A2 = Logn((1 - R1 * P1) / Abs(1 - P1))
747. A3 = 2 - P1 * (1 + R1 - (1 + (R1) ^ 2)) ^ 0.5 'up
748. A4 = Abs(2 - P1 * (1 + R1 + (1 + (R1) ^ 2)) ^ 0.5) 'down
749. A5 = Logn(A3 / A4)
750. FCORF = (A1 * A2) / A5
751. If Abs(FCORF) > 1 Then
752. FCORF = 1

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753. End If
754. If FLAG = 1 Then
755. LMTD = Q / (U * AREAHEX * FCORF)
756. CHOT = Q / (TH1 - TH2)
757. HFR = CHOT * 24 * 3600 / SCHOT
758. GoTo 800
759. End If
760. If FLAG = 2 Then
761. LMTD = Q / (U * AREAHEX * FCORF)
762. CCOLD = Q / (TH1 - TH2)
763. HFR = CCOLD * 24 * 3600 / SCHOT
764. End If
765. 'EFFECTIVENESS
766. 800 If CCOLD > CHOT Then
767. CMIN = CHOT
768. C1 = CHOT
769. EPS = (C1 * (TC2 - TC1)) / (CMIN * (TH1 - TC1))
770. GoTo 900
771. Else
772. CMIN = CCOLD
773. C1 = CCOLD
774. EPS = (C1 * (TH1 - TH2)) / (CMIN * (TH1 - TC1))
775. 900 End If
776. QEFF = EPS * CMIN * (TH1 - TC1)
777. 'Number of ELEMENT
778. NTU = U * AREAHEX / CMIN
779. If NTU <= 1 Then
780. NTU = 1
781. Else
782. End If
783. End Sub
784. Private Static Sub COMPRESSOR(GASTEMPC, COMPOP, COMPPI, GAMMA, GASVOL, OUTADIATEMP, COMETREFF, WATT, ENTCC, DRMOTWATT, DRMOTHP, MOTOREFF1, MOTO
REFF3, SPHASVOL, THREPAEVOL, CURRENT1, CURRENT3)
785. A1 = 1000
786. A2 = 60
787. WATT = 745.7 '1 Horse power to Watt
788. 'OUTADIATEMP = ((GASTEMPC + 273) * ((COMPOP / COMPPI) ^ ((GAMMA - 1) / GAMMA))) - 273 ' OUTLET ADIABATIC TEMPERATURE
789. 'DRMOTWATT = ((GASVOL / (A1 * A2)) * ENTCC * OUTADIATEMP) / (COMETREFF / 100)
790. 'DRMOTHP = DRMOTWATT / WATT
791. 'CURRENT1 = (DRMOTWATT / (MOTOREFF1 / 100)) / SPHASVOL
792. ' CURRENT3 = ((DRMOTWATT / (MOTOREFF3 / 100)) * (3 ^ 0.5)) / (3 * THREPAEVOL)
793. End Sub
794. Private Static Function AIRDENSITY(AIRTEMP) 'Air Density (Kg/m^3) oC
795. A1 = 1.2910739
796. B1 = 279.63468
797. C1 = 0.0036989433
798. D1 = 1.0050404
799. AIRDENSITY = (A1 * B1 + C1 * AIRTEMP ^ D1) / (B1 + AIRTEMP ^ D1) 'Air Density (Kg/m^3) oC
800. End Function
801. Private Static Function O2DENSITY(TC) 'Temperature TC in oC g/L
802. A = 0.70879975: B = 0.0026206143: C = 0.9987447
803. O2DENSITY = 1 / (A + B * (TC) ^ C) '(A * B + C * (TC) ^ (D)) / (B + (TC) ^ (D))
804. End Function

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Heat Balance results

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1. Sub Sheet11_Button1_Click()
2.
3. '
4.
5. '=====
6.
7. '-----
8. ' HEAT BALANCE
9. '=====

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10. '=====  

11. DFBTANK = ActiveWorkbook.Worksheets("DFB-ADB").Cells(100, 4) 'Energy IN DARK CSTR -(kW)  

12. ADBTANK = ActiveWorkbook.Worksheets("DFB-ADB").Cells(101, 4) 'Energy IN ADB CSTR -(kW)  

13. WESTANK1 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(102, 4) 'Energy IN ADB TANK1 -(kW)  

14. WESTANK2 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(103, 4) 'Energy IN ADB TANK2 -(kW)  

15. WESTANK2QW = ActiveWorkbook.Worksheets("SOFC").Cells(35, 11) 'Energy IN ADB TANK2 -(kW)  

16. WESTANK2ER = ActiveWorkbook.Worksheets("SOFC").Cells(52, 4) 'Energy IN ADB TANK2 -(kW)  

17. WESTANK2PY = ActiveWorkbook.Worksheets("SOFC").Cells(53, 4) 'Energy IN ADB TANK2 -(kW)  

18. WESTANK2PYT = ActiveWorkbook.Worksheets("SOFC").Cells(28, 11) 'Energy IN ADB TANK2 -(kW)  

19. ASDF = ActiveWorkbook.Worksheets("EMS").Cells(43, 11) 'Energy IN ADB TANK2 -(kW)  

20.  

21. '=====  

22.  

23. '=====  

24. SOFCTEMP = ActiveWorkbook.Worksheets("SOFC").Cells(13, 4) 'SOFC Cell Temperature (oC)  

25. '=====  

26. UREAENIN = ActiveWorkbook.Worksheets("UREA").Cells(9, 31) 'UREA ENERGY IN (kW)  

27. UREAENOUT = ActiveWorkbook.Worksheets("UREA").Cells(15, 32) 'UREA ENERGY OUT (kW)  

28. '=====  

29. AIRDARK = ActiveWorkbook.Worksheets("DFB-ADB").Cells(85, 11) ' AIR REQUIRED FOR DARK (Kg/day)  

30. AIRADB = ActiveWorkbook.Worksheets("DFB-ADB").Cells(85, 18) ' AIR REQUIRED FOR ADB (Kg/day)  

31. AIRSOFC = ActiveWorkbook.Worksheets("SOFC").Cells(10, 4) ' AIR REQUIRED FOR SOFC cell (Kg/day)  

32. AIRSOFEC = ActiveWorkbook.Worksheets("SOFEC").Cells(26, 16) ' AIR REQUIRED FOR SOFEC HECH (Kg/day)  

33. AIRITM = ActiveWorkbook.Worksheets("ITM").Cells(5, 4) ' AIR REQUIRED FOR (ITM)HE (Kg/day)  

34. AIRSSAS1 = ActiveWorkbook.Worksheets("SSAS").Cells(27, 16) ' AIR REQUIRED FOR SSAS HE (Kg/day)  

35. AIRSSAS2 = ActiveWorkbook.Worksheets("SSAS").Cells(14, 16) ' AIR REQUIRED FOR SSAS HE (Kg/day)  

36. AIRSSAS3 = ActiveWorkbook.Worksheets("SSAS").Cells(40, 16) ' AIR REQUIRED FOR SSAS Condenser(Kg/day)  

37. AIREMS = ActiveWorkbook.Worksheets("EMS").Cells(32, 11) ' AIR REQUIRED FOR EMS Condenser(Kg/day)  

38. AIRTEMP = ActiveWorkbook.Worksheets("ITM").Cells(8, 4) ' AIR TEMPERATURE from (ITM) (oC)  

39. '=====  

40. COM1 = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(28, 11) 'Compressor No1[MFI(ZM)](kW)-  

41. COM3 = ActiveWorkbook.Worksheets("SSAS").Cells(31, 11) 'Compressor No3[SSAS] (kW)-  

42. COM4 = ActiveWorkbook.Worksheets("SSAS").Cells(52, 11) 'Compressor No4[SSAS] (kW)-  

43. COM5 = ActiveWorkbook.Worksheets("SOFC").Cells(32, 4) 'Compressor No5[SOFC] (kW)-  

44. COM6 = ActiveWorkbook.Worksheets("SOFC").Cells(49, 16) 'Compressor No6[SOFC] (kW)-  

45. COM8 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(117, 4) 'Hydrolic Compressor (KW)-  

46. '=====  

47. SP1 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(68, 4) 'SLURY PUMP DARK REACTOR (w)-  

48. SP2 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(74, 4) 'SLURY PUMP DARK REACTOR (kW)-  

49. SP3 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(108, 4) 'SLURY PUMP DIGESTER (kW)-  

50. SP4 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(116, 4) 'SLURY PUMP DIGESTER (kW)-  

51. '=====  

52. HE1 = ActiveWorkbook.Worksheets("ITM").Cells(38, 4) 'Heat Exchanger No1 [ITM] (KW)-  

53. HE2 = ActiveWorkbook.Worksheets("EMS").Cells(12, 16) 'Heat Exchanger No2 [EMS] (KW)+  

54. HE3 = ActiveWorkbook.Worksheets("EMS").Cells(24, 16) 'Heat Exchanger No3 [EMS] (KW)-  

55. HE4 = ActiveWorkbook.Worksheets("SOFEC").Cells(13, 16) 'Heat Exchanger No4 [ITM] (KW)+  

56. HE5 = ActiveWorkbook.Worksheets("SOFEC").Cells(26, 16) 'Heat Exchanger No5 [SOFEC] (KW)+  

57. HE6 = ActiveWorkbook.Worksheets("SSAS").Cells(13, 16) 'N2 Heat Exchanger No6 [SSAS](KW)+  

58. HE7 = ActiveWorkbook.Worksheets("SSAS").Cells(26, 16) 'H2 Heat Exchanger No7 [SSAS](KW)+  

59. HE8 = ActiveWorkbook.Worksheets("SOFC").Cells(34, 11) 'Heat Exchanger BOX 8 [SOFC] (KW)-  

60. HE9 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(97, 4) 'Heat Exchanger No9 [INNOCULUM] (KW)-  

61. HE10 = ActiveWorkbook.Worksheets("SOFC").Cells(51, 4) 'Heat Exchanger BOX 8 [SOFC] (KW)-  

62. 'Condenser  

63. COND1 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(84, 11) 'Energy OUT DARK Condenser (kW)+  

64. COND2 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(84, 18) 'Energy OUT ADB Condenser (kW)+  

65. COND3 = ActiveWorkbook.Worksheets("EMS").Cells(30, 11) 'Heat Condenser No1 [EMS](KW)+  

66. COND4 = ActiveWorkbook.Worksheets("SSAS").Cells(39, 16) 'Heat Condenser No2 [SSAS](KW)+  

67. COND5 = ActiveWorkbook.Worksheets("SSAS").Cells(54, 16) 'Heat Condenser No5 [SSAS](KW)+  

68. 'Membranes Heat Loss  

69. HLMFI = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(54, 9) 'Heat Loss from MFI Cell (kW)  

70. HLITM = ActiveWorkbook.Worksheets("ITM").Cells(41, 4) 'Heat Loss from ITM Cell (kW)  

71. HLEMS = ActiveWorkbook.Worksheets("EMS").Cells(29, 16) 'Heat Loss from ITM Cell (kW)  

72. HLSOFEC = ActiveWorkbook.Worksheets("SOFEC").Cells(29, 11) 'Heat Loss from SOFEC Cell (kW)  

73. HLSSAS = ActiveWorkbook.Worksheets("SSAS").Cells(38, 11) 'Heat Loss from SSAS Cell (kW)  

74. HLSOFC = ActiveWorkbook.Worksheets("SOFC").Cells(40, 11) 'Heat Loss from SOFC Cell (kW)

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75. HLMFIX = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(20, 11) 'Heat Loss from MFI Cell (kW)
76. 'CO2 CALCULATIONS
77. 'CO2
78. CO2MFI = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(4, 11) 'CO2 From MFI(Kg/Day)
79. CO2SOFEC = ActiveWorkbook.Worksheets("SOFEC").Cells(6, 11) 'CO2 From SOFEC(kg/hr)
80. CO2MFITEMP = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(10, 4) 'CO2 TEMPERATURE From Dark oC
81. CO2TEMPUREA = ActiveWorkbook.Worksheets("UREA").Cells(4, 4) 'CO2 TEMPERATURE to Urea oC
82. CO2SOFECTEMP = ActiveWorkbook.Worksheets("SOFEC").Cells(15, 4) 'CO2 TEMPERATURE From Dark oC
83. CO2PRESIN = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(11, 4) 'CO2 Pressure atm.
84. CO2PRESOUT = ActiveWorkbook.Worksheets("UREA").Cells(3, 4)
85. H2OHEXRECY = ActiveWorkbook.Worksheets("SOFC").Cells(15, 17)
86. SSASAIRFLOW = ActiveWorkbook.Worksheets("SSAS").Cells(55, 16)
87. SSASAIRFLOW1 = ActiveWorkbook.Worksheets("SSAS").Cells(40, 16)
88. SOFECAIRFLOW1 = ActiveWorkbook.Worksheets("SOFEC").Cells(8, 11)
89. MFIZMAIRFLW1 = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(50, 11)
90. MFIZMAIRFLW2 = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(49, 11)
91. MFIZMAIRFLW3 = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(20, 11)
92. MFIZMAIRFLW4 = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(19, 11)
93. '=====
94. 'CO2 Calculations
95. R = 8.314 'J/K.mol
96. CO2MW = 44 'Molecular Weight
97. 'CO2 Total Flowrate
98. CO2TOTAL = CO2MFI + CO2SOFEC
99. 'MIXED CO2 Temperature
100. CO2MIXTEMP = (CO2MFI * CO2MFITEMP + CO2SOFEC * CO2SOFECTEMP) / CO2TOTAL 'Mixed CO2 Temperature
101. '===== COMPRESSORE FOR CO2 COM10 =====
102. Cells(67, 16) = CO2PRESIN 'Inlet Pressure atm
103. Cells(68, 16) = CO2PRESOUT 'OUTLET Pressure atm
104. Cells(69, 16) = CO2MIXTEMP 'Inlet Temperature
105. 'CALCULATIONS
106. COMPIP = CO2PRESIN 'Compressor Inlet Pressure (atm.)
107. COMPOP = CO2PRESOUT 'Compressor Outlet Pressure (atm.)
108. COMETREFF = Cells(70, 16) 'Compressor Entropy Efficieny (%)
109. SPHASVOL = Cells(71, 16) 'Single Phase Voltage (Volts)
110. MOTOREFF1 = Cells(72, 16) 'Single Phase Motor Efficiency (%)
111. THREPASEVOL = Cells(73, 16) '3 Phase Voltage (Volts)
112. MOTOREFF3 = Cells(74, 16) '3 Phase Motor Efficiency (%)
113. 'COMPRESSOR DATA
114. GASTK = CO2MIXTEMP + 273 'Inlet Gas Temperature (oK)
115. CO2SPCHEAT = CO2SPEHEAT(GASTK) 'CO2 SPECIFIC HEAT ' Cp of CO2 kJ/Kg K 'NH3 Specific Heat (kJ/Kg.K)kJ/kg.K (>1atm)
116. T = CO2MIXTEMP
117. RHOCO2 = CO2DENSITY(T) 'NH3 Density (Kg/m^3)
118. GAMMA = 1.18 'GAMMA=Cp/Cv
119. CO2VOLD = CO2TOTAL / RHOCO2 'CO2 Volume m^3/day
120. CO2VOLM = (CO2VOLD / 24) / 60 'CO2 Volume m^3/min
121. CO2VOLIT = CO2VOLM * 1000 'CO2 Volume L/min
122. Cells(66, 16) = CO2VOLIT 'CO2 Volume L/min,<=====
123. CO2MOL = CO2TOTAL / CO2MW 'CO2 Mol
124. ENTCC = CO2MOL * R * Logn(COMPOP / COMPIP)
125. GASTEMPC = CO2MIXTEMP: GASVOL = CO2VOLIT
126. OUTADIATEMP = ((CO2MIXTEMP + 273) * ((CO2PRESOUT / CO2PRESIN) ^ ((1.18 - 1) / 1.18))) - 273 ' OUTLET ADIABATIC TEMPERATURE
127. DRMOTWATT = (((OUTADIATEMP + 273) - (CO2MIXTEMP + 273)) * CO2SPCHEAT * (CO2TOTAL / 86400)) / (MOTOREFF1 / 100) 'KW
128. Call COMPRESSOR(GASTEMPC, COMPOP, COMPIP, GAMMA, GASVOL, OUTADIATEMP, COOLSYS, COMETREFF, WATT, ENTCC, DRMOTWATT, DRMOTHP, MOTOREFF1, MOTOR
EFF3, SPHASVOL, THREPASEVOL, CURRENT1, CURRENT3)
129. Cells(65, 21) = OUTADIATEMP
130. Cells(66, 21) = DRMOTWATT
131. Cells(67, 21) = DRMOTHP
132. Cells(68, 21) = CURRENT1
133. Cells(69, 21) = CURRENT3
134. CO2CONPW = DRMOTWATT
135. '===== CO2 COOLING Heat EXCHANGER N011 =====
136. TL = Cells(81, 16)
137. TOD = Cells(82, 16)
138. 'CO2

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139. TH1 = OUTADIATEMP + 273
140. TH2 = CO2TEMPUREA + 273
141. GASTK = TH2
142. SCCO2 = CO2SPEHEAT(GASTK)
143. CO2 = ((CO2TOTAL / 24) / 3600) * SCCO2 'O2 Heat capacity (KW/oK)
144. QO2 = CO2 * (TH1 - TH2)
145. 'Air Flow rate needed to Cool CO2
146. Cells(78, 16) = 25 'AIR TEMPERATURE IN oC
147. TC1 = 25 + 273
148. AIRINTK1 = TC1
149. AIRINTK1 = 25 + 273
150. SCAIR = AIRSPECIFICHEAT(AIRINTK1)
151. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
152. FLAG = 2
153. U = 0.02
154. CHOT = CO2: Q = QO2: SCHOT = SCCO2: SCCOLD = SCAIR
155. Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN
GER
156. 'OUTPUT
157. AIRCO2 = HFR
158. Cells(77, 16) = OUTADIATEMP
159. Cells(78, 16) = CO2TEMPUREA
160. Cells(79, 16) = 25 'AIR TEMPERATURE IN oC
161. Cells(80, 16) = TC2 - 273 'AIR TEMPERATURE IN oC
162. Cells(83, 16) = NTU
163. Cells(84, 16) = AREAHEX
164. Cells(85, 16) = EPS
165. Cells(86, 16) = QEFF
166. Cells(87, 16) = AIRCO2
167. HE11 = QEFF
168. 'Waste Eanks Heat Losses
169. '=====
170. 'TOTAL STEAM'
171. MSTEAMTOT = ((H2OHEXRECY + WESTANK2QW + (WESTANK2ER - WESTANK2PY)) / 86400) * (1000 - WESTANK2PYT) * 4.18
172. Cells(70, 21) = MSTEAMTOT
173. 'Waste Tanks Heat Losses
174. '=====
175. ' CALCULATIONS
176. '=====
177. '===== ENERGY OUT (kW)
178. ' STEATURB = ActiveWorkbook.Worksheets("SOFC").Cells(36, 16) 'Steam Turbine [SOFC] (kW)+
179. GASTURB = ActiveWorkbook.Worksheets("SOFC").Cells(57, 16) 'Steam Turbine [SOFC] (kW)+
180. '=====
181. 'POWER and Voltage
182. EMSPower = ActiveWorkbook.Worksheets("EMS").Cells(18, 11) 'POWER IN OF EMS(kw)-
183. SOFECPOWER = ActiveWorkbook.Worksheets("SOFEC").Cells(25, 11) 'POWER IN OF SOFEC (kW)-
184. ITMPOWER = ActiveWorkbook.Worksheets("ITM").Cells(26, 11) 'POWER OUT OF ITM (kW)+
185. SOFCPOWER = ActiveWorkbook.Worksheets("SOFC").Cells(22, 11) 'POWER OUT OF SOFC (kW)+
186. NH3HHV = ActiveWorkbook.Worksheets("SSAS").Cells(53, 3) 'NH3 Equivalent Power HHV of NH3(KW)+
187. NH3LHV = ActiveWorkbook.Worksheets("SSAS").Cells(54, 3) 'NH3 Equivalent Power LHV of NH3(KW)+
188. SSASPOWER = ActiveWorkbook.Worksheets("SSAS").Cells(49, 3)
189. '=====
190. ' IMPELLERS
191. IMPDFB = ActiveWorkbook.Worksheets("DFB-ADB").Cells(48, 12) 'IMPELLER DARK TEACTOR (HP)
192. IMPADB = ActiveWorkbook.Worksheets("DFB-ADB").Cells(48, 19) 'IMPELLER BIO TEACTOR (HP)
193. IMPINOC = ActiveWorkbook.Worksheets("DFB-ADB").Cells(65, 12) 'IMPELLER BIO TEACTOR (HP)
194. IMPMIX = ActiveWorkbook.Worksheets("DFB-ADB").Cells(8, 23) 'IMPELER MIXING TANK
195. CB1W = ActiveWorkbook.Worksheets("DFB-ADB").Cells(85, 4) 'BLOWER BIO REACTOR (WATT)
196. CB1 = CB1W 'BLOWER BIO REACTOR (KW)
197. '=====
198. ' TOTAL AIR REQUIRED PUMPING)
199. COOLAIR = 25
200. AIRSSAS = AIRSSAS1 + AIRSSAS2 + AIRSSAS3 + SSASAIRFLOW
201. TOTAIR = AIRSOFC + AIRITM + AIRSSAS + AIREMS + AIRDARK + AIRADB + AIRCO2 + MFIZMAIRFLW1 'TOTAL AIR REQUIRED for the SYSTEM (Kg/day)
202. 'Air Density

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203. COOLAIR = AIRTEMP
204. AIRDEN = AIRDENSITY(AIRTEMP) 'Air Density(Kg/m^3)
205. 'Volumetric Flow
206. AIRVOL1 = TOTAIR / AIRDEN 'Air Volume (m^3/day)
207. AIRVOL2 = AIRVOL1 * 1000 'Air Volume (Lt/day)
208. AIRVOL = (AIRVOL2 / 24) / 60 'Air Volume (Lt/min)
209. 'Compressor DATA IN
210. Cells(42, 4) = AIRADB '(Kg/day)
211. Cells(43, 4) = AIRDARK '(Kg/day)
212. Cells(44, 4) = AIREMS '(Kg/day)
213. Cells(45, 4) = AIRSOFC '(Kg/day)
214. Cells(46, 4) = AIRITM '(Kg/day)
215. Cells(47, 4) = AIRSOFEC '(Kg/day)
216. Cells(48, 4) = AIRSSAS '(Kg/day)
217. Cells(49, 4) = AIRVOL 'Air Volume (Lt/min)
218. COMPIN = Cells(50, 4) 'Compressor Inlet Pressure (Atm)
219. COMPOT = Cells(51, 4) 'Compressor Outlet Pressure (Atm)
220. COMPIT = Cells(52, 4) 'Compressor Inlet Temperature (oC)
221. COMETREFF = Cells(53, 4) 'Compressor ENTROPY Efficiency (%)
222. MOTOREFF1 = Cells(47, 11) 'Motor Efficiency 1-Phase (%)
223. SPHASVOL = Cells(48, 11) 'Single Phase Voltage (Volt)
224. MOTOREFF3 = Cells(50, 11) 'Motor Efficiency 3-Phase (%)
225. THREPASEVOL = Cells(51, 11) '3-Phase Voltage (Volt)
226. ' CONSTANT
227. RAIR = 408.97 'J/Kg.K
228. GAMMA = 2.0339 'Constant for Diatomic gas compression adiabatic temperature rise
229. ENTCC = AIRDEN * RAIR 'Entropy Change Constant (J/K.M^3)
230. '
231. '===== Compressor-1 Calculations =====
232. GASTEMPC = COMPIT: GASVOL = AIRVOL
233. OUTADIATEMP = ((GASTEMPC + 273) * ((COMPOT / COMPIN) ^ ((1.401 - 1) / 1.401))) - 273 ' OUTLET ADIABATIC TEMPERATURE
234. DRMOTWATT = (((OUTADIATEMP + 273) - (GASTEMPC + 273)) * 1.15 * (TOTAIR / 86400)) / (75 / 100) 'KW
235. Call COMPRESSOR(GASTEMPC, COMPOT, COMPIN, GAMMA, GASVOL, OUTADIATEMP, COOLSYS, COMETREFF, WATT, ENTCC, DRMOTWATT, DRMOTHP, MOTOREFF1, MOTOR
EFF3, SPHASVOL, THREPASEVOL, CURRENT1, CURRENT3)
236. '..... DATA OUTPUT ....
237. Cells(42, 11) = OUTADIATEMP
238. Cells(43, 11) = COOLAIR
239. Cells(44, 11) = COOLSYS
240. Cells(45, 11) = OUTADIATEMP
241. Cells(45, 11) = DRMOTWATT
242. Cells(46, 11) = DRMOTHP
243. Cells(49, 11) = CURRENT1
244. Cells(52, 11) = CURRENT3
245. '===== Energy =====
246. COM9 = DRMOTWATT 'Air Compressor
247. TOTALINKW = COM1 + COM2 + COM3 + COM4 + COM5 + COM6 + COM7 + COM8 + COM9 + SP1 + SP2 + SP3 + SP8 + CB1 'kw
248. ' DATA OUTPUT
249. '=====
250. ' ENERGY IN
251. '=====
252. 'ENERGY IN for Compressors
253. TOTALCOM = COM1 + COM3 + COM4 + COM5 + COM6 + COM7 + COM8 + COM9 + COM10 + COOLSYS 'Compressors
254. Cells(56, 3) = COM1 'Compressor No1[MFI(ZM)](kw)
255. Cells(57, 3) = COM2 'Compressor No1[SOFEC](kw)
256. Cells(58, 3) = COM3 'Compressor No3[SSAS] (kw)
257. Cells(59, 3) = COM4 'Compressor No4[SSAS] (kw)
258. Cells(60, 3) = COM5 'Compressor No5[SOFEC] (kw)
259. Cells(61, 3) = COM6 'Compressor No6[SOFEC] (kw)
260. Cells(62, 3) = COM7 'Compressor No7[SOFEC] (kw)
261. Cells(63, 3) = COM8 'Compressor No7[ADB] CAKING (kw)
262. Cells(64, 3) = COM9 'Compressor No9 [For Total AIR required [ENERGY (kw)]]
263. Cells(65, 3) = TOTALCOM 'TOTAL Compressors
264. 'ENERGY IN for PUMPS & Fan
265. Cells(67, 3) = SP1 'Sludge Pump[DARK.REACTOR] (kw)
266. Cells(68, 3) = SP2 'Sludge Pump[DARK.REACTOR] (kw)

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267. Cells(69, 3) = SP3 'For Digester Sludge (kW)
268. Cells(70, 3) = SP4 'For Digester Sludge (kW)
269. Cells(72, 3) = CB1 'Centrifugal fan[BIOREACTOR] (kW)
270. TOTALF = SP1 / 1000 + SP2 / 1000 + SP3 + SP4 + CB1
271. Cells(73, 3) = TOTALF 'Total (kW)
272. 'ENERGY IN for Heat-Exchangers
273. Cells(75, 3) = HE1
274. Cells(76, 3) = HE3
275. Cells(77, 3) = HE5
276. Cells(78, 3) = HE8
277. Cells(79, 3) = HE9
278. Cells(80, 3) = HE10
279. TOTALHEXIN = HE1 + HE3 + HE5 + HE8 + HE9 + HE10 + HE4 + HE2
280. Cells(81, 3) = TOTALHEXIN
281. 'ENERGY IN FOR IMPELLER
282. IMPDFBW = IMPDFB * 0.745 'Dark Impeller (kW)
283. IMPADBW = IMPADB * 0.745 'BIO Impeller (kW)
284. IMPINOCW = IMPINOC * 0.745 'Inoculum Impeller (kW)
285. IMPMIXT = IMPMIX * 0.745 'Mixing Tank (kW)
286. TOTALIMP = IMPDFBW + IMPADBW + IMPINOCW + IMPMIXT
287. 'Cells
288. Cells(83, 3) = IMPDFBW 'Dark Impeller (kW)
289. Cells(84, 3) = IMPADBW 'BIO Impeller (kW)
290. Cells(85, 3) = IMPINOCW 'Inoculum Impeller (kW)
291. Cells(86, 3) = IMPMIXT 'Mixer Impeller (kW)
292. Cells(87, 3) = TOTALIMP
293. 'ENERGY IN FOR WASTE TANKS
294. TOTALTANKS = DFBTANK + ADBTANK + WESTANK1 + WESTANK2
295. Cells(89, 3) = DFBTANK 'Energy IN DARK CSTR -(kW)
296. Cells(90, 3) = ADBTANK 'Energy IN ADB CSTR -(kW)
297. Cells(91, 3) = WESTANK1 'Energy IN ADB TANK1 -(kW)
298. Cells(92, 3) = WESTANK2 'Energy IN ADB TANK2 -(kW)
299. Cells(93, 3) = TOTALTANKS
300. 'Membranes Heat Loss
301. TOTALHLMEMB = HLMFI + HLITM + HLEMS + HLSOFEC + HLSSAS + HLSOFC 'Total MEMBRANE HEAT LOSS (kW)
302. Cells(95, 3) = HLMFI 'Heat Loss from MFI Cell (kW)
303. Cells(96, 3) = HLITM 'Heat Loss from ITM Cell (kW)
304. Cells(97, 3) = HLEMS 'Heat Loss from EMS Cell (kW)
305. Cells(98, 3) = HLSOFEC 'Heat Loss from SOFEC Cell (kW)
306. Cells(99, 3) = HLSSAS 'Heat Loss from SSAS Cell (kW)
307. Cells(100, 3) = HLSOFC 'Heat Loss from SOFC Cell (kW)
308. Cells(101, 3) = TOTALHLMEMB 'Total MEMBRANE HEAT LOSS (kW)
309. '
310. '=====
311. ' ENERGY OUT
312. '=====
313. '...ENERGY OUT of Turbines
314. TOTALOUTTURBKW = STEATURB + GASTURB '+ GASTURB2
315. Cells(54, 11) = STEATURB
316. Cells(55, 11) = GASTURB
317. Cells(43, 15) = GASTURB2
318. Cells(56, 11) = TOTALOUTTURBKW
319. '...ENERGY OUT for Heat-Exchangers and Condensers
320. 'HEAT-EXCHANGERS
321. Cells(58, 11) = HE2
322. Cells(59, 11) = HE4
323. Cells(60, 11) = HE6
324. Cells(61, 11) = HE7
325. 'Condensers
326. Cells(62, 11) = COND1
327. Cells(63, 11) = COND2
328. Cells(64, 11) = COND3
329. Cells(65, 11) = COND4
330. Cells(66, 11) = COND5
331. TOTALHEXCONOUT = COND1 + COND2 + HE6 + HE7 + COND3 + COND4 + COND5 + HE11 + MFIZMAIRFLW2

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332. BXC = TOTALHEXCONOUT * 0.1 'Loss in heat condenser; based on 10%
333. Cells(67, 11) = TOTALHEXCONOUT
334. 'TOTAL PRODUCED
335. TOTAPRO = TOTALOUTTURBKW + TOTALHEXCONOUT 'Total Produced (kW)
336. Cells(68, 11) = TOTAPRO '(A+B)
337. 'Total Balance (1)
338. ENERGYIN = TOTALCOM + ((SP1 + SP2)) + CB1 + TOTALHEXIN + TOTALIMP + TOTALTANKS + TOTALHLMEMB + SP4 + BXC 'Total IN from compressor + .....
339. TOTALGIVEN = TOTAPRO - ENERGYIN 'ENERGY BALANCE (1)OUT
340. Cells(70, 11) = ENERGYIN 'Energy Consumed (kW)
341. Cells(71, 11) = TOTAPRO 'Energy Produced(kW)
342. Cells(72, 11) = TOTALGIVEN 'ENERGY BALANCE (1)
343. 'TOTAL OUT
344. TOTALOUTHEXTURB = TOTALOUTTURBKW + TOTALHEXCONOUT
345. Cells(69, 11) = TOTALOUTHEXTURB '(A+B)
346. '=====
347. ' Cell Voltages to Power + NH3 + UREA
348. '=====
349. 'Total Energy from Voltage
350. TOTALVOLTAGE = -SOFECPOWER - EMSPower + ITMPower + SOFCPOWER - SSASPOWER 'Total Voltage Power (kW)(2)
351. 'Energy From NH3
352. NH3HHV = NH3HHV 'Energy From NH3 (kW) (4)
353. 'Energy From Urea
354. UREAETOTNEEDED = UREAENOUT - UREAENIN 'ENERGY FROM UREA (kW) (3)
355. 'TOTAL ENERGY WITHOUT NH3
356. TOTENER3 = TOTALGIVEN + TOTALVOLTAGE + UREAETOTNEEDED - CO2CONPW + COM2 - MSTEAMTOT - MFIZMAIRFLW4 - MFIZMAIRFLW3 - ASDF '(1)+(2)-(3)
357. 'TOTAL ENERGY WITHOUT NH3
358. TOTENERWNH3 = NH3HHV + TOTENER3 'Total Energy with NH3 (1)+(2)-(3)+(4)
359. 'Cells
360. Cells(65, 6) = EMSPower 'Voltage in Kw from EMS
361. Cells(66, 6) = SOFECPOWER 'Voltage in Kw from SOFEC
362. Cells(67, 6) = ITMPower 'Voltage in Kw from ITM
363. Cells(68, 6) = SOFCPOWER 'Voltage in Kw from SOFC
364. Cells(69, 6) = TOTALVOLTAGE 'Energy OUT From Voltages (kW)
365. Cells(70, 6) = UREAETOTNEEDED 'ENERGY IN FROM UREA (kW)
366. Cells(71, 6) = NH3HHV 'ENERGY IN from NH3
367. Cells(72, 6) = TOTENER3 'ENERGY BALANCE (2)
368. Cells(73, 6) = TOTENERWNH3 'ENERGY BALANCE (3)
369. End Sub
370. Static Function Logn(X)
371. Logn = Log(X) / Log(2.718282)
372. End Function
373. Private Static Function AIRDENSITY(AIRTEMP)
374. A1 = 1.2910739
375. B1 = 279.63468
376. C1 = 0.0036989433
377. D1 = 1.0050404
378. AIRDENSITY = (A1 * B1 + C1 * AIRTEMP ^ D1) / (B1 + AIRTEMP ^ D1) 'Air Density(Kg/m^3) oC
379. End Function
380. Private Static Sub COMPRESSOR(GASTEMPC, COMPOP, COMPIP, GAMMA, GASVOL, OUTADIATEMP, COOLSYS, COMETREFF, WATT, ENTCC, DRMOTWATT, DRMOTHP, MOTORE
FF1, MOTOREFF3, SPHASVOL, THREPAEVL, CURRENT1, CURRENT3)
381. A1 = 1000
382. A2 = 60
383. End Sub
384. Private Static Function CO2SPEHEAT(GASTK) 'CO2 SPECIFIC HEAT ' Cp of CO2 kJ/Kg K)
385. Z1 = 0.51476288
386. Z2 = 5820.1918
387. Z3 = 1.4877831
388. Z4 = 1.404349
389. CO2SPEHEAT = (Z1 * Z2 + Z3 * GASTK ^ Z4) / (Z2 + GASTK ^ Z4)
390. End Function
391. Private Static Function AIRSPECIFICHEAT(AIRTK) 'AIRSPECIFICHEAT (kJ/kg.K)
392. TA = 1.0828694; TB = -0.00063119116; TC = 0.000016253087; TD = -1.3949526E-09; TE = 5.3826153E-13; TF = -7.9021928E-17
393. AIRSPECIFICHEAT = TA + TB * AIRTK + TC * AIRTK ^ 2 + TD * AIRTK ^ 3 + TE * AIRTK ^ 4 + TF * AIRTK ^ 5
394. End Function

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395. Private Static Function WATERSPECIFICHEAT(H2OTEMP) 'WATER SPECIFIC HEAT (kJ/kg.K)
396. WATERSPECIFICHEAT = 1.224986 + 0.0014072339 * H2OTEMP - 0.00000039722778 * H2OTEMP ^ 2 + 5.3431749E-11 * H2OTEMP ^ 3 + -2.7473115E-
15 * H2OTEMP ^ 4
397. End Function
398. Private Static Function CO2DENSITY(T) 'T=oC,kg/m^3
399. A = 0.50649907: B = 0.0019289299: C = 1.0174749
400. CO2DENSITY = (A + B * T) ^ (-1 / C)
401. End Function
402. Private Static Sub HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'H
EAT EXCHANGER
403. AREAHEX = 3.14 * TOD * TL
404. LMTD = Q / (U * AREAHEX)
405. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
406. '----- HEATING -----
407. If FLAG = 1 Then
408. DELTAA = TH1 - TC2
409. LMTD = Q / (U * AREAHEX)
410. X1 = 1
411. 300 S1 = DELTAA / (LMTD - Logn(DELTAA))
412. S2 = X1 / (LMTD - Logn(X1))
413. If S2 >= S1 Then
414. GoTo 400
415. Else
416. X1 = X1 + 0.1
417. GoTo 300
418. 400 End If
419. DELTAB = X1
420. TH2 = DELTAB + TC1
421. GoTo 700
422. End If
423. '-----
424. '----- COOLING -----
425. If FLAG = 2 Then
426. 'DELTAA = TH1 - TC2
427. DELTAB = TH2 - TC1
428. LMTD = Q / (U * AREAHEX)
429. X1 = 2
430. 500 S1 = Logn(X1) - X1 / LMTD
431. S2 = Logn(DELTAB) - DELTAB / LMTD
432. If S1 >= S2 Then
433. GoTo 600
434. Else
435. X1 = X1 + 0.1
436. GoTo 500
437. 600 End If
438. DELTAA = X1
439. TC2 = TH1 - DELTAA
440. End If
441. '-----
442. 700 P = (TC2 - TC1) / (TH1 - TC1)
443. R = (TH1 - TH2) / (TC2 - TC1)
444. If R > 1 Then
445. R1 = 1 / R
446. P1 = P * R
447. Else
448. P1 = P
449. R1 = R
450. End If
451. A1 = (((R1) ^ 2 + 1) ^ 0.5) / (1 - R1)
452. A2 = Logn((1 - R1 * P1) / Abs(1 - P1))
453. A3 = 2 - P1 * (1 + R1 - (1 + (R1) ^ 2)) ^ 0.5 'up
454. A4 = Abs(2 - P1 * (1 + R1 + (1 + (R1) ^ 2)) ^ 0.5) 'down
455. A5 = Logn(A3 / A4)
456. FCORF = (A1 * A2) / A5
457. If Abs(FCORF) > 1 Then

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458. FCORF = 1
459. End If
460. If FLAG = 1 Then
461. LMTD = Q / (U * AREAHEX * FCORF)
462. CHOT = Q / (TH1 - TH2)
463. HFR = CHOT * 24 * 3600 / SCHOT
464. GoTo 800
465. End If
466. If FLAG = 2 Then
467. LMTD = Q / (U * AREAHEX * FCORF)
468. CCOLD = Q / (TH1 - TH2)
469. HFR = CCOLD * 24 * 3600 / SCHOT
470. End If
471. 'EFFECTIVENESS
472. 800 If CCOLD > CHOT Then
473. CMIN = CHOT
474. C1 = CHOT
475. EPS = (C1 * (TC2 - TC1)) / (CMIN * (TH1 - TC1))
476. GoTo 900
477. Else
478. CMIN = CCOLD
479. C1 = CCOLD
480. EPS = (C1 * (TH1 - TH2)) / (CMIN * (TH1 - TC1))
481. 900 End If
482. QEFF = EPS * CMIN * (TH1 - TC1)
483. 'Number of ELEMENT
484. NTU = U * AREAHEX / CMIN
485. If NTU <= 1 Then
486. NTU = 1
487. Else
488. End If
489. End Sub

```

A.2 DF+AD+CCS Codes

The VBA code for DF+AD+CCS process is similar to the aforementioned DF+AD+UREA process except for the SSAS and energy balance calculations

```

1. Sub Sheet8_Button1_Click()
2. '
3. ' SSAS
4. 'N2
5. N2FRK = ActiveWorkbook.Worksheets("ITM").Cells(10, 11) 'N2 Total Available from (ITM) (Kg/Day)
6. N2EMS = ActiveWorkbook.Worksheets("ITM").Cells(23, 4) 'N2 Needed for EMS (Kg/Day)
7. N2ITMTEMP = ActiveWorkbook.Worksheets("ITM").Cells(11, 4) 'N2 Temperature from (ITM)(oC)
8. N2ITMTPRE = ActiveWorkbook.Worksheets("ITM").Cells(12, 4) 'N2 Pressure from (ITM)(oC)
9. 'CO2
10. CO2MFI = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(4, 11) 'CO2 From Dark(Kg/Day)
11. CO2SOFEC = ActiveWorkbook.Worksheets("SOFEC").Cells(6, 11) 'CO2 From SOFEC(kg/hr)
12. CO2MFITEMP = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(10, 4) 'CO2 TEMPERATURE From Dark oC
13. CO2SOFECTEMP = ActiveWorkbook.Worksheets("SOFEC").Cells(15, 4) 'CO2 TEMPERATURE From Dark oC
14. 'H2
15. H2MFI = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(6, 11) 'H2 From MFI(ZM) (Kg/Day)
16. H2FRKSOFEC = ActiveWorkbook.Worksheets("SOFEC").Cells(5, 11) 'H2 IN From SOFEC(kg/hr)
17. H2FRKSOFEC = ActiveWorkbook.Worksheets("SOFEC").Cells(5, 11) 'H2 IN From SOFEC(kg/hr)
18. 'TEMPERATURE
19. H2MFITEMP = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(10, 4) 'H2 Temperature From MFI(ZM) (oC)
20. H2SOFECTEMP = ActiveWorkbook.Worksheets("SOFEC").Cells(15, 4) 'H2 Temperature From SOFEC(ZM) (oC)
21. H2SOFECTEMP = ActiveWorkbook.Worksheets("SOFEC").Cells(15, 4) 'H2 Temperature From SOFEC(ZM) (oC)
22. '
23. ' INPUT
24. ' N2 Total Available
25. N2TOTAVAILABLE = (N2FRK) - (N2EMS) '+ (N2SOFEC) 'N2 TOTAL AVAILABLE (Kg/day)
26. ' H2 Total Available
27. H2TOTAVAILABLE = H2MFI + H2FRKSOFEC + H2FRKSOFEC
28. ' N2
29. Cells(5, 4) = N2TOTAVAILABLE 'N2 Total Available from (ITM) (Kg/Day)
30. Cells(6, 4) = N2ITMTEMP 'N2 Mixed Inlet Temperature (oC)
31. Cells(7, 4) = N2ITMTPRE 'N2 Inlet Pressure (atm)
32. ' H2
33. Cells(10, 4) = H2TOTAVAILABLE 'H2 Flow Rate (kg/hr)
34. HIP = Cells(12, 4) 'H2 Inlet Pressure (atm)
35. ' Cell
36. CIT = Cells(15, 4) 'Cell Temperature (oC)
37. CIP = Cells(16, 4) 'Cell Pressure (atm)
38. MC = Cells(17, 4) 'Membrane Conductivity (1/cm.ohm)
39. MSA1 = Cells(18, 4) 'Membrane Surface Area (m^2)
40. MTH = Cells(19, 4) 'Membrane Thickness (cm)
41. APC = Cells(20, 4) 'Applied Current(mA)
42. APV = Cells(21, 4) 'Applied Voltage
43. FU1 = Cells(47, 2)
44. 'N2 Mixed Temperature
45. 'Temperature of Mixed N2 gas
46. N2HIGHTEM = N2TOTAVAILABLE - N2FREXCHANGER 'N2 Flow rate from (ITM) not used at T= 900 (oC)
47. N2FREXCHANGER = N2FREXCHANGER 'N2 Flow rate from (ITM)Used for the Heat Exchanger at T=305.65 (oC)
48. '<===== Input Data =====>
49. ' Constant
50. MSA = MSA1 * 10000
51. N2ITK = N2ITMTEMP + 273
52. H2TK = H2IT + 273
53. CITK = CIT + 273
54. TSTPK = 25 + 273
55. FU = FU1 / 100
56. ECD = 3.5 ' Electrical Current Density Mole/cm^2.sec
57. FA = 96485 ' coulombs/mole
58. R = 8.314 'J/K.mol
59. RG = 82.05746 'cm3 atm/mol.K

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59. DELH0 = 91.88 'kJ/mole
60. AWN2 = 14 'Weight of one N2 atom
61. N2MW = 28
62. H2MW = 2
63. NH3MW = 17
64. UREAMW = 60.6
65. CO2MW = 44
66. THPLUS = 1.11 'Proton transport number
67. '=====  

68. '***** Needed Components for Urea *****  

69. ' CO2 TOTAL PRODUCED  

70. CO2TOTAL = CO2MFI + CO2SOFEC '(Kg/Day)  

71. 'Urea Needed to consume all the CO2  

72. UREA = (CO2TOTAL * UREAMW) / CO2MW 'Urea Prduced'Total CO2 produced is Used For Urea (according to the UREA production ratio)(KG/day)  

73. 'NH3 Needed for this Urea production  

74. NH3TOTUREA = (UREA * (2 * NH3MW)) / UREAMW 'Total NH3 NEEDED FOR UREA PRODUCTION (Kg/day)  

75. 'H2 Needed for this NH3 production for Urea  

76. H2TOTUREA = (NH3TOTUREA * (H2MW * 3)) / (2 * NH3MW) 'H2 Needed for NH3 To UREA (Kg/day)  

77. 'N2 Needed for this NH3 production for Urea  

78. N2TOTUREA = (NH3TOTUREA * N2MW) / (NH3MW * 2) 'N2 Needed for NH3 To UREA (Kg/day)  

79. '***** Component Availability *****  

80. 'H2 Available  

81. H2AVAILABLE = H2TOTAVAILABLE - H2TOTUREA 'H2 Available (Kg/day)  

82. 'N2 Available  

83. N2AVAILABLE = N2TOTAVAILABLE - N2TOTUREA 'N2 Available (Kg/day)  

84. '.....  

85. 'Ratio of Available H2 for Extra NH3 and SOFC  

86. NR = Cells(32, 3)  

87. If NR <= 0 Then  

88. Cells(22, 6) = "ERROR N=0"  

89. End  

90. Else  

91. Cells(22, 6) = ""  

92. End If  

93. 'H2 For NH3  

94. H2NH3EXTRA = H2AVAILABLE / NR 'H2 for Extra NH3 (Kg/day)  

95. 'H2 For SOFC  

96. H2SOFEC = H2AVAILABLE - H2NH3EXTRA 'H2 for SOFC (Kg/day)  

97. If H2SOFEC < 0 Then  

98. Cells(31, 3) = H2SOFEC  

99. Cells(22, 6) = "ERROR H2 is NEGATIVE"  

100. End  

101. Else  

102. Cells(22, 6) = "H/N OK for SOFC"  

103. End If  

104. 'H2 Needed For Membrane  

105. H2MEMBRANE = H2TOTUREA + H2NH3EXTRA 'H2 Total For SSAS Membrane (Kg/day)  

106. '.....Extra NH3 .....  

107. NH3EXTRA = (H2NH3EXTRA * (NH3MW * 2)) / (H2MW * 3) 'Extra NH3 (Kg/day)  

108. 'N2 Needed For Extra NH3  

109. N2NH3EXTRA = (NH3EXTRA * N2MW) / (NH3MW * 2) 'N2 Used For Extra NH3 (Kg/day)  

110. 'N2 Remaining  

111. N2REMAIN = N2FRK - N2EMS - N2TOTUREA - N2NH3EXTRA  

112. '  

113. '***** TOTAL NH3 *****  

114. '.....TOTAL H2 and N2 Needed For A TOTAL of NH3.....  

115. 'N2 Needed for a Total of NH3  

116. N2TOTNH3 = N2TOTUREA + N2NH3EXTRA 'N2 Needed For a Total of NH3 (Kg/day)  

117. 'H2 Needed for a Total of NH3  

118. H2TOTNH3 = H2TOTUREA + H2NH3EXTRA  

119. 'Total NH3 Needed  

120. NH3TOTALNEEDED = NH3TOTUREA + NH3EXTRA  

121. '*****  

122. '=====  

123. 'NH3 For Urea

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189. NH3TOTAL = NH3TOTUREA + NH3EXTRA
190. ' TOTAL Moles
191. N2MOLTOT = N2FRKUSED / N2MW 'N2 Moles/day
192. H2MOLTOT = H2TOTALIN / H2MW 'H2 Moles/day
193. NH3MOLTOT = NH3TOTAL / NH3MW 'NH3 Moles/day
194. 'AT Cathode
195. H2PERCTOT = H2MOLTOT / H2MOLTOT 'H2 %
196. 'AT Anode
197. TOTMOLTOT = N2MOLTOT + NH3MOLTOT 'Total Moles
198. N2PERCTOT = N2MOLTOT / TOTMOLTOT 'N2 %
199. NH3PERCTOT = NH3MOLTOT / TOTMOLTOT 'NH3 %
200. 'Partial Pressure
201. PPN2TOT = N2PERCTOT * CIP
202. PPH2TOT = H2PERCTOT * CIP
203. PPNH3TOT = NH3PERCTOT * CIP
204. '=====
205. PPN2 = PPN2TOT
206. PPH2 = PPH2TOT
207. PPNH3 = PPNH3TOT
208. '=====
209. ' Thermodynamics - DELTA : C,H, S, G in fuction of T
210. A = TSTPK
211. B = 573 'CITK
212. N = 263
213. ' DELTA(H)with TK
214. Call DELTAH(A, B, N, INTEGRALH) 'Simpson integrator for DELTA(H)263
215. DELH = INTEGRALH - 91.88 'DELTA(H) (kJ/mole)
216. ' DELTA(S)with TK
217. N = 108
218. Call DELTAH(A, B, N, INTEGRALS) 'Simpson integrator for DELTA(S)108
219. DELS = (-198.091 + INTEGRALS) / 1000 'DELTA(S) (J/mole)
220. ' DELTA(G)with TK
221. DELTAGKJ = DELH - CITK * DELS 'DELTA (G)(kJ/mole)
222. DELTAG = DELTAGKJ * 1000 'DELTA (G)(J/mole)
223. ' Reversible Voltage E0
224. E0 = (DELTAG / (6 * FA)) ' * 1000 'Gibbs Free Energy in(Volt)Ref:75969 Page-
225. ENERST = E0 + ((R * CITK) / (6 * FA)) * Logn((PPN2) * (PPH2) ^ 1 / 3) / (PPNH3) ^ 1 / 2) 'Nerst Voltage Ref: Fogler Reactor design SOFC
226. 'Area Specific Resistance
227. ASR = (MTH / MC)
228. 'RATE OF NH3 at MEMBRANE(FLUX)
229. RNH3 = -((ENERST - APV) / (ASR * 6 * FA)) * 2 / 3 'Rate of NH3 'At MEMBRANE(FLUX) RATE OF Reaction of NH3 moles/cm^2.s
230. 'Maximum RATE OF NH3 at Working Electrode
231. RNH3MAX = 1.13 * (10) ^ -8 'Maximum Rate of NH3 moles/cm^2.sec Ref:XU209 Page-4 or 75969 Page-12
232. 'Exchange Current Density io
233. IO = RNH3 * 3 * FA * MSA1 'mAmp/cm^2
234. 'Faradaic Efficiency
235. FE = ((3 * FA * RNH3MAX * (MSA1) * 100) / (APC * 1.07))
236. 'Current il Needed for maximum fuel efficiency of this RNH3MAX => ICUR = 0.005972+>Limited current desity
237. ' or-Electrochemical_Synthesis_of_Ammonia_in_Solid_Elec Page-7
238. ICURL = (6 * FA * MSA * RNH3MAX) / THPLUS '(0.904 * TH) 'AMP Ref:XU209 Page-4 or 75969 Page-12
239. 'Limited Current Density
240. IL = ICURL / MSA 'mAmp/cm^2
241. 'Current Density
242. II = APC / MSA
243. 'Moles of NH3 Required
244. NH3MOLNEED = (NH3TOTAL * 1000) / NH3MW 'Moles/day
245. NH3MOLSEC = (NH3MOLNEED / 24) / 3600 'Moles /sec
246. 'AREA
247. AREANEED = NH3MOLSEC / RNH3
248. 'Number Of Electrode
249. NUMBCELLS = AREANEED / MSA
250. 'Activation Energy
251. ETAACT = ((R * CITK) / (0.5 * FA)) * Logn(II / IO)
252. 'Concentration Energy
253. ETACONT = ((R * CITK) / (6 * FA)) * Logn(1 - II / IL)

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254. 'Ohmic Energy
255.   IOHM = II * (MTH / MC)
256. 'TOTAL VOLTAGE
257.   TOTVOLT = -((ENERST) + (APV) + (ETAAC) + (ETACONT) + (IOHM)) * NUMBCELLS
258. '===== PLOT =====
259. 'Plot of Butler-Volmer equation to find II
260.   II1 = 0.1
261.   For I = 1 To 10
262.     TACT1 = ((R * CITK) / (0.5 * FA)) * Logn(II1)
263.     II1 = II1 + 0.1
264.     Cells(64 + I, 1) = -TACT1
265.     Cells(64 + I, 2) = II1
266.   Next I
267. 'Resistance R
268.   RES = 1 / 0.051
269. '***** COMPONENT OUT *****
270. 'N2 Out at Cathode
271.   N2OUT = N2REMAIN
272.   Cells(5, 11) = N2OUT      'N2 OUT UNUSED (kg/hr)
273.   If N2OUT <= 0 Then
274.     Cells(4, 7) = "ERROR"
275.     Cells(5, 7) = "N2 OUT LOW"
276.     Cells(6, 7) = "First Check H/N"
277.     Cells(7, 7) = "AGAIN, if N2<0"
278.     Cells(8, 7) = "RUN ITM"
279.     Cells(9, 7) = "AGAIN"
280.   End
281.   Else
282.     Cells(5, 11) = N2OUT      'N2 OUT UNUSED (kg/hr)
283.     Cells(4, 7) = " "
284.     Cells(5, 7) = " "
285.     Cells(6, 7) = " "
286.     Cells(7, 7) = " "
287.     Cells(8, 7) = " "
288.     Cells(9, 7) = " "
289.   End If
290. '----- CELL POWER IN          CELLPWER = (TOTAPPLI * TOTALEV) / 1000
291.   IVMC = 1 / MC      '(Ohm.cm) Inverse of conductivity
292.   RESISTANCE = IVMC / MTH '(Ohm)
293.   TOTALCURRENT = (TOTVOLT / RESISTANCE) 'Total Current (Amp)
294.   CELLPWER = (TOTALCURRENT * TOTVOLT * NUMBCELLS) / 1000 '(kW)
295.   Cells(49, 3) = CELLPWER
296.   Cells(50, 3) = RESISTANCE
297.   Cells(51, 3) = FE      'Faradaic Efficiency
298. 'OUTPUT
299.   Cells(13, 4) = H2SOFC
300.   Cells(4, 11) = NH3TOTAL 'NH3(kg/Day)Formed
301.   Cells(5, 11) = N2OUT    'N2 OUT UNUSED (kg/hr)
302.   Cells(6, 11) = RNH3MAX  'Maximum Reaction Rate
303.   Cells(7, 11) = RNH3     'Actual Reaction Rate
304.   Cells(8, 11) = AREANEDED 'Required Area from Reaction
305.   Cells(9, 11) = NUMBCELLS 'Number of Cells
306.   Cells(10, 11) = APC     'Current Imposed (Amp)
307.   Cells(11, 11) = TOTALCURRENT 'Total Current (Amp)
308.   Cells(12, 11) = TOTVOLT 'Voltage (Volt)
309.   Cells(13, 11) = H2SOFC  'H2 Out(kg/Day)
310.   Cells(14, 11) = NH3TUREA 'NH3 for Urea (kg/hr)
311.   Cells(15, 11) = NH3EXTRA 'Extra NH3 produced (kg/hr)
312.   Cells(16, 11) = CO2TOTAL 'Total CO2 For Urea (kg/hr)
313.   Cells(17, 11) = UREA    'Amount of Urea (kg/day) for complete CO2 Elimination
314. '
315. '===== END OF CELL CALCULATIONS =====
316. '
317. '===== HEAT EXCHANGER-6
318.   H2TEMPMIXED1 = (H2FRKSOFC * H2SOFCTEMP + H2MFI * H2MFIEMP) / (H2FRKSOFC + H2MFI)

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319.   If H2TEMPMIXED1 < CIT Then
320.     H2TEMPMIXED2 = CIT - H2TEMPMIXED1
321.     H2TEMPMIXED = H2TEMPMIXED2 + H2TEMPMIXED1 + H2TEMPMIXED2 * 0.16
322.     GoTo 5
323.   Else
324.     H2TEMPMIXED1 = (H2FRKSOFECC * H2SOFECCTEMP + H2MFI * H2MFITEMP) / (H2FRKSOFECC + H2MFI)
325.     H2TEMPMIXED = H2TEMPMIXED1
326. 5   End If
327.   Cells(11, 4) = H2TEMPMIXED
328.   TL = Cells(8, 16)
329.   TOD = Cells(9, 16)
330. '=====
331. '..... Heat Exchanger No6 for H2 cooling .....
332. '=====
333. TL = Cells(8, 16)
334.   TOD = Cells(9, 16)
335. ' Hydrogen
336.   H2TK = H2TEMPMIXED + 273
337.   SCH2 = HYDROGENSPECHEAT(H2TK)           'H2 Specific Heat (kJ/kg.K)
338.   CH2 = ((H2TOTAVAILABLE / 24) / 3600) * SCH2 'H2 Heat capacity (KW/oK)
339.   TH1 = (H2TEMPMIXED) + 273              'H2 Hot Side (oK)
340.   TH2 = CIT + 273 'Cell Temperature in Kelvin 'H2 Cold Side (oK)
341.   QH2 = CH2 * (TH1 - TH2)
342. 'Air
343.   TC1 = 25 + 273
344.   'TC2=?
345.   AIRINTK = TC1
346.   SCAIR = AIRSPECIFICHEAT(AIRINTK)
347. 'Air Flow rate needed to Cool H2
348. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
349.   FLAG = 2
350.   U = 0.02
351.   CCOLD = CH2: CHOT = CH2: Q = QH2: SCHOT = SCH2: SCCOLD = SCAIR
352.   Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN
GER
353. '----- OUTPUT DATA FOR HEAT-EXCHANGER No-6 -----
354.   AIRFLR = HFR
355.   Cells(4, 16) = TH1 - 273 'H2 Temperature IN (oC)
356.   Cells(5, 16) = TH2 - 273 'H2 Temperature OUT (oC)
357.   Cells(6, 16) = TC1 - 273 'AIR Temperature In (oC)
358.   Cells(7, 16) = TC2 - 273 'AIR Temperature OUT (oC)
359.   Cells(10, 16) = NTU 'Number of Elements (No)
360.   Cells(11, 16) = AREAHEX 'Shell Area (m^2)
361.   Cells(12, 16) = EPS * 100 'Effectiveness (%)
362.   Cells(13, 16) = QEFF 'Heat Transfer Rate (KW)
363.   Cells(14, 16) = AIRFLR 'N2 Flow Rate (Kg/hr)
364. '-----
365. '===== HEAT EXCHANGER-7 CALCULATION =====
366. 'Cooling remaining of N2 With air
367.   TL = Cells(21, 16)
368.   TOD = Cells(22, 16)
369. 'NITROGEN
370.   N2FRREM = N2TOTAVAILABLE - N2FLR 'N2 remaining to be cooled (Kg/day)
371.   TH1 = N2ITMTEMP + 273           'N2 Temperature IN
372.   TH2 = CIT + 273
373.   N2ITK = TH2
374.   SCN2 = NITROSPCHEAT(N2ITK)           'N2 Specific Heat (kJ/kg.K)
375.   CN2 = ((N2FRREM / 24) / 3600) * SCN2 'N2 Heat capacity (KW/oK)
376.   QN2 = CN2 * (TH1 - TH2)           'Q-N2 (kW)
377. 'Air Flow rate needed to Cool N2
378.   Cells(19, 16) = AIRTEMIN
379.   TC1 = 25 + 273
380.   AIRINTK1 = 25 + 273
381.   SCAIR = AIRSPECIFICHEAT(AIRINTK1)
382. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.

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383. FLAG = 2
384. U = 0.02
385. CHOT = CN2: Q = QN2: SCHOT = SCN2: SCCOLD = SCAIR
386. Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN
GER
387. 'DATA
388. AIRFR = HFR
389. Cells(17, 16) = N2ITMTEMP 'N2 Temperature IN (oC)
390. Cells(18, 16) = TH2 - 273 'N2 Temperature OUT (oC)
391. Cells(19, 16) = 25 'AIR Temperature IN (oC)
392. Cells(20, 16) = TC2 - 273 'AIR Temperature OUT(oC)
393. Cells(23, 16) = NTU 'Number of Elements (No)
394. Cells(24, 16) = AREAHEX 'Shell Area (m^2)
395. Cells(25, 16) = EPS * 100 'Effectiviness (%)
396. Cells(26, 16) = QEFF 'Heat Transfer Rate (KW)
397. Cells(27, 16) = AIRFR 'Air Flow Rate (Kg/hr)
398. Cells(28, 16) = COMPOP 'Condenser inside Pressure (Atm.)
399. '===== COMPRESSOR-3 ===== NH3TOTAL
400. '...INPUT
401. COMPIP = Cells(21, 11) 'Compressor Inlet Pressure (atm.)
402. COMPOP = Cells(22, 11) 'Compressor Outlet Pressure (atm.)
403. Cells(23, 11) = CIT 'Gas Temperature (oC)
404. COMETREFF = Cells(24, 11) 'Compressor Entropy Efficiency (%)
405. SPHASVOL = Cells(25, 11) 'Single Phase Voltage (Volts)
406. MOTOREFF1 = Cells(26, 11) 'Single Phase Motor Efficiency (%)
407. THREPASEVOL = Cells(27, 11) '3 Phase Voltage (Volts)
408. MOTOREFF3 = Cells(28, 11) '3 Phase Motor Efficiency (%)
409. '...Chemical Calculation
410. TK = CIT + 273 'Inlet Gas Temperature (oK)
411. NH3SPECHEAT = NH3SPECHEAT(TK) 'NH3 Specific Heat (kJ/Kg.K)kJ/kg.K (>1atm)
412. NH3TEMPC = CIT
413. GAMMA = 1.289 'NH3GAMMA(NH3TEMPC) 'GAMMA=Cp/Cv
414. RHONH3 = NH3DENSITY(NH3TEMPC) 'NH3 Density (Kg/m^3)
415. NH3KG = NH3TOTUREA 'NH3 Rquired for Urea(Kg/day)
416. NH3VOLD = NH3KG / RHONH3 'NH3 Volume m^3/day
417. NH3VOLM = (NH3VOLD / 24) / 60 'NH3 Volume m^3/min
418. NH3VOLIT = NH3VOLM * 1000 'NH3 Volume L/min
419. Cells(20, 11) = NH3VOLIT 'NH3 Volume L/min,<=====
420. NH3MOL = NH3KG / NH3MW 'NH3 Mols
421. ENTCC = NH3MOL * R * Logn(COMPOP / COMPIP)
422. GASTEMPC = NH3TEMPC: GASVOL = NH3VOLIT
423. MASSMIXCP = 2.22 '1.13
424. STGE = 5
425. Call COMPRESSOR(GASTEMPC, COMPOP, COMPIP, GAMMA, GASVOL, OUTADIATEMP, COMETREFF, WATT, ENTCC, DRMOTWATT, DRMOTHP, MOTOREFF1, MOTOREFF3, SPH
ASVOL, THREPASEVOL, CURRENT1, CURRENT3)
426. '===== CONDENSER-2 (EXCHANGER) CALCULATION =====
427. T1L = Cells(34, 16)
428. TOD1 = Cells(35, 16)
429. T1HC = OUTADIATEMP
430. Cells(30, 11) = T1HC
431. T1H = T1HC + 273
432. T2HC = Cells(31, 16)
433. T2H = T2HC + 273
434. '...NH3
435. TK = T1H
436. CCNH3 = NH3SPECHEAT(TK)
437. CNH3 = ((NH3TOTUREA / 24) / 3600) * CCNH3
438. QNH3 = CNH3 * (T1H - T2H)
439. '...AIR
440. T1C = 25 + 273
441. AIRINTK1 = T1C
442. CCAIR2 = AIRSPECIFICHEAT(AIRINTK1)
443. AIRFR2 = 1
444. 50 CAIR2 = ((AIRFR2 / 24) / 3600) * CCAIR2
445. T2C = QNH3 / CAIR2 + T1C 'Air Temperature OUT (K)

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446. QAIR1 = CAIR2 * (T2C - T1C)
447. If T1H - T2C >= 0 Then
448. GoTo 60
449. Else
450. AIRFR2 = AIRFR2 + 0.1
451. GoTo 50
452. 60 End If
453. P1 = (T2C - T1C) / (T1H - T1C)
454. R1 = (T1H - T2H) / (T2C - T1C)
455. DELTAA = T1H - T2C
456. DELTAB = T2H - T1C
457. FCORF = 1
458. LMTD = (DELTAA - DELTAB) / Logn(DELTAA / DELTAB) ' (K)
459. COLD = CAIR2: CHOT = CNH3: CFLUIDH = CNH3: TL = TL1: TOD = TOD1: AX1 = 1.2
460. '...DATA OUT
461. Cells(30, 16) = OUTADIATEMP
462. Cells(33, 16) = T2C - 273 'Air Temperature OUT (oC)
463. '=====
464. ' NH3 --> POWER
465. '=====
466. NH3HHV = NH3EXTRA * 2.604 'High Heating Value (kW)
467. NH3LHV = NH3EXTRA * 2.15 'Low Heating Value (kW)
468. Cells(53, 3) = NH3HHV 'High Heating Value (kW)
469. Cells(54, 3) = NH3LHV 'High Heating Value (kW)
470. '=====
471. ' Cell Heat Losses
472. '=====
473. '----- HEAT IN -----
474. '...N2
475. N2ITK = CITK
476. CN2 = NITROSPCHEAT(N2ITK) 'kJ/kg.K
477. QN2IN = ((N2TOTAVAILABLE / 24) / 3600) * CN2 * N2ITK '(kW)
478. '...H2
479. H2TK = CITK
480. CH2 = HYDROGENSPEHEAT(H2TK) 'kJ/kg.K (T=K)
481. QH2IN = ((H2TOTAVAILABLE / 24) / 3600) * CH2 * H2TK '(kW)
482. 'Total Heat IN
483. QTOTIN = QN2IN + QH2IN + CELLPower '(kW)
484. '----- HEAT OUT -----
485. '...NH3
486. TK = CITK
487. CNH3 = NH3SPECIFICHEAT(TK) 'kJ/kg.K (1atm)
488. QNH3OUT = ((NH3TOTAL / 24) / 3600) * CNH3 * TK '(kW)
489. '...H2
490. H2TK = CITK
491. CH2 = HYDROGENSPEHEAT(H2TK) 'kJ/kg.K (T=K)
492. QH2IN = ((H2SOFC / 24) / 3600) * CH2 * H2TK '(kW)
493. 'Total Heat OUT
494. QTOTOUT = QNH3OUT + QH2IN '(kW)
495. '----- HEAT LOSSES -----
496. QLOSSES = QTOTIN - QTOTOUT
497. 'Cells OUTPUT
498. Cells(36, 11) = QTOTIN
499. Cells(37, 11) = QTOTOUT
500. Cells(38, 11) = QLOSSES
501. '===== COMPRESSOR-4 ===== NH3 EXTRA
502. '...INPUT
503. COMPIN = Cells(42, 11) 'Compressor Inlet Pressure (atm.)
504. COMPOT = Cells(43, 11) 'Compressor Outlet Pressure (atm.)
505. Cells(44, 11) = CIT 'Gas Temperature (oC)
506. COMETREFF = Cells(45, 11) 'Compressor Entropy Efficiency (%)
507. SPHASVOL = Cells(46, 11) 'Single Phase Voltage (Volts)
508. MOTOREFF1 = Cells(47, 11) 'Single Phase Motor Efficiency (%)
509. THREPASEVOL = Cells(48, 11) '3 Phase Voltage (Volts)
510. MOTOREFF3 = Cells(49, 11) '3 Phase Motor Efficiency (%)

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511. '...Chemical Calculation
512. TK = CIT + 273 'Inlet Gas Temperature (oK)
513. NH3SPECHEAT = NH3SPECHEAT(TK) 'NH3 Specific Heat (kJ/Kg.K)kJ/kg.K (>1atm)
514. NH3TEMP = CIT
515. GAMMA = NH3GAMMA(NH3TEMP) 'GAMMA=Cp/Cv
516. RHONH3 = NH3DENSITY(NH3TEMP) 'NH3 Density (Kg/m^3)
517. NH3KGX = NH3EXTRA 'NH3 Required for Urea(Kg/day)
518. NH3VOLD = NH3KGX / RHONH3 'NH3 Volume m^3/day
519. NH3VOLM = (NH3VOLD / 24) / 60 'NH3 Volume m^3/min
520. NH3VOLIT = NH3VOLM * 1000 'NH3 Volume L/min
521. Cells(41, 11) = NH3VOLIT 'NH3 Volume L/min,<=====
522. NH3MOL = NH3KG / NH3MW 'NH3 MoIs
523. ENTCC = NH3MOL * R * Logn(COMPOP / COMPIP)
524. GASTEMPC = NH3TEMP: GASVOL = NH3VOLIT
525. OUTADIATEMP = ((GASTEMPC + 273) * ((COMPOP / COMPIP) ^ ((GAMMA - 1) / GAMMA))) - 273 ' OUTLET ADIABATIC TEMPERATURE
526. DRMOTWATT = ((OUTADIATEMP + 273) - (GASTEMPC + 273)) * 2.22 * ((NH3KGX + NH3TOTUREA) / 86400) / 0.75 'KW
527. Cells(51, 11) = OUTADIATEMP
528. Cells(52, 11) = DRMOTWATT
529. Cells(53, 11) = DRMOTHP
530. Cells(54, 11) = CURRENT1
531. Cells(55, 11) = CURRENT3
532. '===== CONDENSER-3 (EXCHANGER) CALCULATION =====
533. COMPIP = COMPOP
534. TL1 = Cells(49, 16) 'TUBE LENGTH (m)
535. TOD1 = Cells(50, 16) 'TUBE DIAMETER (m)
536. TH1 = OUTADIATEMP + 273 'NH3 TEMPERATURE IN (K)
537. TH2 = CIT + 273
538. '...NH3
539. TK = TH1
540. SCNH3 = NH3SPECHEAT(TK)
541. CNH3 = (((NH3EXTRA + NH3TOTUREA) / 24) / 3600) * SCNH3
542. QNH3 = CNH3 * (TH1 - TH2)
543. '...AIR
544. TC1 = 25 + 273
545. AIRINTK1 = TC1
546. SCAIR2 = AIRSPECIFICHEAT(AIRINTK1)
547. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
548. FLAG = 2
549. U = 0.02
550.
551. CHOT = CNH3: Q = QNH3: SCHOT = SCNH3: SCCOLD = SCAIR2
552. Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN
GER
553. '...DATA OUT
554. AIRFR2 = HFR
555. Cells(44, 16) = COMPIP 'Condenser inlet Pressure (atm)
556. Cells(45, 16) = OUTADIATEMP 'Inlet NH3 Temperature (oC)
557. Cells(46, 16) = TH2 - 273 'Outlet NH3 Temperature (oC)
558. Cells(47, 16) = 25 'Inlet Air Temperature (oC)
559. Cells(48, 16) = TC2 - 273 'Outlet Air Temperature (oC)
560. Cells(51, 16) = NTU 'Number of Elements (No)
561. Cells(52, 16) = AREAHEX 'Shell Area (m^2)
562. Cells(53, 16) = EPS * 100 'Effectiviness (%)
563. Cells(54, 16) = QEFF 'Heat Transfer Rate (KW)
564. Cells(55, 16) = AIRFR2 'Air Flow Rate (Kg/hr)
565. '===== CO2 =====
566.
567. 70 End Sub
568. Static Function Logn(X)
569. Logn = Log(X) / Log(2.718282)
570. End Function
571. Private Static Sub DELTAH(A, B, N, INTEGRALH)
572. H = (B - A) / N
573. T = A
574. SUMM = DELCP(T): C = 2

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575. For K = 1 To N - 1
576. C = 6 - C ' Rem GENERATES COEFFICIENTS 4,2,4,2,...
577. T = A + K * H
578. SUMM = SUMM + C * DELCP(T)
579. Next K
580. SUMM = Sum + DELCP(T)
581. INTEGRALH = (H / 3) * SUMM
582. End Sub
583. Private Static Function DELCP(T)
584. DELCP = -55.169 + 49.856 * 10 ^ -3 * T - 4.05 * 10 ^ 5 * T ^ -2 - 1.976 * 10 ^ -6 * T ^ 2
585. End Function
586. Private Static Function DELCPT(T)
587. DELCPT = (-55.169 + 49.856 * 10 ^ -3 * T - 4.05 * 10 ^ 5 * T ^ -2 - 1.976 * 10 ^ -6 * T ^ 2) ' / T
588. End Function
589. Private Static Function NH3SPECIFICHEAT(TK) 'kJ/kg.K (1atm)
590. A = 1.0948345: B = 0.002555016: C = 27119.844
591. NH3SPECIFICHEAT = A + B * GASTK + C / (TK) ^ 2
592. End Function
593. Private Static Function NH3SPECHEAT(TK) 'kJ/kg.K (>1atm)
594. A = 2.200434: B = -0.001750475: C = 0.000026445871: D = -0.0000000741651: E = 7.330493E-11
595. NH3SPECHEAT = A + B * TK + C * TK ^ 2 + D * TK ^ 3 + E * TK ^ 4
596. End Function
597. Private Static Function HYDROGENSPECHEAT(H2TK) 'T=oK kJ/kg.K
598. ZA = 8.3580785: ZB = 0.046774926: ZC = -0.00014346423: ZD = 0.00000023506381: ZE = -2.3076196E-10: ZF = 1.4608608E-13
599. ZG = -6.1673082E-17: ZH = 1.7508367E-20: ZI = -3.2962768E-24: ZJ = 3.9405226E-28: ZK = -2.7046605E-32: ZL = 8.1083083E-37
600. HYDROGENSPECHEAT = ZA + ZB * H2TK + ZC * H2TK ^ 2 + ZD * H2TK ^ 3 + ZE * H2TK ^ 4 + ZF * H2TK ^ 5 + ZG * H2TK ^ 6 + ZH * H2TK ^ 7 + ZI * H2TK ^ 8 + ZJ * H2TK ^ 9 + ZK * H2TK ^ 10 + ZL * H2TK ^ 11
601. End Function
602. Private Static Function NITROSPCHEAT(N2ITK) 'kJ/kg.K
603. SA = 1.100752
604. SB = -0.00053474045
605. SC = 0.0000013971884
606. SD = -1.2555363E-09
607. se = 6.0109266E-13
608. SF = -1.6836213E-16
609. SG = 2.7735985E-20
610. SH = -2.5125233E-24
611. SI = 1.0066147E-28
612. SJ = -5.1950017E-34
613. NITROSPCHEAT = SA + SB * N2ITK + SC * N2ITK ^ 2 + SD * N2ITK ^ 3 + se * N2ITK ^ 4 + SF * N2ITK ^ 5 + SG * N2ITK ^ 6 + SH * N2ITK ^ 7 + SI * N2ITK ^ 8 + SJ * N2ITK ^ 9
614. End Function
615. Private Static Function AIRSPECIFICHEAT(AIRINTK) 'T=oK
616. TA = 1.0828694: TB = -0.00063119116: TC = 0.0000016253087: TD = -1.3949526E-09: TE = 5.3826153E-13: TF = -7.9021928E-17
617. AIRSPECIFICHEAT = TA + TB * AIRINTK + TC * AIRINTK ^ 2 + TD * AIRINTK ^ 3 + TE * AIRINTK ^ 4 + TF * AIRINTK ^ 5
618. End Function
619. Private Static Sub HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'H
EAT EXCHANGER
620. AREAHEX = 3.14 * TOD * TL
621. LMTD = Q / (U * AREAHEX)
622. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
623. '----- HEATING -----
624. If FLAG = 1 Then
625. DELTAA = TH1 - TC2
626. DELTAB = TH2 - TC1
627. LMTD = Q / (U * AREAHEX)
628. X1 = 1
629. 300 S1 = DELTAA / (LMTD - Logn(DELTAA))
630. S2 = X1 / (LMTD - Logn(X1))
631. If S2 >= S1 Then
632. GoTo 400
633. Else
634. X1 = X1 + 0.1
635. GoTo 300
636. 400 End If

```



```

637. DELTAB = X1
638. TH2 = DELTAB + TC1
639. GoTo 700
640. End If
641. '-----
642. '----- COOLING -----
643. If FLAG = 2 Then
644. 'DELTA = TH1 - TC2
645. DELTAB = TH2 - TC1
646. LMTD = Q / (U * AREAHEX)
647. X1 = 2
648. 500 S1 = Logn(X1) - X1 / LMTD
649. S2 = Logn(DELTAB) - DELTAB / LMTD
650. If S1 >= S2 Then
651. GoTo 600
652. Else
653. X1 = X1 + 0.1
654. GoTo 500
655. 600 End If
656. DELTAA = X1
657. TC2 = TH1 - DELTAA
658. End If
659. '-----
660. 700 P = (TC2 - TC1) / (TH1 - TC1)
661. R = (TH1 - TH2) / (TC2 - TC1)
662. If R > 1 Then
663. R1 = 1 / R
664. P1 = P * R
665. Else
666. P1 = P
667. R1 = R
668. End If
669. A1 = (((R1) ^ 2 + 1) ^ 0.5) / (1 - R1)
670. A2 = Logn((1 - R1 * P1) / Abs(1 - P1))
671. A3 = 2 - P1 * (1 + R1 - (1 + (R1) ^ 2)) ^ 0.5 'up
672. A4 = Abs(2 - P1 * (1 + R1 + (1 + (R1) ^ 2)) ^ 0.5) 'down
673. A5 = Logn(A3 / A4)
674. FCORF = (A1 * A2) / A5
675. If Abs(FCORF) > 1 Then
676. FCORF = 1
677. End If
678. If FLAG = 1 Then
679. LMTD = Q / (U * AREAHEX * FCORF)
680. CHOT = Q / (TH1 - TH2)
681. HFR = CHOT * 24 * 3600 / SCHOT
682. GoTo 800
683. End If
684. If FLAG = 2 Then
685. LMTD = Q / (U * AREAHEX * FCORF)
686. CCOLD = Q / (TH1 - TH2)
687. HFR = CCOLD * 24 * 3600 / SCHOT
688. End If
689. 'EFFECTIVENESS
690. 800 If CCOLD > CHOT Then
691. CMIN = CHOT
692. C1 = CHOT
693. EPS = (C1 * (TC2 - TC1)) / (CMIN * (TH1 - TC1))
694. GoTo 900
695. Else
696. CMIN = CCOLD
697. C1 = CCOLD
698. EPS = (C1 * (TH1 - TH2)) / (CMIN * (TH1 - TC1))
699. 900 End If
700. QEFF = EPS * CMIN * (TH1 - TC1)
701. 'Number of ELEMENT

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702. NTU = U * AREAHEX / CMIN
703. If NTU <= 1 Then
704. NTU = 1
705. Else
706. End If
707. End Sub
708.
709. Private Static Function FCORF1(P, R)
710. S1 = (2 - P * (1 + R - (1 + R ^ 2) ^ 0.5)) / (2 - P * (1 + R + (1 + R ^ 2) ^ 0.5))
711. S2 = (1 - R * P) / (1 - P)
712. S3 = ((1 + R ^ 2) ^ 0.5) / (1 - R)
713. FCORF1 = S3 * Logn(S2) * (Logn(S1)) ^ -1
714. End Function
715. Private Static Function NH3DENSITY(NH3TEMPC) ' T=oC
716. Dim F As Double
717. A = 0.76249107: B = -0.0030065503: C = 0.000012095274: D = -0.00000038570889: E = 7.2102508E-11: F = -5.5332429E-14
718. NH3DENSITY = A + B * NH3TEMPC + C * NH3TEMPC ^ 2 + D * NH3TEMPC ^ 3 + E * NH3TEMPC ^ 4 + F * NH3TEMPC ^ 5
719. End Function
720. Private Static Function NH3GAMMA(NH3TEMPC) ' T=oC
721. A = 1.3320734: B = -0.0049999747: C = 0.000010911546: D = -0.00000002975822: E = 3.4313946E-12
722. NH3GAMMA = A + B * NH3TEMPC + C * NH3TEMPC ^ 2 + D * NH3TEMPC ^ 3 + E * NH3TEMPC ^ 4
723. End Function
724. Private Static Sub COMPRESSOR(GASTEMPC, COMPOP, COMPPI, GAMMA, GASVOL, OUTADIATEMP, COMETREFF, WATT, ENTCC, DRMOTWATT, DRMOTHP, MOTOREFF1, MOTO
REFF3, SPHASVOL, THREPAEVL, CURRENT1, CURRENT3)
725. A1 = 1000
726. A2 = 60
727. End Sub

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HEAT BALANCE CCS with dark fermentation

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1. Sub Sheet11_Button1_Click()
2.
3. '
4. '=====
5. ' HEAT BALANCE
6. '=====
7. '===== OUTPUT and INPUT FROM DARK
8. DFBTANK = ActiveWorkbook.Worksheets("DFB-ADB").Cells(100, 4) 'Energy IN DARK CSTR -(kW)
9. ADBTANK = ActiveWorkbook.Worksheets("DFB-ADB").Cells(101, 4) 'Energy IN ADB CSTR -(kW)
10. WESTANK1 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(102, 4) 'Energy IN ADB TANK1 -(kW)
11. WESTANK2 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(103, 4) 'Energy IN ADB TANK2 -(kW)
12. STEAMFRA = ActiveWorkbook.Worksheets("SOFC").Cells(35, 11) 'Energy IN ADB TANK2 -(kW)
13. STEAMFRAXX = ActiveWorkbook.Worksheets("SOFC").Cells(52, 4) 'Energy IN ADB TANK2 -(kW)
14. STEAMFRAYY = ActiveWorkbook.Worksheets("SOFC").Cells(53, 4) 'Energy IN ADB TANK2 -(kW)
15. WESTANK2BBTTT = ActiveWorkbook.Worksheets("SOFC").Cells(28, 11) 'Energy IN ADB TANK2 -(kW)
16. ASDF = ActiveWorkbook.Worksheets("EMS").Cells(43, 11)
17. '===== INPUT FROM ADB
18.
19. '===== SOFC TEMPERATURE
20. SOFCTEMP = ActiveWorkbook.Worksheets("SOFC").Cells(13, 4) 'SOFC Cell Temperature (oC)
21. '===== INPUT DATA FOR TOTAL AIR REQUIRED FOR THE COMPRESSOR
22. AIRDARK = ActiveWorkbook.Worksheets("DFB-ADB").Cells(85, 11) ' AIR REQUIRED FOR DARK (Kg/day)
23. AIRADB = ActiveWorkbook.Worksheets("DFB-ADB").Cells(85, 18) ' AIR REQUIRED FOR ADB (Kg/day)
24. AIRSOFC = ActiveWorkbook.Worksheets("SOFC").Cells(10, 4) ' AIR REQUIRED FOR SOFC cell (Kg/day)
25. AIRSOFEC = ActiveWorkbook.Worksheets("SOFEC").Cells(26, 16) ' AIR REQUIRED FOR SOFEC HECH (Kg/day)
26. AIRITM = ActiveWorkbook.Worksheets("ITM").Cells(5, 4) ' AIR REQUIRED FOR (ITM)HE (Kg/day)
27. AIRSSAS1 = ActiveWorkbook.Worksheets("SSAS").Cells(27, 16) ' AIR REQUIRED FOR SSAS HE (Kg/day)
28. AIRSSAS2 = ActiveWorkbook.Worksheets("SSAS").Cells(14, 16) ' AIR REQUIRED FOR SSAS HE (Kg/day)
29. AIREMS = ActiveWorkbook.Worksheets("EMS").Cells(32, 11) ' AIR REQUIRED FOR EMS Condenser(Kg/day)
30. AIRTEMP = ActiveWorkbook.Worksheets("ITM").Cells(8, 4) ' AIR TEMPERATURE from (ITM) (oC)
31. '===== ENERGY IN COMPRESSORS & PUMPMS (kW)
32. COM1 = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(28, 11) 'Compressor No1[MFI(ZM)](kW)-
33. COM4 = ActiveWorkbook.Worksheets("SSAS").Cells(52, 11) 'Compressor No4[SSAS] (kW)-
34. COM5 = ActiveWorkbook.Worksheets("SOFC").Cells(32, 4) 'Compressor No5[SOFC] (kW)-

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35. COM6 = ActiveWorkbook.Worksheets("SOFC").Cells(49, 16) 'Compressor No6[SOFC] (kW)-
36. COM8 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(117, 4) 'Hydrolic Compressor (KW)-
37. '===== SLUDGE PUMPS =====
38. SP1 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(68, 4) 'SLURY PUMP DARK REACTOR (W)-
39. SP2 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(74, 4) 'SLURY PUMP DARK REACTOR (kW)-
40. SP3 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(108, 4) 'SLURY PUMP DIGESTER (kW)-
41. SP4 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(116, 4) 'SLURY PUMP DIGESTER (kW)-
42. '===== ENERGY IN HEAT EXCHANGER & CONDENSER(kw)
43. HE1 = ActiveWorkbook.Worksheets("ITM").Cells(38, 4) 'Heat Exchanger No1 [ITM] (KW)-
44. HE2 = ActiveWorkbook.Worksheets("EMS").Cells(12, 16) 'Heat Exchanger No2 [EMS] (KW)+
45. HE3 = ActiveWorkbook.Worksheets("EMS").Cells(24, 16) 'Heat Exchanger No3 [EMS] (KW)-
46. HE4 = ActiveWorkbook.Worksheets("SOFEC").Cells(13, 16) 'Heat Exchanger No4 [ITM] (KW)+
47. HE5 = ActiveWorkbook.Worksheets("SOFEC").Cells(26, 16) 'Heat Exchanger No5 [SOFEC] (KW)+
48. HE6 = ActiveWorkbook.Worksheets("SSAS").Cells(13, 16) 'N2 Heat Exchanger No6 [SSAS](KW)+
49. HE7 = ActiveWorkbook.Worksheets("SSAS").Cells(26, 16) 'H2 Heat Exchanger No7 [SSAS](KW)+
50. HE8 = ActiveWorkbook.Worksheets("SOFC").Cells(34, 11) 'Heat Exchanger BOX 8 [SOFC] (KW)-
51. HE9 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(97, 4) 'Heat Exchanger No9 [INNOCULUM] (KW)-
52. HE10 = ActiveWorkbook.Worksheets("SOFC").Cells(51, 4) 'Heat Exchanger BOX 8 [SOFC] (KW)-
53. 'Condenser
54. COND1 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(84, 11) 'Energy OUT DARK Condenser (kW)+
55. COND2 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(84, 18) 'Energy OUT ADB Condenser (kW)+
56. COND3 = ActiveWorkbook.Worksheets("EMS").Cells(30, 11) 'Heat Condenser No1 [EMS](KW)+
57. COND5 = ActiveWorkbook.Worksheets("SSAS").Cells(54, 16) 'Heat Condenser No5 [SSAS](KW)+
58. 'Membranes Heat Loss
59. HLMFI = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(54, 9) 'Heat Loss from MFI Cell (kW)
60. HLITM = ActiveWorkbook.Worksheets("ITM").Cells(41, 4) 'Heat Loss from ITM Cell (kW)
61. HLEMS = ActiveWorkbook.Worksheets("EMS").Cells(29, 16) 'Heat Loss from ITM Cell (kW)
62. HLSOFEC = ActiveWorkbook.Worksheets("SOFEC").Cells(29, 11) 'Heat Loss from SOFEC Cell (kW)
63. HLSASAS = ActiveWorkbook.Worksheets("SSAS").Cells(38, 11) 'Heat Loss from SSAS Cell (kW)
64. HLSOFC = ActiveWorkbook.Worksheets("SOFC").Cells(40, 11) 'Heat Loss from SOFC Cell (kW)
65. HLMFIX = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(20, 11) 'Heat Loss from MFI Cell (kW)
66. 'CO2 CALCULATIONS
67. 'CO2
68. CO2MFI = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(4, 11) 'CO2 From MFI(Kg/Day)
69. CO2SOFEC = ActiveWorkbook.Worksheets("SOFEC").Cells(6, 11) 'CO2 From SOFEC(kg/hr)
70. CO2MFIEMP = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(10, 4) 'CO2 TEMPERATURE From Dark oC
71. CO2SOFECTEMP = ActiveWorkbook.Worksheets("SOFEC").Cells(15, 4) 'CO2 TEMPERATURE From Dark oC
72. CO2PRESIN = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(11, 4) 'CO2 Pressure atm.
73. H2OHEXRECY = ActiveWorkbook.Worksheets("SOFC").Cells(15, 17)
74. SSASAIRFLOW = ActiveWorkbook.Worksheets("SSAS").Cells(55, 16)
75. SOFECAIRFLOW1 = ActiveWorkbook.Worksheets("SOFEC").Cells(8, 11)
76. MFIZMAIRFLW1 = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(50, 11)
77. MFIZMAIRFLW2 = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(49, 11)
78. MFIZMAIRFLW3 = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(20, 11)
79. MFIZMAIRFLW4 = ActiveWorkbook.Worksheets("MFI(ZM)").Cells(19, 11)
80. '=====
81. 'CO2 Calculations
82. R = 8.314 'J/K.mol
83. CO2MW = 44 'Molecular Weight
84. 'CO2 Total Flowrate
85. CO2TOTAL = CO2MFI + CO2SOFEC
86. 'MIXED CO2 Temperature
87. CO2MIXTEMP = (CO2MFI * CO2MFIEMP + CO2SOFEC * CO2SOFECTEMP) / CO2TOTAL 'Mixed CO2 Temperature
88. '===== COMPRESSORE FOR CO2 COM10 =====
89. Cells(67, 16) = CO2PRESIN + 1 'Inlet Pressure atm
90. CO2PRESOUT = Cells(68, 16)
91. CO2PRESOUT = 100 'Compressor Outlet Pressure (atm.)'OUTLET Pressure atm
92. Cells(69, 16) = CO2MIXTEMP 'Inlet Temperature
93. 'CALCULATIONS
94. COMPIP = CO2PRESIN 'Compressor Inlet Pressure (atm.)
95. COMETREFF = Cells(70, 16) 'Compressor Entropy Efficiency (%)
96. SPHASVOL = Cells(71, 16) 'Single Phase Voltage (Volts)
97. MOTOREFF1 = Cells(72, 16) 'Single Phase Motor Efficiency (%)
98. THREPASEVOL = Cells(73, 16) '3 Phase Voltage (Volts)
99. MOTOREFF3 = Cells(74, 16) '3 Phase Motor Efficiency (%)

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100. 'COMPRESSOR DATA
101. GASTK = CO2MIXTEMP + 273 'Inlet Gas Temperature (oK)
102. CO2SPCHEAT = CO2SPEHEAT(GASTK) 'CO2 SPECIFIC HEAT ' Cp of CO2 kJ/Kg K) 'NH3 Specific Heat (kJ/Kg.K)kJ/kg.K (>1atm)
103. T = CO2MIXTEMP
104. RHOCO2 = CO2DENSITY(T) 'NH3 Density (kg/m^3)
105. GAMMA = 1.208 '1.189 'GAMMA=Cp/Cv
106. CO2VOLD = CO2TOTAL / RHOCO2 'CO2 Volume m^3/day
107. CO2VOLM = (CO2VOLD / 24) / 60 'CO2 Volume m^3/min
108. CO2VOLIT = CO2VOLM * 1000 'CO2 Volume L/min
109. Cells(66, 16) = CO2VOLIT 'CO2TOTAL 'CO2 Volume L/min,<=====
110. CO2MOL = CO2TOTAL / CO2MW 'CO2 Mol
111. GASTEMPC = CO2MIXTEMP: GASVOL = CO2VOLIT
112. Call COMPRESSOR(GASTEMPC, COMPOP, COMPIP, GAMMA, GASVOL, OUTADIATEMP, COOLSYS, COMETREFF, WATT, ENTCC, DRMOTWATT, DRMOTHP, MOTOREFF1, MOTOR
EFF3, SPHASVOL, THREPASEVOL, CURRENT1, CURRENT3)
113. OUTADIATEMP = ((CO2MIXTEMP + 273) * ((CO2PRESOUT / (CO2PRESIN + 1)) ^ ((1.18 - 1) / 1.18))) - 273 ' OUTLET ADIABATIC TEMPERATURE
114. DRMOTWATT = (((OUTADIATEMP + 273) - (CO2MIXTEMP + 273)) * CO2SPCHEAT * (CO2TOTAL / 86400)) / (MOTOREFF1 / 100) 'KW
115. Cells(65, 21) = OUTADIATEMP
116. Cells(66, 21) = DRMOTWATT
117. Cells(67, 21) = DRMOTHP
118. Cells(68, 21) = CURRENT1
119. Cells(69, 21) = CURRENT3
120. COM10 = DRMOTWATT
121. '----- CO2 COOLING Heat EXCHANGER N011
122. TL = Cells(81, 16)
123. TOD = Cells(82, 16)
124. 'CO2
125. TH1 = OUTADIATEMP + 273
126. TH2 = 25.1 + 273
127. GASTK = TH2
128. SCCO2 = CO2SPEHEAT(GASTK)
129. CCO2 = ((CO2TOTAL / 24) / 3600) * SCCO2 'O2 Heat capacity (KW/oK)
130. QO2 = CCO2 * (TH1 - TH2)
131. 'Air Flow rate needed to Cool CO2
132. Cells(78, 16) = 25 'AIR TEMPERATURE IN oC
133. TC1 = 25 + 273
134. AIRINTK1 = TC1
135. AIRINTK1 = 25.1 + 273
136. SCAIR = AIRSPECIFICHEAT(AIRINTK1)
137. FLAG = 2
138. U = 0.02
139. CHOT = CCO2: Q = QO2: SCHOT = SCCO2: SCCOLD = SCAIR
140. Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN
GER
141. 'OUTPUT
142. AIRCO2 = HFR
143. Cells(77, 16) = OUTADIATEMP
144. 'Cells(78, 16) = CO2TEMPUREA
145. Cells(79, 16) = 25 'AIR TEMPERATURE IN oC
146. Cells(80, 16) = TC2 - 273 'AIR TEMPERATURE IN oC
147. Cells(83, 16) = NTU
148. Cells(84, 16) = AREAHEX
149. Cells(85, 16) = EPS
150. Cells(86, 16) = QEFF
151. Cells(87, 16) = AIRCO2
152. HE11 = QEFF
153. 'INJECTION
154. Depth = Cells(91, 16)
155. MASSCO2KG = ((CO2TOTAL / 24) / 3600) 'kg.s-1
156. VOLWAT = MASSCO2KG / 0.472 ' m3.s-1 (volume of CO2gas)
157. VOLMATE1 = MASSCO2KG / 818 'm3.s-1 (volume of CO2Liquid)
158. 'Assuming pump diameter =0.1 m'
159. PIP1 = Cells(88, 16)
160. AREAPUMP12 = (3.14) * (PIP1 * PIP1) / 4
161. VOLPUMP = VOLMATE1 / AREAPUMP12 'Velocity m/s'
162. 'k = 1.35

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163. VISCOS = 0.0989 / 1000000 '(m2/s)
164. RYNOL = (PIP1 * VOLPUMP) / VISCOS
165. FRIC = 0.25 / Log((1.8 / (3.7 * PIP1)) + (5.7 / RYNOL)) ^ 2 '
166. PIPELENGTH = 1000 + Depth 'Length of pipe (m)'
167. KPIPE = FRIC * PIPELENGTH / PIP1
168. KFIT = 1.8 + KPIPE
169. HTE1 = KFIT * (VOLPUMP * VOLPUMP) / (19.6)
170. HESDF2 = HTE1 + Depth
171. PUMPEFF = Cells(89, 16)
172. POWEPUM = (HESDF2 * 9.81 * 818 * VOLMATE1) / PUMPEFF
173. Cells(90, 16) = POWEPUM / 1000
174. PRESSURE1 = MASSCO2KG / AREAPUMP12 'kg/m2.s
175. DELTAPRESSURE = 818 * 9.81 * Depth * 0.00000987
176. CO2PRESOUT92 = DELTAPRESSURE - CO2PRESOUT
177. Cells(92, 16) = CO2PRESOUT92 'atm
178. '=====
179. 'TOTAL STEAM'
180. MSTEAMTOT = ((H2OHEXRECY + (STEAMFRAXX - STEAMFRAYY) + STEAMFRA) / 86400) * (1000 - WESTANK2BBTTT) * 4.18
181. Cells(70, 21) = MSTEAMTOT
182. 'Waste Eanks Heat Losses
183. '=====
184. '                                CALCULATIONS
185. '=====
186. '===== ENERGY OUT (kW)
187. GASTURB = ActiveWorkbook.Worksheets("SOFC").Cells(57, 16) 'Steam Turbine [SOFC] (kW)+
188. '=====
189. 'POWER and Voltage
190. EMSPower = ActiveWorkbook.Worksheets("EMS").Cells(18, 11) 'POWER IN OF EMS(kW)-
191. SOFECPOWER = ActiveWorkbook.Worksheets("SOFEC").Cells(25, 11) 'POWER IN OF SOFEC (kW)-
192. ITMPOWER = ActiveWorkbook.Worksheets("ITM").Cells(26, 11) 'POWER OUT OF ITM (kW)+
193. SOFCPOWER = ActiveWorkbook.Worksheets("SOFC").Cells(22, 11) 'POWER OUT OF SOFC (kW)+
194. NH3HHV = ActiveWorkbook.Worksheets("SSAS").Cells(53, 3) 'NH3 Equivalent Power HHV of NH3(KW)+
195. NH3LHV = ActiveWorkbook.Worksheets("SSAS").Cells(54, 3) 'NH3 Equivalent Power LHV of NH3(KW)+
196. SSASPOWER = ActiveWorkbook.Worksheets("SSAS").Cells(49, 3)
197. '=====
198. ' IMPELLERS
199. IMPDFB = ActiveWorkbook.Worksheets("DFB-ADB").Cells(48, 12) 'IMPELLER DARK TEACTOR (HP)
200. IMPADB = ActiveWorkbook.Worksheets("DFB-ADB").Cells(48, 19) 'IMPELLER BIO TEACTOR (HP)
201. IMPINOC = ActiveWorkbook.Worksheets("DFB-ADB").Cells(65, 12) 'IMPELLER BIO TEACTOR (HP)
202. IMPMIX = ActiveWorkbook.Worksheets("DFB-ADB").Cells(8, 23) 'IMPELLER MIXING TANK
203. CB1W = ActiveWorkbook.Worksheets("DFB-ADB").Cells(85, 4) 'BLOWER BIO REACTOR (WATT)
204. CB1 = CB1W 'BLOWER BIO REACTOR (KW)
205. '=====
206. ' TOTAL AIR REQUIRED PUMPING)
207. COOLAIR = 25
208. AIRSSAS = AIRSSAS1 + AIRSSAS2 + AIRSSAS3 + SSASAIRFLOW
209. TOTAIR = AIRSOFC + AIRITM + AIRSSAS + AIREMS + AIRDARK + AIRADB + MFIZMAIRFLW1 + AIRCO2 'TOTAL AIR REQUIRED for the SYSTEM (Kg/day)
210. 'Air Density
211. COOLAIR = AIRTEMP
212. AIRDEN = AIRDENSITY(AIRTEMP) 'Air Density(Kg/m^3)
213. 'Volumetric Flow
214. AIRVOL1 = TOTAIR / AIRDEN 'Air Volume (m^3/day)
215. AIRVOL2 = AIRVOL1 * 1000 'Air Volume (Lt/day)
216. AIRVOL = (AIRVOL2 / 24) / 60 'Air Volume (Lt/min)
217. 'Compressor DATA IN
218. Cells(42, 4) = AIRADB '(Kg/day)
219. Cells(43, 4) = AIRDARK '(Kg/day)
220. Cells(44, 4) = AIREMS '(Kg/day)
221. Cells(45, 4) = AIRSOFC '(Kg/day)
222. Cells(46, 4) = AIRITM '(Kg/day)
223. Cells(47, 4) = AIRSOFEC '(Kg/day)
224. Cells(48, 4) = AIRSSAS '(Kg/day)
225. Cells(49, 4) = AIRVOL 'Air Volume (Lt/min)
226. COMPIN = Cells(50, 4) 'Compressor Inlet Pressure (Atm)
227. COMPPOP = Cells(51, 4) 'Compressor Outlet Pressure (Atm)

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228. COMPIT = Cells(52, 4) 'Compressor Inlet Temperatur (oC)
229. COMETREFF = Cells(53, 4) 'Compressor ENTROPY Efficiency (%)
230. MOTOREFF1 = Cells(47, 11) 'Motor Efficiency 1-Phase (%)
231. SPHASVOL = Cells(48, 11) 'Single Phase Voltage (Volt)
232. MOTOREFF3 = Cells(50, 11) 'Motor Efficiency 3-Phase (%)
233. THREPASEVOL = Cells(51, 11) '3-Phase Voltage (Volt)
234. ' CONSTANT
235. RAIR = 408.97 'J/Kg.K
236. GAMMA = 2.0339 'Constant for Diatomic gas compression adiabatic temperature rise
237. ENTCC = AIRDEN * RAIR 'Entropy Change Constant (J/K.M^3)
238. '
239. '=====  
Compressor-1 Calculations  
=====
240. GASTEMPC = COMPIT: GASVOL = AIRVOL
241. OUTADIATEMP = ((GASTEMPC + 273) * ((COMPOP / COMPIP) ^ ((1.4 - 1) / 1.4))) - 273 ' OUTLET ADIABATIC TEMPERATURE
242. DRMOTWATT = (((OUTADIATEMP + 273) - (GASTEMPC + 273)) * 1.15 * (TOTAIR / 86400)) / (MOTOREFF1 / 100) 'KW
243. Call COMPRESSOR(GASTEMPC, COMPOP, COMPIP, GAMMA, GASVOL, OUTADIATEMP, COOLSYS, COMETREFF, WATT, ENTCC, DRMOTWATT, DRMOTHP, MOTOREFF1, MOTOREFF3
, SPHASVOL, THREPASEVOL, CURRENT1, CURRENT3)
244. '..... DATA OUTPUT ....
245. Cells(42, 11) = OUTADIATEMP
246. Cells(43, 11) = COOLAIR
247. Cells(44, 11) = COOLSYS
248. Cells(45, 11) = OUTADIATEMP
249. Cells(45, 11) = DRMOTWATT
250. Cells(46, 11) = DRMOTHP
251. Cells(49, 11) = CURRENT1
252. Cells(52, 11) = CURRENT3
253. '=====  
Energy  
=====
254. COM9 = DRMOTWATT 'Air Compressor
255. TOTALINKW = COM1 + COM3 + COM4 + COM5 + COM6 + COM7 + COM8 + COM9 + SP1 + SP2 + SP3 + SP8 + CB1 'kw
256. ' DATA OUTPUT
257. '=====  
ENERGY IN
258. '
259. '=====  
ENERGY IN for Compressors
260. 'ENERGY IN for Compressors
261. TOTALCOM = COM1 + COM3 + COM4 + COM5 + COM6 + COM7 + COM8 + COM10 + COOLSYS 'Compressors
262. Cells(56, 3) = COM1 'Compressor No1[MFI(ZM)](kW)
263. Cells(58, 3) = COM3 'Compressor No3[SSAS] (kW)
264. Cells(59, 3) = COM4 'Compressor No4[SSAS] (kW)
265. Cells(60, 3) = COM5 'Compressor No5[SOFC] (kW)
266. Cells(61, 3) = COM6 'Compressor No6[SOFC] (kW)
267. Cells(62, 3) = COM7 'Compressor No7[SOFC] (kW)
268. Cells(63, 3) = COM8 'Compressor No7[ADB] CAKING (kW)
269. Cells(64, 3) = COM9 'Compressor No9 [For Total AIR required [ENERGY (kW)]
270. Cells(65, 3) = TOTALCOM 'TOTAL Compressors
271. 'ENERGY IN for PUMPS & Fan
272. Cells(67, 3) = SP1 'Sludge Pump[DARK.REACTOR] (kW)
273. Cells(68, 3) = SP2 'Sludge Pump[DARK.REACTOR] (kW)
274. Cells(69, 3) = SP3 'For Digester Sludge (kW)
275. Cells(70, 3) = SP4 'For Digester Sludge (kW)
276. Cells(72, 3) = CB1 'Centrifugal fan[BIOREACTOR] (kW)
277. TOTALF = SP1 / 1000 + SP2 / 1000 + SP3 + SP4 + CB1
278. Cells(73, 3) = TOTALF 'Total (kW)
279. 'ENERGY IN for Heat-Exchangers
280. Cells(75, 3) = HE1
281. Cells(76, 3) = HE3
282. Cells(77, 3) = HE5
283. Cells(78, 3) = HE8
284. Cells(79, 3) = HE9
285. Cells(80, 3) = HE10
286. TOTALHEXIN = HE1 + HE9 + HE3 + HE8 + HE10 + HE5 + HE4 + HE2
287. Cells(81, 3) = TOTALHEXIN
288. 'ENERGY IN FOR IMPELLER
289. IMPDFBW = IMPDFB * 0.745 'Dark Impeller (kW)
290. IMPADBW = IMPADB * 0.745 'BIO Impeller (kW)
291. IMPINOCW = IMPINOC * 0.745 'Inoculum Impeller (kW)

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292.    IMPMIXT = IMPMIX * 0.745    'Mixing Tank (kW)
293.    TOTALIMP = IMPDFBW + IMPADBW + IMPINOCW + IMPMIXT
294. 'Cells
295.    Cells(83, 3) = IMPDFBW    'Dark Impeller (kW)
296.    Cells(84, 3) = IMPADBW    'BIO Impeller (kW)
297.    Cells(85, 3) = IMPINOCW  'Inoculum Impeller (kW)
298.    Cells(86, 3) = IMPMIXT    'Mixer Impeller (kW)
299.    Cells(87, 3) = TOTALIMP
300. 'ENERGY IN FOR WASTE TANKS
301.    TOTALTANKS = DFBTANK + ADBTANK + WESTANK1 + WESTANK2
302.    Cells(89, 3) = DFBTANK    'Energy IN DARK CSTR -(kW)
303.    Cells(90, 3) = ADBTANK    'Energy IN ADB CSTR -(kW)
304.    Cells(91, 3) = WESTANK1  'Energy IN ADB TANK1 -(kW)
305.    Cells(92, 3) = WESTANK2  'Energy IN ADB TANK2 -(kW)
306.    Cells(93, 3) = TOTALTANKS
307. 'Membranes Heat Loss
308.    TOTALHLMEMB = HLMFI + HLITM + HLEMS + HLSOFEC + HLSSAS + HLSOFC 'Total MEMBRANE HEAT LOSS (kW)
309.    Cells(95, 3) = HLMFI      'Heat Loss from MFI Cell (kW)
310.    Cells(96, 3) = HLITM      'Heat Loss from ITM Cell (kW)
311.    Cells(97, 3) = HLEMS      'Heat Loss from EMS Cell (kW)
312.    Cells(98, 3) = HLSOFEC    'Heat Loss from SOFEC Cell (kW)
313.    Cells(99, 3) = HLSSAS     'Heat Loss from SSAS Cell (kW)
314.    Cells(100, 3) = HLSOFC     'Heat Loss from SOFC Cell (kW)
315.    Cells(101, 3) = TOTALHLMEMB 'Total MEMBRANE HEAT LOSS (kW)
316. '
317. '=====
318. '          ENERGY OUT
319. '=====
320. '...ENERGY OUT of Turbines
321.    TOTALOUTTURBKW = STEATURB + GASTURB ' + GASTURB2
322.    Cells(54, 11) = STEATURB
323.    Cells(55, 11) = GASTURB
324.    Cells(43, 15) = GASTURB2
325.    Cells(56, 11) = TOTALOUTTURBKW
326. '...ENERGY OUT for Heat-Exchangers and Condensers
327. 'HEAT-EXCHANGERS
328.    Cells(58, 11) = HE2
329.    Cells(59, 11) = HE4
330.    Cells(60, 11) = HE6
331.    Cells(61, 11) = HE7
332. 'Condensers
333.    Cells(62, 11) = COND1
334.    Cells(63, 11) = COND2
335.    Cells(64, 11) = COND3
336.    Cells(65, 11) = COND4
337.    Cells(66, 11) = COND5
338.    TOTALHEXCONOUT = HE6 + HE7 + COND3 + COND4 + COND1 + COND2 + COND5 + HE11 + MFIZMAIRFLW2
339.    Cells(67, 11) = TOTALHEXCONOUT
340. 'TOTAL PRODUCED
341.    TOTAPRO = TOTALOUTTURBKW + TOTALHEXCONOUT    'Total Produced (kW)
342.    BXC = TOTALHEXCONOUT * 0.1
343.    Cells(68, 11) = TOTAPRO '(A+B)
344. 'Total Balance (1)
345.    ENERGYIN = TOTALCOM + ((SP1 + SP2)) + CB1 + TOTALHEXIN + TOTALIMP + TOTALTANKS + TOTALHLMEMB + SP4 + BXC 'Total IN from compressor + .....
346.    TOTALGIVEN = TOTAPRO - ENERGYIN    'ENERGY BALANCE (1)OUT
347.    Cells(70, 11) = ENERGYIN    'Energy Consumed (kW)
348.    Cells(71, 11) = TOTAPRO    'Energy Produced(kW)
349.    Cells(72, 11) = TOTALGIVEN    'ENERGY BALANCE (1)
350. 'TOTAL OUT
351.    TOTALOUTHEXTURB = TOTALOUTTURBKW + TOTALHEXCONOUT
352.    Cells(69, 11) = TOTALOUTHEXTURB '(A+B)
353. '=====
354. '          Cell Voltages to Power + NH3 + UREA
355. '=====

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356. 'Total Energy from Voltage
357. TOTALVOLTAGE = -SOFECPOWER - EMSPOWER + ITMPower + SOFCPOWER - SSASPOWER 'Total Voltage Power (kW)(2)
358. 'Energy From NH3
359. NH3HHV = NH3HHV 'Energy From NH3 (kW) (4)
360. 'TOTAL ENERGY WITHOUT NH3
361. TOTENER3 = TOTALGIVEN + TOTALVOLTAGE - CO2CONPW - MSTEAMTOT - DRMOTWATT - MFIZMAIRFLW4 - MFIZMAIRFLW3 - ASDF - (POWEPUM / 1000) '(1) +(2)-
(3)
362. 'TOTAL ENERGY WITHOUT NH3
363. TOTENERWNH3 = NH3HHV + TOTENER3 'Total Energy with NH3 (1) +(2)-(3) +(4)
364. 'Cells
365. Cells(65, 6) = EMSPOWER 'Voltage in Kw from EMS
366. Cells(66, 6) = SOFECPOWER 'Voltage in Kw from SOFEC
367. Cells(67, 6) = ITMPower 'Voltage in Kw from ITM
368. Cells(68, 6) = SOFCPOWER 'Voltage in Kw from SOFC
369. Cells(69, 6) = TOTALVOLTAGE 'Energy OUT From Voltages (kW)
370. Cells(70, 6) = UREAETOTNEEDED 'ENERGY IN FROM UREA (kW)
371. Cells(71, 6) = NH3HHV 'ENERGY IN from NH3
372. Cells(72, 6) = TOTENER3 'ENERGY BALANCE (2)
373. Cells(73, 6) = TOTENERWNH3 'ENERGY BALANCE (3)
374. End Sub
375. Static Function Logn(X)
376. Logn = Log(X) / Log(2.718282)
377. End Function
378. Private Static Function AIRDENSITY(AIRTEMP)
379. A1 = 1.2910739
380. B1 = 279.63468
381. C1 = 0.0036989433
382. D1 = 1.0050404
383. AIRDENSITY = (A1 * B1 + C1 * AIRTEMP ^ D1) / (B1 + AIRTEMP ^ D1) 'Air Density (Kg/m^3) oC
384. End Function
385. Private Static Sub COMPRESSOR(GASTEMPC, COMPOP, COMPIP, GAMMA, GASVOL, OUTADIATEMP, COOLSYS, COMETREFF, WATT, ENTCC, DRMOTWATT, DRMOTHP, MOTORE
FF1, MOTOREFF3, SPHASVOL, THREPASEVOL, CURRENT1, CURRENT3)
386. A1 = 1000
387. A2 = 60
388. End Sub
389. Private Static Function CO2SPEHEAT(GASTK) 'CO2 SPECIFIC HEAT ' Cp of CO2 kJ/Kg K)
390. Z1 = 0.51476288
391. Z2 = 5820.1918
392. Z3 = 1.4877831
393. Z4 = 1.404349
394. CO2SPEHEAT = (Z1 * Z2 + Z3 * GASTK ^ Z4) / (Z2 + GASTK ^ Z4)
395. End Function
396. Private Static Function AIRSPECIFICHEAT(AIRTK) 'AIRSPECIFICHEAT (kJ/kg.K)
397. TA = 1.0828694: TB = -0.00063119116: TC = 0.0000016253087: TD = -1.3949526E-09: TE = 5.3826153E-13: TF = -7.9021928E-17
398. AIRSPECIFICHEAT = TA + TB * AIRTK + TC * AIRTK ^ 2 + TD * AIRTK ^ 3 + TE * AIRTK ^ 4 + TF * AIRTK ^ 5
399. End Function
400. Private Static Function WATERSPECIFICHEAT(H2OTEMP) 'WATER SPECIFIC HEAT (kJ/kg.K)
401. WATERSPECIFICHEAT = 1.224986 + 0.0014072339 * H2OTEMP - 0.00000039722778 * H2OTEMP ^ 2 + 5.3431749E-11 * H2OTEMP ^ 3 + -2.7473115E-
15 * H2OTEMP ^ 4
402. End Function
403. Private Static Function CO2DENSITY(T) 'T=oC,Kg/m^3
404. A = 0.50649907: B = 0.0019289299: C = 1.0174749
405. CO2DENSITY = (A + B * T) ^ (-1 / C)
406. End Function
407. Private Static Sub HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'H
EAT EXCHANGER
408. AREAHEX = 3.14 * TOD * TL
409. LMTD = Q / (U * AREAHEX)
410. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
411. '----- HEATING -----
412. If FLAG = 1 Then
413. DELTAA = TH1 - TC2
414. 'DELTAB = TH2 - TC1
415. LMTD = Q / (U * AREAHEX)
416. X1 = 1

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417. 300 S1 = DELTAA / (LMTD - Logn(DELTAA))
418. S2 = X1 / (LMTD - Logn(X1))
419. If S2 >= S1 Then
420. GoTo 400
421. Else
422. X1 = X1 + 0.1
423. GoTo 300
424. 400 End If
425. DELTAB = X1
426. TH2 = DELTAB + TC1
427. GoTo 700
428. End If
429. '-----
430. '----- COOLING -----
431. If FLAG = 2 Then
432. 'DELTAA = TH1 - TC2
433. DELTAB = TH2 - TC1
434. LMTD = Q / (U * AREAHEX)
435. X1 = 2
436. 500 S1 = Logn(X1) - X1 / LMTD
437. S2 = Logn(DELTAB) - DELTAB / LMTD
438. If S1 >= S2 Then
439. GoTo 600
440. Else
441. X1 = X1 + 0.1
442. GoTo 500
443. 600 End If
444. DELTAA = X1
445. TC2 = TH1 - DELTAA
446. End If
447. '-----
448. 700 P = (TC2 - TC1) / (TH1 - TC1)
449. R = (TH1 - TH2) / (TC2 - TC1)
450. If R > 1 Then
451. R1 = 1 / R
452. P1 = P * R
453. Else
454. P1 = P
455. R1 = R
456. End If
457. A1 = (((R1) ^ 2 + 1) ^ 0.5) / (1 - R1)
458. A2 = Logn((1 - R1 * P1) / Abs(1 - P1))
459. A3 = 2 - P1 * (1 + R1 - (1 + (R1) ^ 2)) ^ 0.5 'up
460. A4 = Abs(2 - P1 * (1 + R1 + (1 + (R1) ^ 2)) ^ 0.5) 'down
461. A5 = Logn(A3 / A4)
462. FCORF = (A1 * A2) / A5
463. If Abs(FCORF) > 1 Then
464. FCORF = 1
465. End If
466. If FLAG = 1 Then
467. LMTD = Q / (U * AREAHEX * FCORF)
468. CHOT = Q / (TH1 - TH2)
469. HFR = CHOT * 24 * 3600 / SCHOT
470. GoTo 800
471. End If
472. If FLAG = 2 Then
473. LMTD = Q / (U * AREAHEX * FCORF)
474. CCOLD = Q / (TH1 - TH2)
475. HFR = CCOLD * 24 * 3600 / SCHOT
476. End If
477. 'EFFECTIVENESS
478. 800 If CCOLD > CHOT Then
479. CMIN = CHOT
480. C1 = CHOT
481. EPS = (C1 * (TC2 - TC1)) / (CMIN * (TH1 - TC1))

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482.   GoTo 900
483.   Else
484.     CMIN = CCOLD
485.     C1 = CCOLD
486.     EPS = (C1 * (TH1 - TH2)) / (CMIN * (TH1 - TC1))
487. 900 End If
488.     QEFF = EPS * CMIN * (TH1 - TC1)
489. 'Number of ELEMENT
490.     NTU = U * AREAHEX / CMIN
491.     If NTU <= 1 Then
492.       NTU = 1
493.     Else
494.     End If
495. End Sub

```

Anaerobic digestion codes are the same except for the Anaerobic digestion process and heat balance

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1.   Sub Sheet3_Button1_Click()
2.
3.   '=====
4.   '=====
5.   '                DARK-BIO
6.   Dim NUMTANKD As Integer, NUMTANKAB As Integer
7.   '..... FOOD .....
8.   '                Main DATA INPUT
9.   HZOTEMPXX = ActiveWorkbook.Worksheets("SOFC").Cells(31, 4)
10.
11.   FLAG = 0
12.   Pi = 3.14
13.   TAMB = 25
14.   TAMBK = TAMB + 273
15. 10 MF1 = Cells(4, 4)   'Mass of Food (Kg /Day)
16.   FWR = Cells(5, 4)   'Water Dilution Ratio for Feed
17.   WD = MF1 * FWR      'H2O Mass (Kg/day)
18.   Cells(6, 4) = WD    'H2O Mass (Kg/day)
19.   MF = MF1 + WD + VRRKG 'Mass of Food after dilution (Kg/day)
20.   FTOFC = Cells(7, 4) 'Ratio Food to Faeces
21.   MFC = MF1 / FTOFC   'Mass of Faeces (Kg/Day)
22.   Cells(8, 4) = MFC   'Mass of Faeces (Kg/Day)
23.   RPVTS = Cells(32, 4) 'Ratio of VS/TS
24.   PDFB = Cells(40, 4) 'Pressure Bio Reactor IN (atm.)
25.   HRTD = Cells(43, 4)
26.   TEMPD = Cells(42, 4) 'Dark Reactor Temperature oC
27.   TEMPA = Cells(55, 4) 'Anaerobic Reactor Temperature oC
28.   ADBP = Cells(56, 4) 'anaerobic Reactor Pressure (atm.)
29.   HRTB = Cells(50, 4) 'Hydraulic Residence Time (day)
30. 'Densities
31.   RHOFW = Cells(36, 4) 'Density of FW (KG/M^3)
32.   RHOFW = Cells(37, 4) 'Density of FCW (KG/M^3)
33.   GH56 = (WD + MF1) / ((WD / 1000) + (MF1 / RHOFW))
34.   RHOMIX = (WD + MF1 + MFC) / (((WD + MF1) / (GH56)) + (MFC / RHOFW))
35.   Cells(38, 4) = RHOMIX 'Density of Mixture (KG/M^3)
36.   RHOMIXBNM = RHOMIX
37.   Cells(61, 4) = RHOMIXBNM
38. 'Food Input
39.   MFV = MF / RHOFW    'Volume of Food (m^3/day)
40.   Cells(10, 4) = MFV  'Volume of Food (m^3/day)
41.   PTSF = Cells(11, 4) '% TS FOOD
42.   PVSF = Cells(12, 4) '% VS FOOD
43.   TCOF1 = Cells(13, 4) '% TCOD FOOD
44.   SCOF1 = Cells(14, 4) '% SCOD FOOD
45.   TKNF1 = Cells(15, 4) '% TKN FOOD
46.   CHF1 = Cells(16, 4) '% of Carbohydrate content in food
47.   PHF = Cells(17, 4) '% pH of food
48. '..... Food Output

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49.     TSF = MF * PTSF / 100      'TS Food (Kg/day)
50.     VSF = MF * PVSF / 100     'VS Food (Kg/day)
51.     TCOF = MF * TCOF1 / 100   'TCOD Food (Kg/day)
52.     SCOF = MF * SCOF1 / 100   'SCOD Food (Kg/day)
53.     TKNF = MF * TKNF1 / 100   'TKN Food (Kg/day)
54.     CHF = MF * CHF1 / 100     'Carbohydrate content (Kg/day)
55.     NH3F = MF * NH3F1 / 100   'TKN Food (Kg/day)
56.     H2SF = MF * H2SF1 / 100   'H2S Food (Kg/day)
57. ' Cells
58.     Cells(5, 9) = WD          'H2O Mass (Kg/day)
59.     Cells(6, 9) = MF          'Mass of Food after dilution (Kg/day)
60.     Cells(6, 10) = TSF        'TS Food (Kg/day)
61.     Cells(6, 11) = VSF        'VS Food (Kg/day)
62.     Cells(6, 12) = TCOF        'TCOD Food (Kg/day)
63.     Cells(6, 13) = SCOF        'SCOD Food (Kg/day)
64.     Cells(6, 14) = TKNF        'TKN Food (Kg/day)
65.     Cells(6, 15) = CHF         'CHF Food (Kg/day)
66.     ' Cells(6, 16) = NH3F      'NH3F Food (Kg/day)
67.     'Cells(6, 17) = H2SF      'H2SF Food (Kg/day)
68. '..... Faeces Input
69.     MFCV = MFC / RHOFWCW      'Volume of Faecesd (m^3/day)
70.     Cells(19, 4) = MFCV        'Volume of Faeces (m^3/day)
71.     PTSFC = Cells(20, 4)      '% TS Faeces
72.     PVSFC = Cells(21, 4)      '% VS Faeces
73.     TCOF1 = Cells(22, 4)      '% TCOD Faeces
74.     SCOF1 = Cells(23, 4)      '% SCOD Faeces
75.     TKNFC1 = Cells(24, 4)     '% TKN Faeces
76.     CHFC1 = Cells(25, 4)      '% of Carbohydrate content in Faeces
77.     PHFC = Cells(26, 4)       '% pH of Faeces
78. '..... Faeces Output
79.     TSFC = MFC * PTSFC / 100   'TS Faeces (Kg/day)
80.     VSFC = MFC * PVSFC / 100   'VS Faeces (Kg/day)
81.     TCOFC = MFC * TCOF1 / 100  'TCOD Faeces (Kg/day)
82.     SCOFC = MFC * SCOF1 / 100  'SCOD Faeces (Kg/day)
83.     TKNFC = MFC * TKNFC1 / 100 'TKN Faeces (Kg/day)
84.     CHFC = MFC * CHFC1 / 100   'Faeces Carbohydrate content (Kg/day)
85. ' Cells
86.     Cells(7, 9) = MFC          'Mass of Faecesd Kg/day)
87.     Cells(7, 10) = TSFC        'TS Faeces(Kg/day)
88.     Cells(7, 11) = VSFC        'VS Faeces (Kg/day)
89.     Cells(7, 12) = TCOFC        'TCOD Faeces (Kg/day)
90.     Cells(7, 13) = SCOFC        'SCOD Faeces (Kg/day)
91.     Cells(7, 14) = TKNFC        'TKN Faeces (Kg/day)
92.     Cells(7, 15) = CHFC         'CHF Faeces (Kg/day)
93. '..... MIXTURE .....
94. '.....Mixed IN
95.     TCOVMIX = Cells(33, 4)
96.     BODMIX = 0.6 * TCOVMIX
97.     BODMIX = Cells(48, 4)
98.     SCODMIX = Cells(34, 4)
99.     TFVA = Cells(35, 4)
100. '===== Mixed OUT =====
101.     MMIX = MF + MFC + VRRKG     'Mass of Mixture (kg/day)
102.     If FLAG = 0 Then
103.     VOLMIX = MMIX / RHOMIX      'Voume of Mixture (m^3/day)
104.     GoTo 12
105.     Else
106.     VOLMIX = VOLMIX + VRR
107. 12 End If
108.     'TS (FOOD WASTE ) AFTER DILUTION
109.     TSA = PTSF * 0.346 'TS AFTER DILUTION
110.     PTSMIX = (((MF * TSA / 100) + (MFC * PTSFC / 100) + VRRKG * TSREC / 100) / MMIX) * 100 '% TS MIXED (Kg/day)
111.     PVS MIX = PTSMIX * RPVTS     '% VS MIXED (Kg/day)
112.     'Mixed (Kg/day)
113.     MTS MIX = MMIX * PTSMIX / 100 'TS MIXED (Kg/day)

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114.     MVMIX = MMIX * PVMIX / 100      'VS MIXED (Kg/day)
115.     MTCODMIX = MMIX * TCODMIX / 100 'TCOD MIXED (Kg/day)
116.     MSCODMIX = MMIX * SCODMIX / 100 'SCOD MIXED (Kg/day)
117. 'Cells
118.     Cells(28, 4) = MMIX      'Mass of Mixture (kg/day)
119.     Cells(29, 4) = VOLMIX    'Volume of Mixture (m^3/day)
120.     Cells(30, 4) = PTSMIX   '% TS MIXED
121.     Cells(31, 4) = PVMIX    '% VS MIXED
122.     Cells(32, 4) = RPVTS    'Ratio of VS/TS
123.     Cells(8, 9) = MMIX      'Flow Rate of Mixed Waste (kg/day)
124.     Cells(8, 10) = MTSMIX   'TS MIXED (Kg/day)
125.     Cells(8, 11) = MVMIX    'MTCODMIX (Kg/day)
126.     Cells(8, 12) = MTCODMIX 'MTCODMIX (Kg/day)
127.     Cells(8, 13) = MSCODMIX 'MTCODMIX (Kg/day)
128. '=====
129. '..... ACIDOGENIC REACTOR .....
130.     GTSMIX = MTSMIX * 1000 / MMIX   'TS MIX (g/L)
131.     GVMIX = MVMIX * 1000 / MMIX     'VS MIX (g/L)
132.     GTCODMIX = MTCODMIX * 1000 / MMIX 'TCOD MIX (g/L)
133.     GSCODMIX = MSCODMIX * 1000 / MMIX 'TCOD MIX (g/L)
134.     GTVFAMIX = (TFVA * 10)         'TFVA MIX (g/L)
135. 'Cells
136.     Cells(11, 9) = GTSMIX
137.     Cells(12, 9) = GVMIX
138.     Cells(13, 9) = GTCODMIX
139.     Cells(14, 9) = GSCODMIX
140.     Cells(15, 9) = GTVFAMIX
141. 'OUTPUT of INPUT as %
142.     Cells(11, 10) = GTSMIX / 10
143.     Cells(12, 10) = GVMIX / 10
144.     Cells(13, 10) = GTCODMIX / 10
145.     Cells(14, 10) = GSCODMIX / 10
146.     Cells(15, 10) = GTVFAMIX / 10
147. 'Cells Input
148.     PHM = Cells(41, 4)
149.     RMIC = Cells(47, 4)      'Ratio of Micro
150.     H2DARK = Cells(58, 4)   'Ratio of H2 from Dark to Anaerobic
151.     CH4BIORAC = Cells(59, 4)
152. 'Calculations
153. 'Effluent (E)
154.     TSE = (PTSMIX * 0.479) * 10
155.     VSE = (0.5) * GVMIX
156.     KH = -((1 / HRTD) * Logn(VSE / GVMIX))
157.     SRT = 1 / KH
158.     Cells(44, 4) = KH      'First Order Constant for H2 (1/day)
159.     Cells(11, 16) = SRT   'SRT Effluent (g/L)
160.     TCODE = GTCODMIX * 0.36
161.     SCODEF = TCODE * 0.413
162.     TVFAE = (TCODMIX * 0.07) * 10
163.     OLR = (GVMIX * KH * VSE) / (GVMIX - VSE) 'Organic Loading Rate (gVS/L.day)
164. 'Cells Out
165.     Cells(44, 4) = KH      'First Order Constant for H2 (1/day)
166.     Cells(46, 4) = OLR    'Organic Loading Rate (gVS/L.day)
167.     Cells(11, 12) = TSE   'TSE Effluent (g/L)
168.     Cells(12, 12) = VSE   'VSE Effluent (g/L)
169.     Cells(13, 12) = TCODE 'TCODE Effluent (g/L)
170.     Cells(14, 12) = SCODEF 'SCODE Effluent (g/L)
171.     Cells(15, 12) = TVFAE 'TVFAE Effluent (g/L)
172. 'Effluent (%)
173.     TSEP = TSE / 10
174.     VSEP = VSE / 10
175.     TCODEP = TCODE / 10
176.     SCODEP = SCODEF / 10
177.     TVFAEP = TVFAE / 10
178. 'Cells out

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179. Cells(11, 13) = TSEP      'TSE Effluent (%)
180. Cells(12, 13) = VSEP      'VSE Effluent (%)
181. Cells(13, 13) = TCODEP    'TCODE Effluent (%)
182. Cells(14, 13) = SCODEP    'SCODE Effluent (%)
183. Cells(15, 13) = TVFAEP    'TVFAE Effluent (%)
184. 'Reactor
185. 'Substrate
186. H2PERD = H2DARK
187. Cells(17, 16) = H2PERD
188. VW = VOLMIX * HRTB      'Useful Volume (m^3)
189. SOBSRT = OLR * HRTD      'Amount of Substrate [Yield of Biogas] (kgCs/m^3) ...[S]
190. MU = 0.83 - (0.028 * VSEP) 'Theoretical Biogas Yield (m^3/kgVS)
191. YGPR = (MU * KH * VSE) / SOBSRT 'Biogas Yield = Specific Gas Production Rate (m^3/kgVS)
192. QBIOGAS = MMIX * YGPR
193. GASPR = YGPR * OLR      'Gas Production Rate (1/day)
194. Cells(17, 10) = GASPR
195. Cells(18, 10) = QBIOGAS 'Biogas Production Rate (m^3/day)
196. Cells(19, 10) = YGPR    'Biogas Yield (m^3/kgVS)
197. Cells(17, 16) = H2PERD
198. '
199. 'Useful Volume of Dark Bioreactor
200. VOLREACTOR = VW + 0.15 * VW      'Volume of Dark Bioreactor (m^3)
201. 'YIELD
202. ' BIOYIELD = YGPR      'BIOGAS Yield (m^3/kgVS)
203. YEXP = (H2PERD / 100) * YGPR
204. TOTBIOR = 100
205. CO2PER = TOTBIOR - H2PERD      'H2Yield (m^3/kgVS)
206. CO2YIELD = YGPR - YEXP      'CO2 Yield (m^3/kgVS)
207. BIOYIELD = YGPR
208. 'Cells Output-1
209. Cells(18, 16) = CO2PER
210. Cells(19, 16) = TOTBIOR
211. Cells(10, 16) = VOLREACTOR      'Working Volume (m^3)
212. Cells(12, 16) = OLR      'OLR Effluent (g/L)
213. Cells(13, 16) = MU      'Theoretical Biogas Yield (m^3/kgVS)
214. 'Cells Output-2
215. Cells(17, 13) = YEXP      'H2 Yield (m^3/kgVS)
216. Cells(18, 13) = CO2YIELD    'CO2 Yield (m^3/kgVS)
217. Cells(19, 13) = BIOYIELD    'BIOGAS Yield (m^3/kgVS)
218. H2VAR = QBIOGAS * H2PERD / 100
219. CO2VAR = QBIOGAS * CO2PER / 100
220. TOTVAR = QBIOGAS
221. TOTVARGT = H2VAR + CO2VAR
222. Cells(17, 20) = H2VAR
223. Cells(18, 20) = CO2VAR
224. Cells(19, 20) = TOTVARGT
225. '=====
226. '..... CSTR'DF' .....
227. '=====
228. 'CSTRT = HRTD      '<<<===== Digested Time
229. CSTRDARKV = VOLREACTOR      'VOLUME of CSTR (m3)
230. CSTRDARKD = (CSTRDARKV * 2 / 3.14) ^ (1 / 3)      'Diameter of CSTR (m)
231. CSTRDARKH = CSTRDARKD * 2      'Height of CSTR (m)
232. CSTR = (2 * 3.14 * (CSTRDARKD / 2) * CSTRDARKH) + (2 * 3.14 * ((CSTRDARKD / 2) ^ 2)) 'Area of CSTR (m2)'To be print'
233. CSTRDARKV1 = VW      'VOLUME of CSTR (m3)
234. CSTRDARKD1 = (CSTRDARKV1 * 2 / 3.14) ^ (1 / 3)      'Diameter of CSTR (m)
235. CSTRDARKH1 = CSTRDARKD1 * 2      'Height of CSTR (m)
236. 'Cells..... CSTR
237. Cells(14, 16) = CSTRDARKD      'Diameter of CSTR (m)
238. Cells(15, 16) = CSTRDARKH      'Height of CSTR (m)
239. '=====
240. ' TANK DESIGN (DARK MIXER)
241. '=====
242. RHOACETACID = 1037.38 'DENSITY OF ACETIC ACID 'Density of Acetic Acid (kg/m3)
243. MMIXG = MMIX * 1000

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244.   FAO = MMIXG / RHOACETACID
245.   TANKV9 = VW
246.   MAXVOL = 50
247.   NUMTANKD = VW / MAXVOL
248.   If NUMTANKD < 1 Then
249.     NUMTANKD = 1
250.   Else
251.     End If
252. '...RATE
253.   'Input Feed of Mixture (mol/g)
254.   X1 = (1 - (VSE / GVSMIX)) 'Conversion Rate of Dark Fermentation'
255. 'AGITATOR DIMENSIONS FOR Dark fermentation'
256.   IMPDAD = (CSTRDARKD / 3) 'Impeller diameter (m)
257.   EMDAD = IMPDAD 'Impeller height above bottom of vessel(m)
258.   LMPDAD = (IMPDAD / 4) 'Length of Impeller blade (m)
259.   WMPDAD = (IMPDAD / 5) 'Width of Impeller blade(m)
260.   WBAFD = (CSTRDARKD / 10) 'Width of baffle(m)
261.   NOIMPD = 2 'Number of impellers
262.   NOIMBPLD = 6 'Number of impeller blades
263. 'SHAPE FACTORS OF BLADES AS FOLLOWS 6BLADE'
264.   DISTBD = IMPDAD 'Distance between two consecutive impellers (m)
265.   S1BIOD = IMPDAD / CSTRDARKD 'Shape Factor(m)
266.   S2BIOD = EMDAD / CSTRDARKD 'Shape Factor(m)
267.   S3BIOD = LMPDAD / IMPDAD 'Shape Factor(m)
268.   S4BIOD = WMPDAD / IMPDAD 'Shape Factor(m)
269.   S5BIOD = WBAFD / CSTRDARKD 'Shape Factor(m)
270.   S6BIOD = CSTRDARKH1 / CSTRDARKD 'Shape Factor(m)
271. 'Velocity of agitation
272.   TVELAGD = 2 'Velocity of agitation
273. 'Speed of impellers'
274.   SPEIMPD = ((TVELAGD) / (3.14 * IMPDAD)) * 60 '(RPM)
275.   FT5 = (RHOMIX * (0.99))
276.   DENDARK7 = (MMIX + KGOUTR) / ((KGOUTR / FT5) + (MMIX / RHOMIX)) 'DENSITY'
277.   'Energy impellers HORSEPOWER'
278.   IMPHPD = (((NOIMBPLD) * (((SPEIMPD) * (0.016)) ^ (3)) * ((IMPDAD) ^ (5)) * (DENDARK7)) / (2447.578)) * NUMTANKD '(HP)'
279.   RTEEQWSTDARK = (KGINADBR / FT5) - (KGINADARK / RHOMIX) 'Volume of solid in the DF'
280.   POWBIO5 = IMPHPD * NUMTANKD 'Total Power for Total number of Vessels
281. 'IMPELLER EFFICIENCY'
282.   EFF1G = Cells(47, 12) 'Efficiency of impellers(%)<=====
283.   'Power by considering the efficiency of impeller'
284.   POWBIO5G = IMPHPD * ((EFF1G / 100))
285. 'Baffle design'
286.   NOBAFD = 4 'Number of Baffles
287.   WBAFD = ((CSTRDARKD) / (10)) 'Width of baffle (m)
288.   HBAFD = CSTRDARKH1 'HEIGHT of baffle (m)
289. 'corrosion allowance'
290.   CORAL4 = ((2) * (10) ^ (-3)) 'Corrosion allowance (m)
291. 'Wall thickness'
292.   PSBIORACF = (RHOFW * (9.81) * CSTRDARKH) * 0.0000986 'Static pressure (atm)
293.   POP1T = 0.0144 'OPERATIONAL PRESSURE (atm)
294.   PTOTH5 = POP1T + PSBIORACF 'Maximum allowance pressure(atm)
295. 'Cells
296.   Cells(35, 12) = NUMTANKD
297.   Cells(36, 12) = FAO 'INPUT FLOW OF WASTE in (g/day)
298.   Cells(37, 12) = X1 'Conversion Rate %
299.   Cells(38, 12) = IMPDAD 'Impeller diameter (m)
300.   Cells(39, 12) = EMDAD 'Impeller height above bottom of vessel(m)
301.   Cells(40, 12) = LMPDAD 'Length of Impeller blade (m)
302.   Cells(41, 12) = WMPDAD 'Width of Impeller blade(m)
303.   Cells(42, 12) = NOIMPD 'Number of Propellers
304.   Cells(43, 12) = NOIMBPLD 'Number of impeller blades
305.   Cells(44, 12) = TVELAGD 'Velocity of agitation
306.   Cells(45, 12) = SPEIMPD 'Rotation per minute (RPM)
307.   Cells(46, 12) = IMPHPD 'Impeller Horse Power (HP)
308.   Cells(48, 12) = POWBIO5G 'Impeller Horse Power at EFFICIENCY (HP)

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309. Cells(49, 12) = NOBAFD 'number of Baffles
310. Cells(50, 12) = WBAF1D 'Width of baffle (m)
311. Cells(51, 12) = HBAFLD 'HEIGHT of baffle (m)
312. Cells(52, 12) = CORAL4 'Corrosion allowance (m)
313. Cells(53, 12) = PSBIORACF 'Static pressure (atm)
314. Cells(54, 12) = POP1T 'OPERATIONAL PRESSURE (atm)
315. Cells(55, 12) = PTOTH5 'Maximum allowance pressure(atm)
316. 'Shape Factor
317. Cells(57, 12) = S1BIOD 'Shape Factor(m)
318. Cells(58, 12) = S2BIOD 'Shape Factor(m)
319. Cells(59, 12) = S3BIOD 'Shape Factor(m)
320. Cells(60, 12) = S4BIOD 'Shape Factor(m)
321. Cells(61, 12) = S5BIOD 'Shape Factor(m)
322. Cells(62, 12) = S6BIOD 'Shape Factor(m)
323. '=====
324. ' ANAEROBIC DIGESTER
325. '=====
326. H2SP = Cells(53, 4) 'H2S Percent %
327. NH3P = Cells(54, 4) 'NH3 Percent %
328. '.....EFFLUENT
329. TSEBP = TSEP * 2.4 / 4.3 'TS OUT as (%)
330. VSREM = 100 - 80 'VS removed as (%)
331. VSEPB = (VSE / 10) * VSREM / 100 'VS OUT as (%)
332. CODREM = 100 - 81 'COD Removed (%)
333. CODEP = TCODEP * CODREM / 100 'Chemical Oxygen Demand (%)
334. VFAEP = TCODMIX * 0.035 'Volatile Fatty Acid (%)
335. 'Cells Kg/m^3 OUT
336. TSEBG = TSEBP * 10 'TS effluent (g/L) or (Kg/m3)
337. VSEG = VSEPB * 10 'VS effluent (g/L) or (Kg/m3)
338. CODEG = CODEP * 10 'COD effluent (g/L) or (Kg/m3)
339. VFAEG = VFAEP * 10 'Volatile Faty Acids (g/L) or (Kg/m3)
340. 'Cells
341. Cells(23, 9) = TSEBG 'TS effluent (g/L) or (Kg/m3)
342. Cells(24, 9) = VSEG 'VS effluent (g/L) or (Kg/m3)
343. Cells(25, 9) = CODEG 'COD effluent (g/L) or (Kg/m3)
344. Cells(26, 9) = VFAEG 'Volatile Faty Acids (g/L) or (Kg/m3)
345. 'Cells % OUT
346. Cells(23, 10) = TSEBP 'TS effluent(%)
347. Cells(24, 10) = VSEPB 'VS effluent(%)
348. Cells(25, 10) = CODEP 'COD effluent(%)
349. Cells(26, 10) = VFAEP 'Volatile Fatty Acids Produced (%)
350. Cells(22, 13) = VSREM 'Volatile Fatty Acids Removed (%)
351. Cells(23, 13) = CODREM 'COD Removed (%)
352. 'Sludge
353. TSOUT = TSEBP * 1.1 / 2.7 'TS rejected (%)
354. TSREC = TSEBP - TSOUT 'TS recycled (%)
355. Cells(27, 9) = TSREC * 10 '<=====
356. 'Cells OUT
357. Cells(25, 13) = TSREC 'TS RECYCLED (%)
358. Cells(26, 13) = TSOUT 'TS rejected (%)
359. 'Recycle, Rates and Volume
360. MAXPRO = 2 'Recirculation rate (m^3/day)
361. VRR = VOLMIX * MAXPRO 'Recycled Volume (m^3/day)
362. VRRKG = MMIX * TSREC / PTSMIX 'Recycled Volume (Kg/day) Ratio of Mixed to racycling
363. RB1 = (MMIX * TSREC) / (PTSMIX) 'To be print''flow rate of recycled(kg/day)'
364. QBIOL = MMIX + RB1 - TOTALGDK
365. VOLUSEFULBIO = VOLREACTOR / 1.15 'Useful Volume (m^3)
366. '=====
367. 'ADB CSTR'
368. '=====
369. 'Height of CSTR (m)
370. CSTRBD2E = (VOLREACTOR * 2 / 3.14) ^ (1 / 3) 'Diameter of CSTR (m)
371. CSTRBH2 = CSTRBD2E * 2 'Height of CSTR (m)
372. CSTRBA2 = (2 * 3.14 * (CSTRBD2E / 2) * CSTRBH2) + (2 * 3.14 * ((CSTRBD2E / 2) ^ 2)) 'Area of CSTR (m2)'to be print'
373. 'Cells..... CSTR

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374. Cells(26, 16) = CSTRBD2E 'Diameter of CSTR (m)
375. Cells(27, 16) = CSTRBH2 'Height of CSTR (m)
376. '=====
377. ' ADB MIXER (CSTR)
378. '=====
379. C6H12O6MOL = 180.156 'g/mol
380. MMIXG = MMIX * 1000 'INPUT FLOW OF WASTE in (g/day)
381. FAOQ = MMIXG / C6H12O6MOL
382. NUMTANKAB = VOLUSEFULBIO / MAXVOL 'Number Of Tanks
383. If NUMTANKAB < 1 Then
384. NUMTANKAB = 1
385. Else
386. End If
387. Cells(35, 19) = NUMTANKAB
388. '=====
389. ' TANK DESIGN (ADB MIXER)
390. '=====
391. '..... X1 From above (Dark Fermenter)Line 238
392. '....RATE
393. X2 = (1 - (VSEG / VSE)) 'Conversion Aaerobic
394. RA2 = -((FAO * (X2 - X1)) / (VOLUSEFULBIO)) 'Total reaction rate
395. 'DENSITY OF THE EFFLUENT GOING TO COMPOST'
396. DENRTP = (DENDARK7 * 4.4) / (8.98)
397. '=====
398. IMPDA = (CSTRBD2E / (3)) 'Impeller diameter(m)
399. EMDA = IMPDA 'Impeller height above vessel floor(m)
400. LMPDA = (IMPDA / (4)) 'Length of Impeller blade(m)
401. WMPDA = (IMPDA / (5)) 'Width of Impeller blade(m)
402. QWPDA = (CSTRBD2E / (10)) 'Width of baffle(m)'
403. NOIMP = 3 'Number of impellers
404. NOBLAD = 6 'Number of impeller blades
405. 'SHAPE FACTORS OF BLADES AS FOLLOWS 6BLADE'
406. DISTB = IMPDA 'Distance between two consecutive impellers (m)'
407. S1BIO = IMPDA / CSTRBD2E 'Shape Factor(m)
408. S2BIO = EMDA / CSTRBD2E 'Shape Factor(m)
409. S3BIO = LMPDA / IMPDA 'Shape Factor(m)
410. S4BIO = WMPDA / IMPDA 'Shape Factor(m)
411. S5BIO = QWPDA / CSTRBD2E 'Shape Factor(m)
412. S6BIO = CSTRBH2 / CSTRBD2E 'Shape Factor(m)
413. 'Velocity of agitation
414. 'Density of Dark Mixture
415. FT5 = (RHOMIX * (0.733333))
416. TIPVELO = 5 'Velocity of agitation
417. FT0Y = (DENDARK7 * (1.5))
418. 'Speed of impellers'
419. SPEIMP = ((TIPVELO) / (3.14 * IMPDA)) * 60 '(RPM)
420. 'Energy impellers HORSEPOWER'
421. POWBIOA = (((NOBLAD) * (((SPEIMP) * (0.016)) ^ (3)) * ((IMPDA) ^ (5)) * (RHOMIX)) / (2447.578)) * NUMTANKAB '(HP)
422. POWBIOAN = POWBIOA 'Total Power for Total number of Vessels
423. 'IMPELLER EFFICIENCY'
424. EFF1 = Cells(47, 19) 'Efficiency of impellers(%)<*****
425. POWBIO = POWBIOA * ((EFF1 / 100)) 'Power by considering the efficiency of impeller
426. 'Baffle design'
427. NOBLADQ = 6
428. WBAFF = ((CSTRBD2E) / (10)) 'width of baffle (m)
429. HBAFF = CSTRBH2 'HEIGHT of baffle (m)
430. 'corrosion allowance'
431. CORAL = ((2) * (10) ^ (-3)) 'Corrosion allowance (m)
432. 'Wall thickness'
433. PSBIORAC = (RHOFW * (9.81) * CSTRBH2) * 0.0000986 'Static pressure (atm)
434. POP1 = 0.0144 'OPERATIONAL PRESSURE (atm)
435. PTOTH = POP1 + PSBIORAC 'Maximum allowance pressure(atm)
436. 'Cells
437. Cells(36, 19) = FAOQ 'INPUT FLOW OF WASTE in (g/day)
438. Cells(37, 19) = X2 'Conversion Rate %

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439. Cells(38, 19) = IMPDA      'Impeller diameter (m)
440. Cells(39, 19) = EMDA      'Impeller height above bottom of vessel(m)
441. Cells(40, 19) = LMPDA     'Length of Impeller blade (m)
442. Cells(41, 19) = WMPDA     'Width of Impeller blade(m)
443. Cells(42, 19) = NOIMP     'Number of Propellers
444. Cells(43, 19) = NOBLAD    'Number of impeller blades
445. Cells(44, 19) = TIPVELO   'Velocity of agitation
446. Cells(45, 19) = SPEIMP    'Rotation per minute (RPM)
447. Cells(46, 19) = POWBIOAN  'Impeller Horse Power (HP)
448. Cells(48, 19) = POWBIO    'Impeller Horse Power at EFFICIENCY (HP)
449. Cells(49, 19) = NOBLADQ   'number of Baffles
450. Cells(50, 19) = WBAFF     'Width of baffle (m)
451. Cells(51, 19) = HBAFF     'HEIGHT of baffle (m)
452. Cells(52, 19) = CORAL     'Corrosion allowance (m)
453. Cells(53, 19) = PSBIORAC  'Static pressure (atm)
454. Cells(54, 19) = POP1     'OPERATIONAL PRESSURE (atm)
455. Cells(55, 19) = PTOTH     'Maximum allowance pressure(atm)
456. 'Shape Factor
457. Cells(57, 19) = S1BIO
458. Cells(58, 19) = S2BIO
459. Cells(59, 19) = S3BIO
460. Cells(60, 19) = S4BIO
461. Cells(61, 19) = S5BIO
462. Cells(62, 19) = S6BIO
463. '=====
464. '                TANK DESIGN (MIXER INOCULUM)
465. '=====
466. INORESTIME = Cells(62, 4)      'Tank Residence Time (day)
467. INOTIMFACTOR = 1.25          'TANK FACTOR
468. INOTANKVOL = MMIX * (INORESTIME / RHOMIX) * INOTIMFACTOR 'Tank Volume (m^3)
469. MAXVOL = 50                  'Maximum Volume Allowed (m^3)
470. INONUMBTANK = INOTANKVOL / MAXVOL 'Number Of Tanks
471. If INONUMBTANK < 1 Then
472. INONUMBTANK = 1
473. Else
474. End If
475. INODISRATE = (MAXVOL * (INOTANKVOL / INONUMBTANK)) / (10) 'Discharge Rate (m^3/day)
476. INODISRATE = ((INOTANKVOL / INONUMBTANK) / INODISRATE) 'Discharge Rate
477. RTANKD = ((INOTANKVOL / INONUMBTANK) * 2 / 3.14) ^ (1 / 3) 'Diameter of Tank (m)
478. RTANKH = RTANKD * 2 'Height of CSTR (m)
479. 'CELLS OUTPUT
480. Cells(4, 20) = INOTANKVOL     'Tank Volume (m^3)
481. Cells(5, 20) = INONUMBTANK   'NUMTANK
482. Cells(6, 20) = RTANKD        'Diameter of Tank (m)/Tanks
483. Cells(7, 20) = RTANKH        'Height of Tank (m) /Tanks
484. Cells(8, 20) = INODISRATE
485. 'Reactor Input Flow Rate
486. RRT = Cells(64, 17)          'Recycling Ratio (%)
487. TYUI = TOTVARGT - (MMIX / RHOMIX) ' - ( )
488. KGOUTR2 = TYUI * (RRT / 100) 'Amount of Recycled (kg/day)
489. '=====
490. '                'Inoculum tank'
491. '=====
492. IMPDA0Y = RTANKD / 3
493. TIPVELO1Y = 5
494. 'Speed of impellers'
495. SPEIMP2Y = ((TIPVELO1Y) / (3.14 * IMPDA0Y)) * 60 '(RPM)
496. 'Energy impellers HORSEPOWER'
497. POWBIOAINOTANK = ((NOBLAD) * (((SPEIMP2Y) * (0.016)) ^ (3)) * ((IMPDA0Y) ^ (5)) * (RHOMIX)) / (2447.578) '(HP)
498. POWBIOAINOTANKTOT = POWBIOAINOTANK * INONUMBTANK
499. 'IMPELLER EFFICIENCY'
500. POWBIO5U = POWBIOAINOTANKTOT * ((EFF1 / 100)) 'Power by considering the efficiency of impeller
501. Cells(64, 12) = SPEIMP2Y
502. Cells(65, 12) = POWBIO5U
503. 'K constant

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504. KM = ((1 / HRTB) * (-Logn(VSEG / GVSMIX))) 'First Order Constant for CH4 (1/day)
505. SRTB = 1 / KM
506. Cells(51, 4) = KM
507. 'OLR
508. OLRB = VSEG * KM * GVSMIX / (GVSMIX - VSEG) 'OLR-Organic Loading Rate (kgVS/m^3. d)
509. 'SB, MU, and Organic Loading Rate (OLR)
510. 'Experimental Yield (m^3/kgVS)
511. MUB = 0.83 - (0.028 * VSEPB)
512. SGP = (MUB * KM * VSEG) / OLRB 'Specific Gas Production
513. SB = OLRB * HRTB 'Amount of Substract(kgVS/m^3)
514. GPRB = (OLRB * SGP) 'Gas Productio Rate (m3/m3.d)
515. QBIOGAD = MMIX * SGP
516. CH4PERBIO = CH4BIORAC
517. H2SPERBIO = H2SP
518. NH3PERBIO = NH3P
519. TOTALPERBIO = 100
520. CO2PERBIO = TOTALPERBIO - (H2SP + NH3P + CH4PERBIO)
521. 'Rate of Biogas OUT
522. YEXCH4 = (CH4PERBIO / 100) * SGP
523. YEXH2S = (H2SPERBIO / 100) * SGP
524. YEXNH3 = (NH3PERBIO / 100) * SGP
525. YEXCO2 = SGP - YEXCH4 - YEXH2S - YEXNH3
526. YEXCO2 = (CO2PERBIO / 100) * SGP
527. Total = YEXCH4 + YEXCO2 + YEXH2S + YEXNH3
528. 'Cells OUTPUT
529. Cells(29, 13) = YEXCH4
530. Cells(30, 13) = YEXCO2
531. Cells(31, 13) = YEXH2S
532. Cells(32, 13) = YEXNH3
533. Cells(33, 13) = YEXPE
534. CH4RATE = (QBIOGAD * CH4BIORAC) / 100 'CH4 OUT (m^3/day)<-----
535. H2SRATE = QBIOGAD * H2SP / 100 'H2O OUT (m^3/day)<-----
536. NH3RATE = QBIOGAD * NH3P / 100
537. CO2RATE = QBIOGAD - CH4RATE - H2SRATE 'CO2 OUT (m^3/day)<-----
538. TOTALB = CH4RATE + CO2RATE + H2SRATE + NH3RATE
539. '*****
540. 'Cells OUTPUT
541. Cells(29, 16) = CH4PERBIO 'CH4 (%)
542. Cells(30, 16) = CO2PERBIO 'CO2(%)
543. Cells(31, 16) = H2SPERBIO 'H2S (%)
544. Cells(32, 16) = NH3PERBIO 'NH3 (%)
545. Cells(33, 16) = TOTALPERBIO 'Total (%)
546. '*****
547. 'Cells OUT
548. Cells(29, 20) = CH4RATE 'CH4 OUT (m^3/day)
549. Cells(30, 20) = CO2RATE 'CO2 OUT (m^3/day)
550. Cells(31, 20) = H2SRATE 'H2S OUT (m^3/day)
551. Cells(32, 20) = NH3RATE 'NH3 OUT (m^3/day)
552. TOTALB = CH4RATE + CO2RATE + H2SRATE + NH3RATE
553. Cells(33, 20) = TOTALB 'Total (m^3/day)
554. '*****
555. 'Cells
556. 'Cells(50, 4) = HRTB 'Hydrolic Residence Time (day)
557. Cells(22, 16) = VOLUSEFULBIO * 1.15
558. Cells(23, 16) = SRTB
559. Cells(24, 16) = OLRB 'OLR-Organic Loading Rate (kgVS/m^3. d)
560. Cells(25, 16) = MUB
561. 'Cells
562. Cells(27, 12) = VRR 'Recycled Volume (m^3/day)
563. 'YIELD
564. Cells(27, 10) = TSREC 'TS RECYCLED (%)
565. Cells(29, 10) = GPRB 'Gas Production Rate (m3/m3.d)
566. Cells(30, 10) = QBIOGAD 'Rate of Biogas OUT (m^3/day)
567. Cells(31, 10) = SGP 'Experimental Yield of CH4 (m^3/kgVS)
568. TKH5 = SGP

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569. Cells(33, 13) = TKH5
570. *****
571. '                OUTPUT FOR EMS
572. *****
573. T = TEMPA
574. RHOH2S = 1.4341 'Density of H2S (kg/m^3)
575. RHOC2 = CO2DENSITY(T) 'CO2 Density T=oC,Kg/m^3
576. RHOCH4 = CH4DENSITY(T) 'CH4 Density T=oC,Kg/m^3
577. RHONH3 = NH3DENSITY(T) 'NH3 Density T=oC,Kg/m^3
578. CH4AK = CH4RATE * RHOCH4 'CH4 OUT From ADB (kg/day)
579. CO2AK = CO2RATE * RHOC2 'CO2 OUT From ADB (kg/day)
580. H2SAK = H2SRATE * RHOH2S 'H2S OUT From ADB (kg/day)
581. NH3AK = 0.00021
582. TOTALGASOUTADB = CH4AK + CO2AK + H2SAK + NH3AK 'Total gas out (Kg/day)'
583. DENBIOGASAD = TOTALGASOUTADB / (CH4RATE + CO2RATE + H2SRATE + NH3RATE) 'Density of biogas from AD'
584. MASSTOTRTQ = DENBIOGASAD * TOTALB
585. Cells(26, 20) = MASSTOTRTQ
586. RTFDDE = (CH4PERBIO / 100) * 16
587. RTFDDECO2 = (CO2PERBIO / 100) * 44
588. RTFDDEH2S = (H2SPERBIO / 100) * 34.1
589. RTFDDENH3 = (NH3PERBIO / 100) * 17.03
590. TREO0 = RTFDDE + RTFDDECO2 + RTFDDEH2S + RTFDDENH3
591. FTUUOOI = RTFDDE / TREO0
592. FTUUOOICO2 = RTFDDECO2 / TREO0
593. FTUUOOIH2S = RTFDDEH2S / TREO0
594. FTUUOOINH3 = RTFDDENH3 / TREO0
595. FTTRREEQ = MASSTOTRTQ * FTUUOOI
596. FTTRREEQCO2 = MASSTOTRTQ * FTUUOOICO2
597. FTTRREEQH2S = MASSTOTRTQ * FTUUOOIH2S
598. FTTRREEQNH3 = MASSTOTRTQ * FTUUOOINH3
599. Cells(22, 20) = FTTRREEQ 'CH4 OUT From ADB (kg/day)
600. Cells(23, 20) = FTTRREEQCO2 'CO2 OUT From ADB (kg/day)
601. Cells(24, 20) = FTTRREEQH2S 'H2S OUT From ADB (kg/day)
602. Cells(25, 20) = FTTRREEQNH3 'NH3 OUT From ADB (kg/day)
603. FTC3 = QBIOL - TOTALGASOUTADB
604. '=====
605. '***** RECYCLING *****
606. '=====
607. '.....MASS BALANCE WITHOUT RECYCLING
608. KGOUTADB = MMIX - TOTALGDKF - MASSTOTRTQ 'Total kg out of ADB wiyhout recycling
609. KGOUTDF = MMIX - TOTALGDK 'Total out of Dark Fermenter (kg/day)
610. KGINADB = KGOUTDF 'Total Flow into ADB (kg/day)
611. KGOUTADB = KGOUTDF - MASSTOTRTQ 'Total Flow OUT ADB (kg/day)
612. MMIXCV = MMIX
613. '...DATA OUT
614. Cells(67, 10) = MMIXCV 'Input flow to DARK Reactor (kg/day)
615. Cells(68, 10) = TOTALGDKF 'Gas out of DF Dark Fermenter [H2,CO2] (kg/day)
616. Cells(69, 10) = KGOUTDF 'Total out of Dark Fermenter (kg/day)
617. Cells(70, 10) = KGINADB 'Total Flow into ADB (kg/day)
618. Cells(71, 10) = MASSTOTRTQ 'Gas out of ADB [CH4,CO2] (kg/day)
619. Cells(72, 10) = KGOUTADB 'Total Flow out of ADB (kg/day)
620. '.....Mass BALANCE WITH RECYCLING at RRAT % Recycling Ratio
621. '...DATA IN
622. RRT = Cells(64, 17) 'Recycling Ratio (%)
623. '....
624. KGOUTR = KGOUTADB * (RRT / 100) 'Amount of Recycled (kg/day)
625. KGOUTCOM = KGOUTADB - KGOUTR 'Amount of compost Rejected (kg/day)
626. '...Recycling for DB ...
627. KGINDARK = MMIX + KGOUTR 'Amount of kg into Dark with recycling (kg/day)
628. KGGASOUTDFR = TOTALGDKF 'Amount of GAS out of DF (kg/day)
629. ' kg OUT of DF
630. KGOUTDFR = KGINDARK - TOTALGDKF 'Amount of liquid kg out of DF
631. '...Recycling for ADB ...
632. 'kg OUT of DF into ADB
633. KGINADBR = KGINADB 'Amount of liquid kg into ADB from DF

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634. ' Recycling ...
635.   GASOUTADBR = MASSTOTRTQ + KGOUTR   'Amount of gas out of ADB (kg/day)
636. 'kg out of ADB
637.   KGOUTADBR = KGINADB - GASOUTADBR
638. '...DATA OUT
639.   Cells(33, 9) = KGOUTR   'Amount of Recycled (kg/day)
640.   Cells(33, 11) = KGOUTCOM 'Amount of compost Rejected (kg/day)
641.   Cells(65, 17) = KGOUTR   'Amount of Recycled (kg/day)
642.   Cells(65, 19) = KGOUTCOM 'Amount of compost Rejected (kg/day)
643.   Cells(67, 17) = KGINADARK 'Amount of kg into Dark with recycling (kg/day)
644.   Cells(68, 17) = TOTALGDKF 'Amount of Gas out of DF Dark Fermenter [H2,CO2] (kg/day)
645.   Cells(69, 17) = KGOUTDFR   'Amount of liquid kg out of DF
646.   Cells(70, 17) = KGINADBR   'Amount of liquid kg into ADB DF
647.   Cells(71, 17) = GASOUTADBR 'Amount of gas out of ADB (kg/day)
648.   Cells(72, 17) = KGOUTADBR   'Amount of gas out of ADB (kg/day)
649.   '=====
650.   'DISCHARGED TANK'
651.   '=====
652.   TANKV98B = KGOUTADBR * (1 / FT0Y) * 1.25
653.   NUMTANK0 = TANKV98B / 113.562
654.   If NUMTANK0 < 1 Then
655.     NUMTANK0 = 1
656.   Else
657.     End If
658.   DISCHRATE0 = ((300 * (TANKV98B / NUMTANK0)) / (10)   'Discharge Rate (m^3/day)
659.   DISCHRATE5I = ((TANKV98B / NUMTANK0) / (DISCHRATE0)) 'Discharge Rate (m^3/sec)
660.   '=====
661.   RTANKD0 = (((TANKV98B / NUMTANK0) * (2)) / (3.14)) ^ (1 / 3) 'Diameter of Tank (m)
662.   RTANKH0 = (RTANKD0 * (2))   'Height of CSTR (m)
663. 'Cells
664.   Cells(4, 18) = TANKV98B   'Tank Volume (m^3)
665.   Cells(5, 18) = NUMTANK0   'NUMTANK
666.   Cells(6, 18) = RTANKD0   'Diameter of Tank (m)/Tanks
667.   Cells(7, 18) = RTANKH0   'Height of Tank (m) /Tanks
668.   Cells(8, 18) = DISCHRATE5I 'Discharge Rate (m^3/sec)
669.   '=====
670.   '                               SLUDGE PUPMPS
671.   '=====
672. 'To Dark
673. '...INPUT DATA
674.   GR = 9.81
675.   PRESHEAD = (CSTRBH2 / NUMTANKAB) + 0.5
676.   Cells(65, 4) = PRESHEAD
677.   Cells(66, 4) = RHOMIX
678.   Cells(67, 4) = MMIX
679. '...DATA OUT
680.   SLUDGFR1 = (((MMIX / RHOMIX) / 86400) * GR * PRESHEAD * RHOMIX) 'SLUDGE Flow Rate (L/sec)
681.   POWER1 = (SLUDGFR1) / 1000   'KW
682.   WATT3 = 1000 * POWER1
683.   Cells(68, 4) = POWER1   'Watt
684.   Cells(69, 4) = WATT3   'HP
685.   PRESHEAD2 = (RTANKD0 / NUMTANK0) + 0.5
686.   Cells(71, 4) = PRESHEAD2
687.   Cells(72, 4) = FT5
688.
689.   SLUDGFR2 = (((KGOUTADBR / FT5) / 86400) * GR * PRESHEAD2 * FT5)
690.   POWER12 = (SLUDGFR2) / 1000   'KW
691.   Cells(73, 4) = KGOUTADBR
692.   WATT4 = 1000 * POWER12
693.   Cells(74, 4) = POWER12   'Watt
694.   Cells(75, 4) = WATT4
695.
696.   '=====
697.   '                               CONVERSION
698.   '=====

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699. 'Cells OUT
700.   CONVERS = ((MMIX - KGOUTCOM) / (MMIX))           'conversion without recycling (%)
701.   OVERALLCONV = ((CONVERS) * (1 + RRT)) / ((1 + (RRT * CONVERS))) 'Overall conversion of the system'
702.   Cells(63, 4) = CONVERS 'conversion without recycling (%)
703.   Cells(63, 6) = OVERALLCONV 'Overall conversion of the system'
704.   '=====
705.   '                               Centrifugal FAN TO EMS (CV1)
706.   '=====
707.   GACC = 9.81 'Gravity Acceleration
708.   RHOCH4 = 0.656 'kg/m³
709.   RHOC02 = 1.98 'kg/m3
710.   RHOGAS = RHOCH4 * (CH4PERBIO / 100) + RHOC02 * (CO2PERBIO / 100)
711.   GASFR = (TOTALB / 24) / 3600 'GAS Flow Rate OUT(m³/sec)
712.   IPSPEED = 5000
713. '...DATA IN
714.   Cells(78, 4) = GASFR
715.   Cells(79, 4) = PDFB 'INLET Pressure (Atm.)
716.   POUT = Cells(80, 4) 'OUTLET Pressure (Atm.)
717.   EXITPIPIARE = Cells(81, 4) 'Exit Pipe AREA (m)
718.   IPSPEED = Cells(82, 4) 'Impeller Specific Speed (RPM)
719. '...DATA OUT
720.   VDISCH = GASFR / EXITPIPIARE '
721.   HEADCH = POUT / (RHOGAS * GACC) + VDISCH ^ 2 / (GACC * 2) - PIN / (RHOGAS * GACC)
722.   POWERFAN = (RHOGAS * GASFR * GACC * HEADCH) * 10000 'Watt
723.   NS = (IPSPEED * GASFR ^ 0.5) / (HEADCH ^ (3 / 4))
724.   Cells(83, 4) = VDISCH
725.   Cells(84, 4) = NS
726.   Cells(85, 4) = POWERFAN '(W)
727. '=====
728. '=====
729. '                               CALCULATIONS
730. '=====
731. '.....Required Heat for DARK HEAT EXCHANGER N09
732. '=====
733. 'Waste Specific Heat=2629.425 J/kg.K
734.   TL = Cells(92, 4) 'Tube Length (m)
735.   TOD = Cells(93, 4) 'Tube Outside Diameter (m)
736. '.....
737.   TH1 = H2OTEMPXX + 273 'Steam Temperature(K)
738.   TC1 = 2 + 273 'Waste IN Temperature (K)
739.   TC2 = 37 + 273 'Waste OUT Temperature (K)
740.   SCWASTE = 2629.425 / 1000 'WASTE Specific Heat Capacity (kJ/kg.K)
741.   CWASTED = SCWASTE * (MMIX / 24) / 3600 'WASTE Heat Capacity (kW/sec.K)
742.   QWASTED = CWASTED * (TC2 - TC1) '(kW)
743. 'STEAM
744.   H2OTEMP = TH1
745.   SCSTEAM = WATERSPECIFICHEAT(H2OTEMP) 'WATER SPECIFIC HEAT Capacity (kJ/kg.K)
746. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
747.   FLAG = 1
748.   U = 0.227
749.   CCOLD = CWASTED: Q = QWASTED: SCHOT = SCSTEAM: SCCOLD = CWASTED
750. 'Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN
GER
751.   HE9 = QEFF
752.   WASTETEMOUT = TC2 - 273
753. 'OUTPUT
754.   STEAMFR = HFR
755.   Cells(88, 4) = H2OTEMPXX 'Steam Temperature In (oC)
756.   Cells(89, 4) = TH2 - 273 'Steam Temperature OUT (oC)
757.   Cells(90, 4) = TC1 - 273 'Waste Temperature In (oC)
758.   Cells(91, 4) = WASTETEMOUT 'Waste Temperature OUT (oC)
759.   Cells(94, 4) = NTU 'Number of Tubes
760.   Cells(95, 4) = AREAHEX 'Shell Area (m²)
761.   Cells(96, 4) = EPS * 100 'Effectiveness
762.   Cells(97, 4) = QEFF 'Heat Transfer (W)

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763. Cells(98, 4) = STEAMFR 'Steam Flow Rate (kg/day)
764. '=====
765. '.....Required cold for DARK CONDENSER No3
766. '=====
767. 'Waste Specific Heat=2629.425 J/kg.K
768. TL = Cells(79, 11) 'Tube Length (m)
769. TOD = Cells(80, 11) 'Tube Outside Diameter (m)
770. TH1 = WASTETEMOUT + 273 'Waste IN Temperature (K)
771. TH2 = 35 + 273 'Waste OUT Temperature (K)
772. TC1 = 25 + 273 'Air IN Temperature (K)
773. AIRTK = 25 + 273
774. SCAIR = AIRSPECIFICHEAT(AIRTK) 'AIRSPECIFICHEAT (kJ/kg.K)
775. '....
776. SCWASTE = 2629.425 / 1000 'WASTE Specific Heat Capacity (kJ/kg.K)
777. CWASTEDB = SCWASTE * (KGINDARK / 24) / 3600 'WASTE Heat Capacity (kW/sec.K)
778. QWASTEDB = CWASTEDB * (TH1 - TH2) '(kW)
779. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
780. FLAG = 2
781. U = 0.227 '0.02
782. CHOT = CWASTEDB: Q = QWASTEDB: SCHOT = SCWASTE: SCCOLD = SCAIR
783. Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN
GER
784. AIRFRDB = HFR
785. Cells(75, 11) = AIRTK - 273 'Air Temperature In (oC)
786. Cells(76, 11) = TC2 - 273 'Air Temperature OUT (oC)
787. Cells(77, 11) = TH1 - 273 'Waste Temperature In (oC)
788. Cells(78, 11) = TH2 - 273 'Waste Temperature OUT (oC)
789. Cells(81, 11) = NTU 'Number of Tubes
790. Cells(82, 11) = AREAHEX 'Shell Area (m^2)
791. Cells(83, 11) = EPS * 100 'Effectiveness
792. Cells(84, 11) = QEFF 'Heat Transfer (W)
793. Cells(85, 11) = AIRFRDB 'Steam Flow Rate (kg/day)
794.
795. '=====
796. 'Heat LOSS
797. '=====
798. 'Dark fermentation heat loss'
799. TEMPDK = TEMPD + 273
800. 'Anaerobic digestion heat loss'
801. ANAR1 = CSTRBH2 * 2 * Pi * (CSTRBD2E / 2)
802. ANAR2 = 2 * Pi * ((CSTRBD2E / 2) ^ 2)
803. QUP = (0.3 * ANAR1 * (TEMPDK - TAMBK)) / 1000 'Heat loss 1 (kW)'
804. QUP1 = (0.34 * ANAR1 * (TEMPDK - TAMBK)) / 1000 'Heat loss 2 (kW)'
805. QUP2 = (0.15 * ANAR2 * (TEMPDK - TAMBK)) / 1000 'Heat loss 3 (kW)'
806. QUP3 = (2.08 * ANAR2 * (TEMPDK - TAMBK)) / 1000 'Heat loss 4 (kW)'
807. QUP4 = (0.32 * ANAR1 * (TEMPDK - TAMBK)) / 1000 'Heat loss 5 (kW)'
808. 'TOTAL For ANAEROBIC
809. QUPTOT = (QUP + QUP1 + QUP2 + QUP3 + QUP4) * NUMTANKAB 'Total heat loss (kW)'
810. 'Cells Output
811. Cells(100, 4) = QUPTOTDARK
812. Cells(101, 4) = QUPTOT
813. '===== TANKS HEAT LOSSES =====
814. 'heat loss Tank 1'(After ADB)
815. TEMPA00 = Cells(78, 11) + 273
816. TEMPAK = 25 + 273 'ADB Temperature (K)
817. CHT = 0.1 'W/m^2.K
818. TIMCONV = 86400 '=> (3600) * (24)
819. ANAWGH1 = 2 * RTANKH0 * Pi * (RTANKD0 / 2)
820. ANAWGH2 = 2 * Pi * ((RTANKD0 / 2) ^ 2)
821. ATWER56 = ANAWGH1 + ANAWGH2
822. QUPTFERT4 = ((ATWER56 * (TEMPA00 - TEMPAK)) / CHT) / 1000
823. QUPTOTV4 = QUPTFERT4 * NUMTANK0 'Total heat loss (kW)'
824. 'Heat Loss Tank 2'(Before ADB)
825. TEMPHG = Cells(91, 4)
826. ANARDARW1 = 2 * RTANKH * Pi * (RTANKD / 2)

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827. ANARDARW2 = 2 * Pi * ((RTANKD / 2) ^ 2)
828. ATRE12KL = ANARDARW2 + ANARDARW1
829. QUPDARWEYT = ((ATRE12KL * ((TEMPHG + 273) - TEMPAK)) / CHT) / 1000
830. QUPTOTDARFKX1 = QUPDARWEYT * INONUMBTANK      'Total heat loss (kW)'
831. 'Cells OUTPUT
832. Cells(102, 4) = QUPTOTV4
833. Cells(103, 4) = QUPTOTDARFKX1
834.
835. '=====
836. TVELAGDXTAN = 6
837. IMPDADXTAN = (RTANKD / 3)      'Impeller diameter (m)
838. SPEIMPDXTAN = ((TVELAGDXTAN) / (3.14 * IMPDADXTAN)) * 60      '(RPM)'Impeller speed'
839. IMPHPDXTAN = (((NOIMBPLD) * ((SPEIMPD) ^ (3)) * (0.016)) * ((IMPDADXTAN) ^ (5)) * (RHOMIX)) / (2447.578))      '(HP)'impeller
840. POWBIO5XTAN = IMPHPDXTAN * INONUMBTANK
841. TVELAGDXTAN = Cells(4, 23)
842. Cells(5, 23) = IMPDADXTAN
843. Cells(6, 23) = SPEIMPDXTAN
844. Cells(7, 23) = IMPHPDXTAN
845. Cells(8, 23) = POWBIO5XTAN
846. '=====
847.      'Dewatering the Digested Sludge'
848. '=====
849. DENSOLID = (FT5 / 34.429) / 1000      'Density of solid (Cake) (kg/liter)'
850. RTEW2 = 100 - TSOUT      'Moisture content%'
851. MOISTCONT = KGOUTCOM * (RTEW2 / 100)      'MOISTURE CONTENT (kg/day)'
852. SOLIDRT3 = KGOUTCOM - MOISTCONT      'Solid content (kg/day)'
853. 'FILTERFLUX = KGOUTCOM / 92      'Flux of Digested Sludge from Filter Press'(kg/day.m2)'https://www.environmental-
expert.com/files/19732/download/737034/2-Filter-Press-DRACO-Toro-Equipment-ENG.pdf'
854. VOLUY = (KGOUTCOM / FT5) * 1000      '(liter/day) to be dewatered'
855. DFREWQ = (VOLUY * (TSOUT)) / (100)      'Liter of solid'
856. HOYOU = (VOLUY * (TSOUT * 10)) / 1000      '(gram/day) of Solid (For sizing of the filter press)'
857. SFCAKE = ((HOYOU) / KGOUTCOM) * 100      'Dryness of the cakes produced (wet/dry)%'
858. VOLFILT = (100 * HOYOU) / (SFCAKE * (DENSOLID))      'Daily volume of cake produced (Liter/day)'
859. VOLB023 = VOLFILT / 3.2
860. VOLB023HYD = (VOLB023 * SFCAKE * 1000 * DENSOLID) / (TSOUT * 1000)      'Total haydraulic volume to be pumped (Liters)'
861. VOLPUMPFPR = VOLB023HYD / 1440      'flow to be pumped (Liter/min)'
862. BNM = ((1.55 * VOLB023HYD) / 2.25) / 60      'Initial flow rate of membrane pump (Liter/min)'
863. FLOWRATE = BNM
864. PUPMPOWER = FILTERPUMPPOWER(FLOWRATE)      '(kW)
865. 'HYDROLIC PRESSING MOTOR POWER
866. If VOLUY <= 5100 Then
867. HYDROLICPOW = 4
868. End If
869. If VOLUY > 5100 Then
870. HYDROLICPOW = 7.5
871. End If
872. If VOLUY > 8000 Then
873. HYDROLICPOW = 7.5
874. End If
875. If VOLUY > 10660 Then
876. HYDROLICPOW = 11
877. End If
878. If HYDROLICPOW > 17800 Then
879. HYDROLICPOW = 15
880. End If
881.
882. 'OUTPUT CELLS
883. Cells(111, 4) = VOLUY      'Wet Volume of Sludge (L/min)
884. Cells(112, 4) = RTEW2      'Sludge Moisture Contents (%)
885. Cells(113, 4) = VOLFILT      'Daily volume of cake produced (Liter/day)
886. Cells(114, 4) = SFCAKE      'Final Solid Moisture Content (%)
887. Cells(115, 4) = BNM      'Final Solid Moisture Content (%)
888. Cells(116, 4) = PUPMPOWER      'Pump Power (kW)
889. Cells(117, 4) = HYDROLICPOW      'Hydrolic Pressing Motor (kW)
890. '=====

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891.
892. 'MOISTCONT=12428.421 (kg/day)
893. VOLWAT = MOISTCONT / 1000 ' (m3/day)
894. VOLMATE1 = VOLWAT / 86400 '(m3/s)
895. 'assuming pump diameter =0.1 m'
896. PIP1 = Cells(120, 2)
897. AREAPUMP12 = (3.14) * (PIP1 * PIP1) / 4
898. VOLPUMP = VOLMATE1 / AREAPUMP12 'Velocity m/s'
899. 'k = 1.35
900. VISCOS = 8.9 * 10^ - 7 '(m2/s) '1.31*10^-6 (m2/s)
901. RYNOL = (PIP1 * VOLPUMP) / VISCOS
902. FRIC = 0.25 / Log((1.35 / (3.7 * PIP1)) + (5.7 / RYNOL)) ^ 2
903. PIPELENGTH = (NUMTANKAB * 1.47) + (RTANKD0 * NUMTANK0) + 10 + (RTANKD * INONUMBTANK) + (RTANKH / 2) + 2 ' Length of pipe (m)'
904. KPIPE = FRIC * PIPELENGTH / PIP1
905. KFIT = 1.625 + KPIPE
906. HTE1 = KFIT * (VOLPUMP * VOLPUMP) / (19.6)
907. HESDF2 = (RTANKH / 2) + HTE1
908. PUMPEFF = Cells(122, 2)
909. POWEPUM = (HESDF2 * 9.81 * 1000 * VOLMATE1) / 84
910. Cells(123, 2) = POWEPUM / 1000
911. '=====
912. VOLWATSLU = KGOUTR / FT5 ' (m3/day)
913. VOLMATE1X = VOLWATSLU / 86400 '(m3/s)
914. PIP1X = Cells(124, 2)
915. AREAPUMP12X = (3.14) * (PIP1X * PIP1X) / 4
916. VOLPUMP3 = VOLMATE1X / AREAPUMP12X 'Velocity m/s'
917. RYNOLX = (PIP1X * VOLPUMP3) / 0.2
918. FRICX = 0.25 / Log((1.35 / (3.7 * PIP1X)) + (5.7 / RYNOLX)) ^ 2
919. PIPELENGTHX = 0.5 + 2.9 + 2 - 1 + (NUMTANKAB * 1.47) + (RTANKD0 / 2 * NUMTANK0) + 3 ' Length of pipe (m)'
920. KPIPEX = FRICX * PIPELENGTHX / PIP1X
921. KFITX = 1.45 + KPIPEX
922. HTE1X = KFITX * (VOLPUMPX * VOLPUMPX) / (19.6)
923. HESDF2X = (1.47 * NUMTANKAB) + 2.5 - 1 + HTE1X
924. POWEPUMX = (HESDF2X * 9.81 * FT5 * VOLMATE1X) / 84
925. Cells(125, 2) = POWEPUMX / 1000
926. '=====
927. 'From Urea'
928. '=====
929. UREA1 = Cells(130, 2)
930. VOLWATP = UREA1 / 1000 ' (m3/day)
931. VOLMATE1P = VOLWATP / 86400 '(m3/s)
932. 'assuming pump diameter =0.1 m'
933. PIP1 = Cells(120, 2)
934. AREAPUMP12P = (3.14) * (PIP1 * PIP1) / 4
935. VOLPUMPP = VOLMATE1P / AREAPUMP12P 'Velocity m/s'
936. 'k = 1.35
937. VISCOS = 8.9 * 10^ - 7 '(m2/s) '1.31*10^-6 (m2/s)
938. RYNOLP = (PIP1 * VOLPUMPP) / VISCOS
939. FRICP = 0.25 / Log((1.35 / (3.7 * PIP1)) + (5.7 / RYNOLP)) ^ 2
940. PIPELENGTHP = 14 ' Length of pipe (m)'
941. KPIPEP = FRICP * PIPELENGTHP / PIP1
942. KFITP = 1.625 + KPIPEP
943. HTE1P = KFITP * (VOLPUMPP * VOLPUMPP) / (19.6)
944. HESDF2P = 3 + HTE1P
945. PUMPEFF = Cells(122, 2)
946. POWEPUMPP = (HESDF2P * 9.81 * 1000 * VOLMATE1P) / 84
947. Cells(126, 2) = POWEPUMPP / 1000
948.
949. '=====
950. ss = ss
951. End Sub
952. Static Function Logn(X)
953. Logn = Log(X) / Log(2.718282)
954. End Function
955. Private Static Function H2DENSITY(T) 'T=oC,Kg/m^3 1Atm

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956. A = 0.041236128: B = 11.271649
957. H2DENSITY = 1 / ((A * T) + B)
958. End Function
959. Private Static Function CO2DENSITY(T) 'T=oC,Kg/m^3
960. A = 0.50649907: B = 0.0019289299: C = 1.0174749
961. CO2DENSITY = (A + B * T) ^ (-1 / C)
962. End Function
963. Private Static Function CH4DENSITY(T) 'T=oC,Kg/m^3
964. A = 0.70822045: B = 269.39972: C = -0.00035602407: D = 0.99821142
965. CH4DENSITY = (A * B + C * (T) ^ D) / (B + (T) ^ D)
966. End Function
967. Private Static Function NH3DENSITY(T) 'T=oC,Kg/m^3
968. A = 1.3112907: B = 0.0054825167: C = 0.98156027
969. NH3DENSITY = 1 / (A + B * (T) ^ C)
970. End Function
971. Private Static Function WATERSPECIFICHEAT(H2OTEMP) 'WATER SPECIFIC HEAT kJ/Kg.K in oK
972. WATERSPECIFICHEAT = 1.224986 + 0.0014072339 * H2OTEMP - 0.0000039722778 * H2OTEMP ^ 2 + 5.3431749E-11 * H2OTEMP ^ 3 + -2.7473115E-
15 * H2OTEMP ^ 4
973. End Function
974. Private Static Function AIRSPECIFICHEAT(AIRTK) 'AIRSPECIFICHEAT kJ/Kg.K T=oK
975. TA = 1.0828694: TB = -0.00063119116: TC = 0.0000016253087: TD = -1.3949526E-09: TE = 5.3826153E-13: TF = -7.9021928E-17
976. AIRSPECIFICHEAT = TA + TB * AIRTK + TC * AIRTK ^ 2 + TD * AIRTK ^ 3 + TE * AIRTK ^ 4 + TF * AIRTK ^ 5
977. End Function
978. Private Static Sub HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'H
EAT EXCHANGER
979. AREAHEX = 3.14 * TOD * TL
980. DELTAB = TH2 - TC1
981. LMTD = Q / (U * AREAHEX)
982. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
983. '----- HEATING -----
984. If FLAG = 1 Then
985. DELTAA = TH1 - TC2
986. LMTD = Q / (U * AREAHEX)
987. X1 = 1
988. 300 S1 = DELTAA / (LMTD - Logn(DELTAA))
989. S2 = X1 / (LMTD - Logn(X1))
990. If S2 >= S1 Then
991. GoTo 400
992. Else
993. X1 = X1 + 0.1
994. GoTo 300
995. 400 End If
996. DELTAB = X1
997. TH2 = DELTAB + TC1
998. GoTo 700
999. End If
1000. '-----
1001. '----- COOLING -----
1002. If FLAG = 2 Then
1003. DELTAB = TH2 - TC1
1004. LMTD = Q / (U * AREAHEX)
1005. X1 = 2
1006. 500 S1 = Logn(X1) - X1 / LMTD
1007. S2 = Logn(DELTAB) - DELTAB / LMTD
1008. If S1 >= S2 Then
1009. GoTo 600
1010. Else
1011. X1 = X1 + 0.1
1012. GoTo 500
1013. 600 End If
1014. DELTAA = X1
1015. TC2 = TH1 - DELTAA
1016. End If
1017. '-----
1018. 700 P = (TC2 - TC1) / (TH1 - TC1)

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1019. R = (TH1 - TH2) / (TC2 - TC1)
1020. If R > 1 Then
1021. R1 = 1 / R
1022. P1 = P * R
1023. Else
1024. P1 = P
1025. R1 = R
1026. End If
1027. A1 = (((R1) ^ 2 + 1) ^ 0.5) / (1 - R1)
1028. A2 = Logn((1 - R1 * P1) / Abs(1 - P1))
1029. A3 = 2 - P1 * (1 + R1 - (1 + (R1) ^ 2)) ^ 0.5 'up
1030. A4 = Abs(2 - P1 * (1 + R1 + (1 + (R1) ^ 2)) ^ 0.5) 'down
1031. A5 = Logn(A3 / A4)
1032. FCORF = (A1 * A2) / A5
1033. If Abs(FCORF) > 1 Then
1034. FCORF = 1
1035. End If
1036. If FLAG = 1 Then
1037. LMTD = Q / (U * AREAHEX * FCORF)
1038. CHOT = Q / (TH1 - TH2)
1039. HFR = CHOT * 24 * 3600 / SCHOT
1040. GoTo 800
1041. End If
1042. If FLAG = 2 Then
1043. LMTD = Q / (U * AREAHEX * FCORF)
1044. CCOLD = Q / (TH1 - TH2)
1045. HFR = CCOLD * 24 * 3600 / SCHOT
1046. End If
1047. 'EFFECTIVENESS
1048. 800 If CCOLD > CHOT Then
1049. CMIN = CHOT
1050. C1 = CHOT
1051. EPS = (C1 * (TC2 - TC1)) / (CMIN * (TH1 - TC1))
1052. GoTo 900
1053. Else
1054. CMIN = CCOLD
1055. C1 = CCOLD
1056. EPS = (C1 * (TH1 - TH2)) / (CMIN * (TH1 - TC1))
1057. 900 End If
1058. QEFF = EPS * CMIN * (TH1 - TC1)
1059. 'Number of ELEMENT
1060. NTU = U * AREAHEX / CMIN
1061. If NTU <= 1 Then
1062. NTU = 1
1063. Else
1064. End If
1065. End Sub
1066.
1067. Private Static Function FILTERPUMPPOWER(FLOWRATE)
1068. A = 6.1441296: B = 0.0277043
1069. FILTERPUMPPOWER = A * (1 - Exp(-B * FLOWRATE))
1070. End Function

```

Heat Balance results

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1. Sub Sheet11_Button1_Click()
2.
3. '
4. '=====
5. ' HEAT BALANCE
6. '=====
7. '===== OUTPUT and INPUT FROM DARK
8. DFBTANK = ActiveWorkbook.Worksheets("DFB-ADB").Cells(100, 4) 'Energy IN DARK CSTR -(kw)
9. ADBTANK = ActiveWorkbook.Worksheets("DFB-ADB").Cells(101, 4) 'Energy IN ADB CSTR -(kw)
10. WESTANK1 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(102, 4) 'Energy IN ADB TANK1 -(kw)

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11. WESTANK2 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(103, 4) 'Energy IN ADB TANK2 -(kW)
12. WESTANK2XX = ActiveWorkbook.Worksheets("SOFC").Cells(35, 11) 'Energy IN ADB TANK2 -(kW)
13. WESTANK2BB = ActiveWorkbook.Worksheets("SOFC").Cells(52, 4) 'Energy IN ADB TANK2 -(kW)
14. WESTANK2BB123 = ActiveWorkbook.Worksheets("SOFC").Cells(53, 4) 'Energy IN ADB TANK2 -(kW)
15. WESTANK2BBTTT = ActiveWorkbook.Worksheets("SOFC").Cells(28, 11) 'Energy IN ADB TANK2 -(kW)
16. ADS = ActiveWorkbook.Worksheets("EMS").Cells(43, 11) 'Energy IN ADB TANK2 -(kW)
17.
18. '===== INPUT FROM ADB
19.
20. '===== SOFC TEMPERATURE
21. SOFCTEMP = ActiveWorkbook.Worksheets("SOFC").Cells(13, 4) 'SOFC Cell Temperature (oC)
22. '===== UREA INPUT
23. UREAENIN = ActiveWorkbook.Worksheets("UREA").Cells(9, 31) 'UREA ENERGY IN (kW)
24. UREAENOUT = ActiveWorkbook.Worksheets("UREA").Cells(15, 32) 'UREA ENERGY OUT (kW)
25. '===== INPUT DATA FOR TOTAL AIR REQUIRED FOR THE COMPRESSOR
26. AIRDARK = ActiveWorkbook.Worksheets("DFB-ADB").Cells(85, 11) ' AIR REQUIRED FOR DARK (Kg/day)
27. AIRSOFC = ActiveWorkbook.Worksheets("SOFC").Cells(10, 4) ' AIR REQUIRED FOR SOFC cell (Kg/day)
28. AIRSOFEC = ActiveWorkbook.Worksheets("SOFEC").Cells(26, 16) ' AIR REQUIRED FOR SOFEC HECH (Kg/day)
29. AIRITM = ActiveWorkbook.Worksheets("ITM").Cells(5, 4) ' AIR REQUIRED FOR (ITM)HE (Kg/day)
30. AIRSSAS1 = ActiveWorkbook.Worksheets("SSAS").Cells(27, 16) ' AIR REQUIRED FOR SSAS HE (Kg/day)
31. AIRSSAS2 = ActiveWorkbook.Worksheets("SSAS").Cells(14, 16) ' AIR REQUIRED FOR SSAS HE (Kg/day)
32. AIRSSAS3 = ActiveWorkbook.Worksheets("SSAS").Cells(40, 16) ' AIR REQUIRED FOR SSAS Condenser(Kg/day)
33. AIREMS = ActiveWorkbook.Worksheets("EMS").Cells(32, 11) ' AIR REQUIRED FOR EMS Condenser(Kg/day)
34. AIRTEMP = ActiveWorkbook.Worksheets("ITM").Cells(8, 4) ' AIR TEMPERATURE from (ITM) (oC)
35. '===== ENERGY IN COMPRESSORS & PUMPMS(kW)
36. COM3 = ActiveWorkbook.Worksheets("SSAS").Cells(31, 11) 'Compressor No3[SSAS] (kW)-
37. COM4 = ActiveWorkbook.Worksheets("SSAS").Cells(52, 11) 'Compressor No4[SSAS] (kW)-
38. COM5 = ActiveWorkbook.Worksheets("SOFC").Cells(32, 4) 'Compressor No5[SOFC] (kW)-
39. COM6 = ActiveWorkbook.Worksheets("SOFC").Cells(49, 16) 'Compressor No6[SOFC] (kW)-
40. COM8 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(117, 4) 'Hydrolic Compressor (KW)-
41. '===== SLUDGE PUMPS =====
42. SP1 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(68, 4) 'SLURY PUMP DARK REACTOR (W)-
43. SP2 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(74, 4) 'SLURY PUMP DARK REACTOR (kW)-
44. SP3 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(108, 4) 'SLURY PUMP DIGESTER (kW)-
45. SP4 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(116, 4) 'SLURY PUMP DIGESTER (kW)-
46. '===== ENERGY IN HEAT EXCHANGER & CONDENSER (kW)
47. HE1 = ActiveWorkbook.Worksheets("ITM").Cells(38, 4) 'Heat Exchanger No1 [ITM] (KW)-
48. HE2 = ActiveWorkbook.Worksheets("EMS").Cells(12, 16) 'Heat Exchanger No2 [EMS] (KW)+
49. HE3 = ActiveWorkbook.Worksheets("EMS").Cells(24, 16) 'Heat Exchanger No3 [EMS] (KW)-
50. HE4 = ActiveWorkbook.Worksheets("SOFEC").Cells(13, 16) 'Heat Exchanger No4 [ITM] (KW)+
51. HE5 = ActiveWorkbook.Worksheets("SOFEC").Cells(26, 16) 'Heat Exchanger No5 [SOFEC] (KW)+
52. HE6 = ActiveWorkbook.Worksheets("SSAS").Cells(13, 16) 'N2 Heat Exchanger No6 [SSAS](KW)+
53. HE7 = ActiveWorkbook.Worksheets("SSAS").Cells(26, 16) 'H2 Heat Exchanger No7 [SSAS](KW)+
54. HE8 = ActiveWorkbook.Worksheets("SOFC").Cells(34, 11) 'Heat Exchanger BOX 8 [SOFC] (KW)-
55. HE9 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(97, 4) 'Heat Exchanger No9 [INNOCULUM] (KW)-
56. HE10 = ActiveWorkbook.Worksheets("SOFC").Cells(51, 4) 'Heat Exchanger BOX 8 [SOFC] (KW)-
57. 'Condenser
58. COND1 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(84, 11) 'Energy OUT DARK Condenser (kW)+
59. COND3 = ActiveWorkbook.Worksheets("EMS").Cells(30, 11) 'Heat Condenser No1 [EMS](KW)+
60. COND4 = ActiveWorkbook.Worksheets("SSAS").Cells(39, 16) 'Heat Condenser No2 [SSAS](KW)+
61. COND5 = ActiveWorkbook.Worksheets("SSAS").Cells(54, 16) 'Heat Condenser No5 [SSAS](KW)+
62. 'Membranes Heat Loss
63. HLITM = ActiveWorkbook.Worksheets("ITM").Cells(41, 4) 'Heat Loss from ITM Cell (kW)
64. HLEMS = ActiveWorkbook.Worksheets("EMS").Cells(29, 16) 'Heat Loss from ITM Cell (kW)
65. HLSOFEC = ActiveWorkbook.Worksheets("SOFEC").Cells(29, 11) 'Heat Loss from SOFEC Cell (kW)
66. HLSSAS = ActiveWorkbook.Worksheets("SSAS").Cells(38, 11) 'Heat Loss from SSAS Cell (kW)
67. HLSOFC = ActiveWorkbook.Worksheets("SOFC").Cells(40, 11) 'Heat Loss from SOFC Cell (kW)
68. HLSOFCE4 = ActiveWorkbook.Worksheets("SOFC").Cells(73, 2) 'Heat Loss from SOFC Cell (kW)
69. 'CO2 CALCULATIONS
70. 'CO2
71. CO2SOFEC = ActiveWorkbook.Worksheets("SOFEC").Cells(6, 11) 'CO2 From SOFEC(kg/hr)
72. CO2TEMPUREA = ActiveWorkbook.Worksheets("UREA").Cells(4, 4) 'CO2 TEMPERATURE to Urea oC
73. CO2SOFECTEMP = ActiveWorkbook.Worksheets("SOFEC").Cells(15, 4) 'CO2 TEMPERATURE From Dark oC
74. CO2PRESIN = ActiveWorkbook.Worksheets("SOFEC").Cells(9, 4) 'CO2 Pressure atm.
75. CO2PRESOUT = ActiveWorkbook.Worksheets("UREA").Cells(3, 4)

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76. H2OHEXRECY = ActiveWorkbook.Worksheets("SOFC").Cells(15, 17)
77. SSASAIRFLOW = ActiveWorkbook.Worksheets("SSAS").Cells(55, 16)
78. SSASAIRFLOW1 = ActiveWorkbook.Worksheets("SSAS").Cells(40, 16)
79. SOFECAIRFLOW1 = ActiveWorkbook.Worksheets("SOFEC").Cells(9, 11)
80. SFDE44 = ActiveWorkbook.Worksheets("HEAT BALANCE").Cells(87, 16)
81. SFDE44CVP = ActiveWorkbook.Worksheets("SOFEC").Cells(8, 11)
82. '=====
83. 'CO2 Calculations
84. R = 8.314 'J/K.mol
85. CO2MW = 44 'Molecular Weight
86. 'CO2 Total Flowrate
87. CO2TOTAL = CO2SOFEC
88. 'MIXED CO2 Temperature
89. CO2MIXTEMP = CO2SOFECTEMP 'Mixed CO2 Temperature
90. '===== COMPRESSORE FOR CO2 COM10 =====
91. Cells(67, 16) = CO2PRESIN 'Inlet Pressure atm
92. Cells(68, 16) = CO2PRESOUT 'OUTLET Pressure atm
93. Cells(69, 16) = CO2MIXTEMP 'Inlet Temperature
94. 'CALCULATIONS
95. COMPIN = CO2PRESIN 'Compressor Inlet Pressure (atm.)
96. COMPOP = CO2PRESOUT 'Compressor Outlet Pressure (atm.)
97. COMETREFF = Cells(70, 16) 'Compressor Entropy Efficiency (%)
98. SPHASVOL = Cells(71, 16) 'Single Phase Voltage (Volts)
99. MOTOREFF1 = Cells(72, 16) 'Single Phase Motor Efficiency (%)
100. THREPASEVOL = Cells(73, 16) '3 Phase Voltage (Volts)
101. MOTOREFF3 = Cells(74, 16) '3 Phase Motor Efficiency (%)
102. 'COMPRESSOR DATA
103. GASTK = CO2MIXTEMP + 273 'Inlet Gas Temperature (oK)
104. CO2SPCHEAT = CO2SPEHEAT(GASTK) 'CO2 SPECIFIC HEAT ' Cp of CO2 kJ/Kg K 'NH3 Specific Heat (kJ/Kg.K)kJ/kg.K (>1atm)
105. T = CO2MIXTEMP
106. RHOCO2 = CO2DENSITY(T) 'NH3 Density (Kg/m^3)
107. GAMMA = 1.18 'GAMMA=Cp/Cv
108. CO2VOLD = CO2TOTAL / RHOCO2 'CO2 Volume m^3/day
109. CO2VOLM = (CO2VOLD / 24) / 60 'CO2 Volume m^3/min
110. CO2VOLIT = CO2VOLM * 1000 'CO2 Volume L/min
111. Cells(66, 16) = CO2VOLIT 'CO2 Volume L/min,<=====
112. CO2MOL = CO2TOTAL / CO2MW 'CO2 Mol
113. ENTCC = CO2MOL * R * Logn(COMPOP / COMPIN)
114. GASTEMPC = CO2MIXTEMP: GASVOL = CO2VOLIT
115. OUTADIATEMP = ((CO2MIXTEMP + 273) * ((COMPOP / COMPIN) ^ ((GAMMA - 1) / GAMMA))) - 273 ' OUTLET ADIABATIC TEMPERATURE
116. DRMOTWATT = ((OUTADIATEMP - (CO2MIXTEMP + 273)) * CO2SPCHEAT * (CO2TOTAL / 86400)) / (MOTOREFF1 / 100) 'KW
117. Cells(65, 21) = OUTADIATEMP
118. Cells(66, 21) = DRMOTWATT
119. Cells(67, 21) = DRMOTHP
120. Cells(68, 21) = CURRENT1
121. Cells(69, 21) = CURRENT3
122. CO2CONPW = DRMOTWATT
123. '----- CO2 COOLING Heat EXCHANGER N011
124. TL = Cells(81, 16)
125. TOD = Cells(82, 16)
126. 'CO2
127. TH1 = OUTADIATEMP + 273
128. TH2 = CO2TEMPUREA + 273
129. GASTK = TH1
130. SCCO2 = CO2SPEHEAT(GASTK)
131. CCO2 = ((CO2TOTAL / 24) / 3600) * SCCO2 'O2 Heat capacity (KW/oK)
132. QO2 = CCO2 * (TH1 - TH2)
133. 'Air Flow rate needed to Cool CO2
134. Cells(78, 16) = 25 'AIR TEMPERATURE IN oC
135. TC1 = 25 + 273
136. AIRINTK1 = TC1
137. AIRINTK1 = 25 + 273
138. SCAIR = AIRSPECICHEAT(AIRINTK1)
139. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
140. FLAG = 2

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141. U = 0.02
142. CHOT = CC02: Q = Q02: SCHOT = SCC02: SCCOLD = SCAIR
143. Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN
GER
144. 'OUTPUT
145. AIRCO2 = HFR
146. Cells(77, 16) = OUTADIATEMP
147. Cells(78, 16) = CO2TEMPUREA
148. Cells(79, 16) = 25 'AIR TEMPERATURE IN oC
149. Cells(80, 16) = TC2 - 273 'AIR TEMPERATURE IN oC
150. Cells(83, 16) = NTU
151. Cells(84, 16) = AREAHEX
152. Cells(85, 16) = EPS
153. Cells(86, 16) = QEFF
154. Cells(87, 16) = AIRCO2
155. HE11 = QEFF
156. 'Waste Eanks Heat Losses
157. '=====
158. ' CALCULATIONS
159. '=====
160. '===== ENERGY OUT (kW)
161. GASTURB = ActiveWorkbook.Worksheets("SOFC").Cells(57, 16) 'Steam Turbine [SOFC] (kW)+
162. '=====
163. 'POWER and Voltage
164. EMSPower = ActiveWorkbook.Worksheets("EMS").Cells(18, 11) 'POWER IN OF EMS(kW)-
165. SOFECPOWER = ActiveWorkbook.Worksheets("SOFEC").Cells(25, 11) 'POWER IN OF SOFEC (kW)-
166. ITMPOWER = ActiveWorkbook.Worksheets("ITM").Cells(26, 11) 'POWER OUT OF ITM (kW)+
167. SOFCPOWER = ActiveWorkbook.Worksheets("SOFC").Cells(22, 11) 'POWER OUT OF SOFC (kW)+
168. NH3HHV = ActiveWorkbook.Worksheets("SSAS").Cells(53, 3) 'NH3 Equivalent Power HHV of NH3(KW)+
169. NH3LHV = ActiveWorkbook.Worksheets("SSAS").Cells(54, 3) 'NH3 Equivalent Power LHV of NH3(KW)+
170. SSASPOWER = ActiveWorkbook.Worksheets("SSAS").Cells(49, 3)
171. '=====
172. ' IMPELLERS
173. IMPADB = ActiveWorkbook.Worksheets("DFB-ADB").Cells(48, 19) 'IMPELLER BIO TEACTOR (HP)
174. IMPINOC = ActiveWorkbook.Worksheets("DFB-ADB").Cells(65, 12) 'IMPELLER BIO TEACTOR (HP)
175. IMPMIX = ActiveWorkbook.Worksheets("DFB-ADB").Cells(8, 23) 'IMPELLER MIXING TANK
176. CB1W = ActiveWorkbook.Worksheets("DFB-ADB").Cells(85, 4) 'BLOWER BIO REACTOR (WATT)
177. CB1 = CB1W 'BLOWER BIO REACTOR (KW)
178. '=====
179. ' TOTAL AIR REQUIRED PUMPING)
180. COOLAIR = 25
181. AIRSSAS = AIRSSAS1 + AIRSSAS2 + AIRSSAS3 + SSASAIRFLOW
182. TOTAIR = AIRSOFC + AIRITM + AIRSSAS + AIREMS + AIRDARK + AIRADB + AIRCO2 'TOTAL AIR REQUIRED for the SYSTEM (Kg/day)
183. 'Air Density
184. COOLAIR = AIRTEMP
185. AIRDEN = AIRDENSITY(AIRTEMP) 'Air Density(Kg/m^3)
186. 'Volumetric Flow
187. AIRVOL1 = TOTAIR / AIRDEN 'Air Volume (m^3/day)
188. AIRVOL2 = AIRVOL1 * 1000 'Air Volume (Lt/day)
189. AIRVOL = (AIRVOL2 / 24) / 60 'Air Volume (Lt/min)
190. 'Compressor DATA IN
191. Cells(42, 4) = AIRADB '(Kg/day)
192. Cells(43, 4) = AIRDARK '(Kg/day)
193. Cells(44, 4) = AIREMS '(Kg/day)
194. Cells(45, 4) = AIRSOFC '(Kg/day)
195. Cells(46, 4) = AIRITM '(Kg/day)
196. Cells(47, 4) = AIRSOFEC '(Kg/day)
197. Cells(48, 4) = AIRSSAS '(Kg/day)
198. Cells(49, 4) = AIRVOL 'Air Volume (Lt/min)
199. COMPIN = Cells(50, 4) 'Compressor Inlet Pressure (Atm)
200. COMPOT = Cells(51, 4) 'Compressor Outlet Pressure (Atm)
201. COMPIT = Cells(52, 4) 'Compressor Inlet Temperature (oC)
202. COMETREFF = Cells(53, 4) 'Compressor ENTROPY Efficiency (%)
203. MOTOREFF1 = Cells(47, 11) 'Motor Efficiency 1-Phase (%)
204. SPHASVOL = Cells(48, 11) 'Single Phase Voltage (Volt)

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205. MOTOREFF3 = Cells(50, 11) 'Motor Efficiency 3-Phase (%)
206. THREPASEVOL = Cells(51, 11) '3-Phase Voltage (Volt)
207. ' CONSTANT
208. RAIR = 408.97 'J/Kg.K
209. GAMMA = 2.0339 'Constant for Diatomic gas compression adiabatic temperature rise
210. ENTCC = AIRDEN * RAIR 'Entropy Change Constant (J/K.M^3)
211. '
212. '===== Compressor-1 Calculations =====
213. GASTEMPC = COMPIT: GASVOL = AIRVOL
214. GASTEMPC = COMPIT: GASVOL = AIRVOL
215. OUTADIATEMP = ((GASTEMPC + 273) * ((COMPOP / COMPIP) ^ ((1.401 - 1) / 1.401))) - 273 ' OUTLET ADIABATIC TEMPERATURE
216. DRMOTWATT = (((OUTADIATEMP + 273) - (GASTEMPC + 273)) * 1.15 * (TOTAIR / 86400)) / (0.75) 'KW
217. '..... DATA OUTPUT ....
218. Cells(42, 11) = OUTADIATEMP
219. Cells(43, 11) = COOLAIR
220. Cells(44, 11) = COOLSYS
221. Cells(45, 11) = OUTADIATEMP
222. Cells(45, 11) = DRMOTWATT
223. Cells(46, 11) = DRMOTHP
224. Cells(49, 11) = CURRENT1
225. Cells(52, 11) = CURRENT3
226. '===== Energy =====
227. COM9 = DRMOTWATT 'Air Compressor
228. TOTALINKW = COM1 + COM2 + COM3 + COM4 + COM5 + COM6 + COM7 + COM8 + COM9 + SP1 + SP2 + SP3 + SP8 + CB1 'kw
229. ' DATA OUTPUT
230. '=====
231. ' ENERGY IN
232. '=====
233. 'ENERGY IN for Compressors
234. TOTALCOM = COM1 + COM2 + COM3 + COM4 + COM5 + COM6 + COM7 + COM8 + COM9 + COM10 + COOLSYS 'Compressors
235. Cells(56, 3) = COM1 'Compressor No1[MFI(ZM)](kw)
236. Cells(57, 3) = COM2 'Compressor No1[SOFEC](kw)
237. Cells(58, 3) = COM3 'Compressor No3[SSAS] (kw)
238. Cells(59, 3) = COM4 'Compressor No4[SSAS] (kw)
239. Cells(60, 3) = COM5 'Compressor No5[SOFEC] (kw)
240. Cells(61, 3) = COM6 'Compressor No6[SOFEC] (kw)
241. Cells(62, 3) = COM7 'Compressor No7[SOFEC] (kw)
242. Cells(63, 3) = COM8 'Compressor No7[ADB] CAKING (kw)
243. Cells(64, 3) = COM9 'Compressor No9 [For Total AIR required [ENERGY (kw)]]
244. Cells(65, 3) = TOTALCOM 'TOTAL Compressors
245. 'ENERGY IN forPUMPS & Fan
246. Cells(67, 3) = SP1 'Sludge Pump[DARK.REACTOR] (kw)
247. Cells(68, 3) = SP2 'Sludge Pump[DARK.REACTOR] (kw)
248. Cells(69, 3) = SP3 'For Digester Sludge (kw)
249. Cells(70, 3) = SP4 'For Digester Sludge (kw)
250. Cells(72, 3) = CB1 'Centrifugal fan[BIOREACTOR] (kw)
251. TOTALF = SP1 / 1000 + SP2 / 1000 + SP3 + SP4 + CB1
252. Cells(73, 3) = TOTALF 'Total (kw)
253. 'ENERGY IN for Heat-Exchangers
254. Cells(75, 3) = HE1
255. Cells(76, 3) = HE3
256. Cells(77, 3) = HE5
257. Cells(78, 3) = HE8
258. Cells(79, 3) = HE9
259. Cells(80, 3) = HE10
260. TOTALHEXIN = HE1 + HE9 + HE4 + HE3 + HE5 + HE8 + HE10 + HE2
261. Cells(81, 3) = TOTALHEXIN
262. 'ENERGY IN FOR IMPELLER
263. IMPDFBW = IMPDFB * 0.745 'Dark Impeller (kw)
264. IMPADBW = IMPADB * 0.745 'BIO Impeller (kw)
265. IMPINOCW = IMPINOC * 0.745 'Inoculum Impeller (kw)
266. IMPMIXT = IMPMIX * 0.745 'Mixing Tank (kw)
267. TOTALIMP = IMPDFBW + IMPADBW + IMPINOCW + IMPMIXT
268. 'Cells
269. Cells(83, 3) = IMPDFBW 'Dark Impeller (kw)

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270. Cells(84, 3) = IMPADBW 'BIO Impeller (kw)
271. Cells(85, 3) = IMPINOCW 'Inoculum Impeller (kw)
272. Cells(86, 3) = IMPMIXT 'Mixer Impeller (kw)
273. Cells(87, 3) = TOTALIMP
274. 'ENERGY IN FOR WASTE TANKS
275. TOTALTANKS = DFBTANK + ADBTANK + WESTANK1 + WESTANK2
276. Cells(89, 3) = DFBTANK 'Energy IN DARK CSTR -(kw)
277. Cells(90, 3) = ADBTANK 'Energy IN ADB CSTR -(kw)
278. Cells(91, 3) = WESTANK1 'Energy IN ADB TANK1 -(kw)
279. Cells(92, 3) = WESTANK2 'Energy IN ADB TANK2 -(kw)
280. Cells(93, 3) = TOTALTANKS
281. 'Membranes Heat Loss
282. TOTALHLMEMB = HLMFI + HLITM + HLEMS + HLSOFEC + HLSSAS + HLSOFC 'Total MEMBRANE HEAT LOSS (kw)
283. Cells(95, 3) = HLMFI 'Heat Loss from MFI Cell (kw)
284. Cells(96, 3) = HLITM 'Heat Loss from ITM Cell (kw)
285. Cells(97, 3) = HLEMS 'Heat Loss from EMS Cell (kw)
286. Cells(98, 3) = HLSOFEC 'Heat Loss from SOFEC Cell (kw)
287. Cells(99, 3) = HLSSAS 'Heat Loss from SSAS Cell (kw)
288. Cells(100, 3) = HLSOFC 'Heat Loss from SOFC Cell (kw)
289. Cells(101, 3) = TOTALHLMEMB 'Total MEMBRANE HEAT LOSS (kw)
290. '
291. '=====
292. ' ENERGY OUT
293. '=====
294. '...ENERGY OUT of Turbines
295. TOTALOUTTURBKW = STEATURB + GASTURB '+ GASTURB2
296. Cells(54, 11) = STEATURB
297. Cells(55, 11) = GASTURB
298. Cells(43, 15) = GASTURB2
299. Cells(56, 11) = TOTALOUTTURBKW
300. '...ENERGY OUT for Heat-Exchangers and Condensers
301. 'HEAT-EXCHANGERS
302. Cells(58, 11) = HE2
303. Cells(59, 11) = HE4
304. Cells(60, 11) = HE6
305. Cells(61, 11) = HE7
306. 'Condensers
307. Cells(62, 11) = COND1
308. Cells(63, 11) = COND2
309. Cells(64, 11) = COND3
310. Cells(65, 11) = COND4
311. Cells(66, 11) = COND5
312. TOTALHEXCONOUT = COND1 + COND3 + HE7 + COND4 + COND5 + HE11 + HE6
313. BCV = 0.1 * TOTALHEXCONOUT
314. Cells(67, 11) = TOTALHEXCONOUT
315. 'TOTAL PRODUCED
316. TOTAPRO = TOTALOUTTURBKW + TOTALHEXCONOUT 'Total Produced (kw)
317. Cells(68, 11) = TOTAPRO '(A+B)
318. 'Total Balance (1)
319. ENERGYIN = TOTALCOM + ((SP1 + SP2)) + SP4 + CB1 + TOTALHEXIN + TOTALIMP + TOTALTANKS + TOTALHLMEMB 'Total IN from compressor + .....
320. TOTALGIVEN = TOTAPRO - ENERGYIN 'ENERGY BALANCE (1)OUT
321. Cells(70, 11) = ENERGYIN 'Energy Consumed (kw)
322. Cells(71, 11) = TOTAPRO 'Energy Produced(kw)
323. Cells(72, 11) = TOTALGIVEN 'ENERGY BALANCE (1)
324. 'TOTAL OUT
325. TOTALOUTHEXTURB = TOTALOUTTURBKW + TOTALHEXCONOUT
326. Cells(69, 11) = TOTALOUTHEXTURB '(A+B)
327. '=====
328. ' Cell Voltages to Power + NH3 + UREA
329. '=====
330. MSTEAMTOT = ((H2OHEXRECY + WESTANK2XX + (WESTANK2BB - WESTANK2BB123)) / 86400) * (1000 - WESTANK2BBTBT) * 4.18 '+ SOFECALOW1RF
331. Cells(70, 21) = MSTEAMTOT
332. 'Total Energy from Voltage
333. TOTALVOLTAGE = -SOFECPOWER - EMSPower + ITMPower + SOFCPOWER - SSASPOWER 'Total Voltage Power (kw)(2)
334. 'Energy From NH3

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335.   NH3HHV = NH3HHV                                'Energy From NH3 (kw) (4)
336. 'Energy From Urea
337.   UREAETOTNEEDED = UREAENOUT - UREAENIN          'ENERGY FROM UREA (kw) (3)
338. 'TOTAL ENERGY WITHOUT NH3
339.   TOTENER3 = TOTALGIVEN + TOTALVOLTAGE + UREAETOTNEEDED - CO2CONPW - MSTEAMTOT - BCV - ADS '(1)+(2)-(3)
340. 'TOTAL ENERGY WITHOUT NH3
341.   TOTENERWNH3 = NH3HHV + TOTENER3 'Total Energy with NH3 (1)+(2)-(3)+(4)
342. 'Cells
343.   Cells(65, 6) = EMSPower                        'Voltage in Kw from EMS
344.   Cells(66, 6) = SOFECPOWER                      'Voltage in Kw from SOFEC
345.   Cells(67, 6) = ITMPOWER                        'Voltage in Kw from ITM
346.   Cells(68, 6) = SOFCPOWER                      'Voltage in Kw from SOFC
347.   Cells(69, 6) = TOTALVOLTAGE                   'Energy OUT From Voltages (kw)
348.   Cells(70, 6) = UREAETOTNEEDED                'ENERGY IN FROM UREA (kw)
349.   Cells(71, 6) = NH3HHV                         'ENERGY IN from NH3
350.   Cells(72, 6) = TOTENER3                       'ENERGY BALANCE (2)
351.   Cells(73, 6) = TOTENERWNH3                   'ENERGY BALANCE (3)
352. End Sub
353. Static Function Logn(X)
354.   Logn = Log(X) / Log(2.718282)
355. End Function
356. Private Static Function AIRDENSITY(AIRTEMP)
357.   A1 = 1.2910739
358.   B1 = 279.63468
359.   C1 = 0.0036989433
360.   D1 = 1.0050404
361.   AIRDENSITY = (A1 * B1 + C1 * AIRTEMP ^ D1) / (B1 + AIRTEMP ^ D1) 'Air Density (Kg/m^3) oC
362. End Function
363. Private Static Sub COMPRESSOR(GASTEMPC, COMPOP, COMPIP, GAMMA, GASVOL, OUTADIATEMP, COOLSYS, COMETREFF, WATT, ENTCC, DRMOTWATT, DRMOTHP, MOTORE
FF1, MOTOREFF3, SPHASVOL, THREPASEVOL, CURRENT1, CURRENT3)
364.   A1 = 1000
365.   A2 = 60
366. End Sub
367. Private Static Function CO2SPEHEAT(GASTK) 'CO2 SPECIFIC HEAT ' Cp of CO2 kJ/Kg.K)
368.   Z1 = 0.51476288
369.   Z2 = 5820.1918
370.   Z3 = 1.4877831
371.   Z4 = 1.404349
372.   CO2SPEHEAT = (Z1 * Z2 + Z3 * GASTK ^ Z4) / (Z2 + GASTK ^ Z4)
373. End Function
374. Private Static Function AIRSPECIFICHEAT(AIRTK) 'AIRSPECIFICHEAT (kJ/kg.K)
375.   TA = 1.0828694; TB = -0.00063119116; TC = 0.0000016253087; TD = -1.3949526E-09; TE = 5.3826153E-13; TF = -7.9021928E-17
376.   AIRSPECIFICHEAT = TA + TB * AIRTK + TC * AIRTK ^ 2 + TD * AIRTK ^ 3 + TE * AIRTK ^ 4 + TF * AIRTK ^ 5
377. End Function
378. Private Static Function WATERSPECIFICHEAT(H2OTEMP) 'WATER SPECIFIC HEAT (kJ/kg.K)
379.   WATERSPECIFICHEAT = 1.224986 + 0.0014072339 * H2OTEMP - 0.00000039722778 * H2OTEMP ^ 2 + 5.3431749E-11 * H2OTEMP ^ 3 + -2.7473115E-
15 * H2OTEMP ^ 4
380. End Function
381. Private Static Function CO2DENSITY(T) 'T=oC,Kg/m^3
382.   A = 0.50649907; B = 0.0019289299; C = 1.0174749
383.   CO2DENSITY = (A + B * T) ^ (-1 / C)
384. End Function
385. Private Static Sub HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'H
EAT EXCHANGER
386.   AREAHEX = 3.14 * TOD * TL
387.   LMTD = Q / (U * AREAHEX)
388. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
389. '----- HEATING -----
390.   If FLAG = 1 Then
391.     DELTAA = TH1 - TC2
392.     'DELTAB = TH2 - TC1
393.     LMTD = Q / (U * AREAHEX)
394.     X1 = 1
395.   S1 = DELTAA / (LMTD - Logn(DELTAA))
396.   S2 = X1 / (LMTD - Logn(X1))

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397.   If S2 >= S1 Then
398.     GoTo 400
399.   Else
400.     X1 = X1 + 0.1
401.     GoTo 300
402. 400 End If
403.     DELTAB = X1
404.     TH2 = DELTAB + TC1
405.     GoTo 700
406.   End If
407. '-----
408. '----- COOLING -----
409.   If FLAG = 2 Then
410.     'DELTA = TH1 - TC2
411.     DELTAA = TH2 - TC1
412.     LMTD = Q / (U * AREAHEX)
413.     X1 = 2
414. 500 S1 = Logn(X1) - X1 / LMTD
415.     S2 = Logn(DELTAB) - DELTAB / LMTD
416.     If S1 >= S2 Then
417.       GoTo 600
418.     Else
419.       X1 = X1 + 0.1
420.       GoTo 500
421. 600 End If
422.     DELTAA = X1
423.     TC2 = TH1 - DELTAA
424.     End If
425. '-----
426. 700 P = (TC2 - TC1) / (TH1 - TC1)
427.     R = (TH1 - TH2) / (TC2 - TC1)
428.     If R > 1 Then
429.       R1 = 1 / R
430.       P1 = P * R
431.     Else
432.       P1 = P
433.       R1 = R
434.     End If
435.     A1 = (((R1) ^ 2 + 1) ^ 0.5) / (1 - R1)
436.     A2 = Logn((1 - R1 * P1) / Abs(1 - P1))
437.     A3 = 2 - P1 * (1 + R1 - (1 + (R1) ^ 2)) ^ 0.5 'up
438.     A4 = Abs(2 - P1 * (1 + R1 + (1 + (R1) ^ 2)) ^ 0.5) 'down
439.     A5 = Logn(A3 / A4)
440.     FCORF = (A1 * A2) / A5
441.     If Abs(FCORF) > 1 Then
442.       FCORF = 1
443.     End If
444.     If FLAG = 1 Then
445.       LMTD = Q / (U * AREAHEX * FCORF)
446.       CHOT = Q / (TH1 - TH2)
447.       HFR = CHOT * 24 * 3600 / SCHOT
448.       GoTo 800
449.     End If
450.     If FLAG = 2 Then
451.       LMTD = Q / (U * AREAHEX * FCORF)
452.       CCOLD = Q / (TH1 - TH2)
453.       HFR = CCOLD * 24 * 3600 / SCHOT
454.     End If
455. 'EFFECTIVENESS
456. 800 If CCOLD > CHOT Then
457.     CMIN = CHOT
458.     C1 = CHOT
459.     EPS = (C1 * (TC2 - TC1)) / (CMIN * (TH1 - TC1))
460.     GoTo 900
461.   Else

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462.   CMIN = CCOLD
463.   C1 = CCOLD
464.   EPS = (C1 * (TH1 - TH2)) / (CMIN * (TH1 - TC1))
465. 900 End If
466.   QEFF = EPS * CMIN * (TH1 - TC1)
467. 'Number of ELEMENT
468.   NTU = U * AREAHEX / CMIN
469.   If NTU <= 1 Then
470.     NTU = 1
471.   Else
472.     End If
473. End Sub

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Anaerobic digestion with CCS

SSAS

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1. Sub Sheet8_Button1_Click()
2. '           SSAS
3. 'N2
4.   N2FRK = ActiveWorkbook.Worksheets("ITM").Cells(10, 11)      'N2 Total Available from (ITM) (Kg/Day)
5.   N2EMS = ActiveWorkbook.Worksheets("ITM").Cells(23, 4)      'N2 Needed for EMS (Kg/Day)
6.   N2ITMTEMP = ActiveWorkbook.Worksheets("ITM").Cells(11, 4)  'N2 Temperature from (ITM)(oC)
7.   N2ITMTPRE = ActiveWorkbook.Worksheets("ITM").Cells(12, 4)  'N2 Pressure from (ITM)(oC)
8.   CO2SOFEC = ActiveWorkbook.Worksheets("SOFEC").Cells(6, 11)  'CO2 From SOFEC(kg/hr)
9. 'H2
10.  H2FRKSOFEC = ActiveWorkbook.Worksheets("SOFEC").Cells(5, 11) 'H2 IN From SOFEC(kg/hr)
11.  H2FRKSOFC = ActiveWorkbook.Worksheets("SOFC").Cells(5, 11)  'H2 IN From SOFC(kg/hr)
12. 'TEMPERATURE
13.  H2SOFECTEMP = ActiveWorkbook.Worksheets("SOFEC").Cells(15, 4) 'H2 Temperature From SOFEC(ZM) (oC)
14.  H2SOFCTEMP = ActiveWorkbook.Worksheets("SOFC").Cells(13, 4)  'H2 Temperature From SOFC(ZM) (oC)
15. '
16. '   INPUT
17. ' N2 Total Available
18.   N2TOTAVAILABLE = (N2FRK) - (N2EMS) '+ (N2SOFC) 'N2 TOTAL AVAILABLE (Kg/day)
19. ' H2 Total Available
20.   H2TOTAVAILABLE = H2FRKSOFEC + H2FRKSOFC
21. ' N2
22.   Cells(5, 4) = N2TOTAVAILABLE 'N2 Total Available from (ITM) (Kg/Day)
23.   Cells(6, 4) = N2ITMTEMP      'N2 Mixed Inlet Temperature (oC)
24.   Cells(7, 4) = N2ITMTPRE     'N2 Inlet Pressure (atm)
25.   Cells(10, 4) = H2TOTAVAILABLE 'H2 Flow Rate (kg/hr)
26.   HIP = Cells(12, 4)          'H2 Inlet Pressure (atm)
27. ' Cell
28.   CIT = Cells(15, 4) 'Cell Temperature (oC)
29.   CIP = Cells(16, 4) 'Cell Pressure (atm)
30.   MC = Cells(17, 4)  'Membrane Conductivity (1/cm.ohm)
31.   MSA1 = Cells(18, 4) 'Membrane Surface Area (m^2)
32.   MTH = Cells(19, 4) 'Membrane Thickness (cm)
33.   APC = Cells(20, 4) 'Applied Current(mA)
34.   APV = Cells(21, 4) 'Applied Voltage
35.   FU1 = Cells(47, 2)
36. 'N2 Mixed Temperature
37. 'Temperature of Mixed N2 gas
38.   N2HIGHTEM = N2TOTAVAILABLE - N2FREXCHANGER 'N2 Flow rate from (ITM) not used at T= 900 (oC)
39.   N2FREXCHANGER = N2FREXCHANGER           'N2 Flow rate from (ITM)Used for the Heat Exchanger at T=305.65 (oC)
40.
41.   '<===== Input Data =====
42. ' Constant
43.   MSA = MSA1 * 10000
44.   N2ITK = N2ITMTEMP + 273
45.   H2TK = H2IT + 273
46.   CITK = CIT + 273
47.   TSTPK = 25 + 273
48.   FU = FU1 / 100

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49.   ECD = 3.5 ' Electrical Current Density Mole/cm^2.sec
50.   FA = 96485 ' coulombs/mole
51.   R = 8.314 'J/K.mol
52.   RG = 82.05746 'cm3 atm/mol.K
53.   DELH0 = 91.88 'kJ/mole
54.   AWN2 = 14 'Weight of one N2 atom
55.   N2MW = 28
56.   H2MW = 2
57.   NH3MW = 17
58.   UREAMW = 60.6
59.   CO2MW = 44
60.   THPLUS = 1.11 'Proton transport number
61.   '===== Calculation =====
62.   '***** Needed Components for Urea *****
63.   ' CO2 TOTAL PRODUCED
64.   CO2TOTAL = CO2SOFEC '(Kg/Day)
65.   'Urea Needed to consume all the CO2
66.   UREA = (CO2TOTAL * UREAMW) / CO2MW 'Urea Prduced'Total CO2 produced is Used For Urea (according to the UREA production ratio) (KG/day)
67.   'NH3 Needed for this Urea production
68.   NH3TOTUREA = (UREA * (2 * NH3MW)) / UREAMW 'Total NH3 NEEDED FOR UREA PRODUCTION (Kg/day)
69.   'H2 Needed for this NH3 production for Urea
70.   H2TOTUREA = (NH3TOTUREA * (H2MW * 3)) / (2 * NH3MW) 'H2 Needed for NH3 To UREA (Kg/day)
71.   'N2 Needed for this NH3 production for Urea
72.   N2TOTUREA = (NH3TOTUREA * N2MW) / (NH3MW * 2) 'N2 Needed for NH3 To UREA (Kg/day)
73.   '***** Component Availability *****
74.   'H2 Available
75.   H2AVAILABLE = H2TOTAVAILABLE - H2TOTUREA 'H2 Avalable (Kg/day)
76.   'N2 Available
77.   N2AVAILABLE = N2TOTAVAILABLE - N2TOTUREA 'N2 Avalable (Kg/day)
78.   '.....
79.   'Ratio of Available H2 for Extra NH3 and SOFC
80.   NR = Cells(32, 3)
81.   If NR <= 0 Then
82.     Cells(22, 6) = "ERROR N=0"
83.   End
84.   Else
85.     Cells(22, 6) = ""
86.   End If
87.   'H2 For NH3
88.   H2NH3EXTRA = H2AVAILABLE / NR 'H2 for Extra NH3 (Kg/day)
89.   'H2 For SOFC
90.   H2SOFC = H2AVAILABLE - H2NH3EXTRA 'H2 for SOFC (Kg/day)
91.   If H2SOFC < 0 Then
92.     Cells(31, 3) = H2SOFC
93.     Cells(22, 6) = "ERROR H2 is NEGATIVE"
94.   End
95.   Else
96.     Cells(22, 6) = "H/N OK for SOFC"
97.   End If
98.   'H2 Needed For Membrane
99.   H2MEMBRANE = H2TOTUREA + H2NH3EXTRA 'H2 Total For SSAS Membrane (Kg/day)
100.  '.....Extra NH3 .....
101.  NH3EXTRA = (H2NH3EXTRA * (NH3MW * 2)) / (H2MW * 3) 'Extra NH3 (Kg/day)
102.  'N2 Needed For Extra NH3
103.  N2NH3EXTRA = (NH3EXTRA * N2MW) / (NH3MW * 2) 'N2 Used for Extra NH3 (Kg/day)
104.  'N2 Remaining
105.  N2REMAIN = N2FRK - N2EMS - N2TOTUREA - N2NH3EXTRA
106.  '
107.  '***** TOTAL NH3 *****
108.  '.....TOTAL H2 and N2 Needed for A TOTAL of NH3.....
109.  'N2 Needed for a Total of NH3
110.  N2TOTNH3 = N2TOTUREA + N2NH3EXTRA 'N2 Needed for a Total of NH3 (Kg/day)
111.  'H2 Needed for a Total of NH3
112.  H2TOTNH3 = H2TOTUREA + H2NH3EXTRA
113.  'Total NH3 Needed

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179. NH3TOTAL = NH3TOTUREA + NH3EXTRA
180. ' TOTAL Moles
181. N2MOLTOT = N2FRKUSED / N2MW 'N2 Moles/day
182. H2MOLTOT = H2TOTALIN / H2MW 'H2 Moles/day
183. NH3MOLTOT = NH3TOTAL / NH3MW 'NH3 Moles/day
184. 'AT Cathode
185. H2PERCTOT = H2MOLTOT / H2MOLTOT 'H2 %
186. 'AT Anode
187. TOTMOLTOT = N2MOLTOT + NH3MOLTOT 'Total Moles
188. N2PERCTOT = N2MOLTOT / TOTMOLTOT 'N2 %
189. NH3PERCTOT = NH3MOLTOT / TOTMOLTOT 'NH3 %
190. 'Partial Pressure
191. PPN2TOT = N2PERCTOT * CIP
192. PPH2TOT = H2PERCTOT * CIP
193. PPNH3TOT = NH3PERCTOT * CIP
194. '=====
195. PPN2 = PPN2TOT
196. PPH2 = PPH2TOT
197. PPNH3 = PPNH3TOT
198. '=====
199. ' Thermodynamics - DELTA : C,H, S, G in fuction of T
200. A = TSTPK
201. B = 573 'CITK
202. N = 263
203. ' DELTA(H)with TK
204. Call DELTAH(A, B, N, INTEGRALH) 'Simpson integrator for DELTA(H)263
205. DELH = INTEGRALH - 91.88 'DELTA(H) (kJ/mole)
206. ' DELTA(S)with TK
207. N = 108
208. Call DELTAH(A, B, N, INTEGRALS) 'Simpson integrator for DELTA(S)108
209. DELS = (-198.091 + INTEGRALS) / 1000 'DELTA(S) (J/mole)
210. ' DELTA(G)with TK
211. DELTAGKJ = DELH - CITK * DELS 'DELTA (G)(kJ/mole)
212. DELTAG = DELTAGKJ * 1000 'DELTA (G)(J/mole)
213. ' Reversible Voltage E0
214. E0 = (DELTAG / (6 * FA)) ' * 1000 'Gibbs Free Energy in(Volt)Ref:75969 Page-11 or Electrochemical_Synthesis_of_Ammonia_in_Solid_Elec Page-7
215. ENERST = E0 + ((R * CITK) / (6 * FA)) * Logn(((PPN2) * (PPH2) ^ 1 / 3) / (PPNH3) ^ 1 / 2) 'Nerst Voltage Ref: Fogler Reactor design SOFC
216. 'Area Specific Resistance
217. ASR = (MTH / MC)
218. 'RATE OF NH3 at MEMBRANE(FLUX)
219. RNH3 = -((ENERST - APV) / (ASR * 6 * FA)) * 2 / 3 'Rate of NH3 'At MEMBRANE(FLUX) RATE OF Reaction of NH3 moles/cm^2.s
220. 'Maximum RATE OF NH3 at Working Electrode
221. RNH3MAX = 1.13 * (10) ^ -8 'Maximum Rate of NH3 moles/cm^2.sec Ref:XU209 Page-4 or 75969 Page-12
222. 'Exchange Current Density io
223. IO = RNH3 * 3 * FA * MSA1 'mAmp/cm^2
224. 'Faradaic Efficiency
225. FE = ((3 * FA * RNH3MAX * (MSA1) * 100) / (APC * 1.07))
226. 'Current il Needed for maximum fuel efficiency of this RNH3MAX => ICUR = 0.005972+>Limited current desity
227. ' or-Electrochemical_Synthesis_of_Ammonia_in_Solid_Elec Page-7
228. ICURL = (6 * FA * MSA * RNH3MAX) / THPLUS '(0.904 * TH) 'AMP Ref:XU209 Page-4 or 75969 Page-12
229. 'Limited Current Density
230. IL = ICURL / MSA 'mAmp/cm^2
231. 'Current Density
232. II = APC / MSA
233. 'Moles of NH3 Required
234. NH3MOLNEED = (NH3TOTAL * 1000) / NH3MW 'Moles/day
235. NH3MOLSEC = (NH3MOLNEED / 24) / 3600 'Moles /sec
236. 'AREA
237. AREANEED = NH3MOLSEC / RNH3
238. 'Number Of Electrode
239. NUMBCELLS = AREANEED / MSA
240. 'Activation Energy
241. ETAACT = ((R * CITK) / (0.5 * FA)) * Logn(II / IO)
242. 'Concentration Energy

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243.     ETACONT = ((R * CITK) / (6 * FA)) * Logn(1 - II / IL)
244. 'Ohmic Energy
245.     IOHM = II * (MTH / MC)
246. 'TOTAL VOLTAGE
247.     TOTVOLT = -((ENERST) + (APV) + (ETA ACT) + (ETACONT) + (IOHM)) * NUMBCELLS
248. '===== PLOT =====
249. 'Plot of Butler-Volmer equation to find II
250.     III = 0.1
251.     For I = 1 To 10
252.         TACT1 = ((R * CITK) / (0.5 * FA)) * Logn(III)
253.         III = III + 0.1
254.         Cells(64 + I, 1) = -TACT1
255.         Cells(64 + I, 2) = III
256.     Next I
257. 'Resistance R
258.     RES = 1 / 0.051
259. '***** COMPONENT OUT *****
260. 'N2 Out at Cathode
261.     N2OUT = N2REMAIN
262.     Cells(5, 11) = N2OUT      'N2 OUT UNUSED (kg/hr)
263.     If N2OUT <= 0 Then
264.         Cells(4, 7) = "ERROR"
265.         Cells(5, 7) = "N2 OUT LOW"
266.         Cells(6, 7) = "First Check H/N"
267.         Cells(7, 7) = "AGAIN, if N2<0"
268.         Cells(8, 7) = "RUN ITM"
269.         Cells(9, 7) = "AGAIN"
270.     End
271.     Else
272.         Cells(5, 11) = N2OUT      'N2 OUT UNUSED (kg/hr)
273.         Cells(4, 7) = " "
274.         Cells(5, 7) = " "
275.         Cells(6, 7) = " "
276.         Cells(7, 7) = " "
277.         Cells(8, 7) = " "
278.         Cells(9, 7) = " "
279.     End If
280. '----- CELL POWER IN                CELLPWER = (TOTAPPLI * TOTALEV) / 1000
281.     IVMC = 1 / MC      ' (Ohm.cm) Inverse of conductivity
282.     RESISTANCE = IVMC / MTH ' (Ohm)
283.     TOTALCURRENT = (TOTVOLT / RESISTANCE) 'Total Current (Amp)
284.     CELLPWER = (TOTALCURRENT * TOTVOLT * NUMBCELLS) / 1000 '(kW)
285.     Cells(49, 3) = CELLPWER
286.     Cells(50, 3) = RESISTANCE
287.     Cells(51, 3) = FE      'Faradaic Efficiency
288. 'OUTPUT
289.     Cells(13, 4) = H2SOFC
290.     Cells(4, 11) = NH3TOTAL      'NH3(kg/Day)Formed
291.     Cells(5, 11) = N2OUT      'N2 OUT UNUSED (kg/hr)
292.     Cells(6, 11) = RNH3MAX      'Maximum Reaction Rate
293.     Cells(7, 11) = RNH3      'Actual Reaction Rate
294.     Cells(8, 11) = AREANEEDED      'Required Area from Reaction
295.     Cells(9, 11) = NUMBCELLS      'Number of Cells
296.     Cells(10, 11) = APC      'Current Imposed (Amp)
297.     Cells(11, 11) = TOTALCURRENT      'Total Current (Amp)
298.     Cells(12, 11) = TOTVOLT      'Voltage (Volt)
299.     Cells(13, 11) = H2SOFC      'H2 Out(kg/Day)
300.     Cells(14, 11) = NH3TOTUREA      'NH3 for Urea (kg/hr)
301.     Cells(15, 11) = NH3EXTRA      'Extra NH3 produced (kg/hr)
302.     Cells(16, 11) = CO2TOTAL      'Total CO2 For Urea (kg/hr)
303.     Cells(17, 11) = UREA      'Amount of Urea (kg/day) for complete CO2 Elimination
304. '
305. '===== END OF CELL CALCULATIONS =====
306. '
307. '===== HEAT EXCHANGER-6 CALCULATION =====

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308. 'Temperature of Mixed N2 gas
309. 'H2 Temperature Mixed
310. H2TEMPMIXED1 = (H2FRKSOFEC * H2SOFECTEMP) / (H2FRKSOFEC)
311. If H2TEMPMIXED1 < CIT Then
312. H2TEMPMIXED2 = CIT - H2TEMPMIXED1
313. H2TEMPMIXED = H2TEMPMIXED2 + H2TEMPMIXED1 + H2TEMPMIXED2 * 0.16
314. GoTo 5
315. Else
316. H2TEMPMIXED1 = (H2FRKSOFEC * H2SOFECTEMP) / (H2FRKSOFEC)
317. H2TEMPMIXED = H2TEMPMIXED1
318. 5 End If
319. Cells(11, 4) = H2TEMPMIXED
320. TL = Cells(8, 16)
321. TOD = Cells(9, 16)
322. '=====
323. '..... Heat Exchanger No6 for H2 cooling .....
324. '=====
325. TL = Cells(8, 16)
326. TOD = Cells(9, 16)
327. ' Hydrogen
328. H2TK = H2TEMPMIXED + 273
329. SCH2 = HYDROGENSPECHEAT(H2TK) 'H2 Specific Heat (kJ/kg.K)
330. CH2 = ((H2TOTAVAILABLE / 24) / 3600) * SCH2 'H2 Heat capacity (KW/oK)
331. TH1 = (H2TEMPMIXED) + 273 'H2 Hot Side (oK)
332. TH2 = CIT + 273 'Cell Temperature in Kelvin 'H2 Cold Side (oK)
333. QH2 = CH2 * (TH1 - TH2)
334. 'Air
335. TC1 = 25 + 273
336. 'TC2=?
337. AIRINTK = TC1
338. SCAIR = AIRSPECIFICHEAT(AIRINTK)
339. 'Air Flow rate needed to Cool H2
340. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
341. FLAG = 2
342. U = 0.02
343. CCOLD = CH2: CHOT = CH2: Q = QH2: SCHOT = SCH2: SCCOLD = SCAIR
344. Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN
GER
345. '----- OUTPUT DATA FOR HEAT-EXCHANGER No-6 -----
346. AIRFLR = HFR
347. Cells(4, 16) = TH1 - 273 'H2 Temperature IN (oC)
348. Cells(5, 16) = TH2 - 273 'H2 Temperature OUT (oC)
349. Cells(6, 16) = TC1 - 273 'AIR Temperature In (oC)
350. Cells(7, 16) = TC2 - 273 'AIR Temperature OUT (oC)
351. Cells(10, 16) = NTU 'Number of Elements (No)
352. Cells(11, 16) = AREAHEX 'Shell Area (m^2)
353. Cells(12, 16) = EPS * 100 'Effectiveness (%)
354. Cells(13, 16) = QEFF 'Heat Transfer Rate (KW)
355. Cells(14, 16) = AIRFLR 'N2 Flow Rate (Kg/hr)
356. '-----
357. '===== HEAT EXCHANGER-7 CALCULATION =====
358. '===== HEAT EXCHANGER-7 CALCULATION =====
359. 'Cooling remaining of N2 With air
360. TL = Cells(21, 16)
361. TOD = Cells(22, 16)
362. 'NITROGEN
363. N2FRREM = N2TOTAVAILABLE - N2FLR 'N2 remaining to be cooled (Kg/day)
364. TH1 = N2ITMTEMP + 273 'N2 Temperature IN
365. TH2 = CIT + 273
366. N2ITK = TH2
367. SCN2 = NITROSPCHEAT(N2ITK) 'N2 Specific Heat (kJ/kg.K)
368. CN2 = ((N2FRREM / 24) / 3600) * SCN2 'N2 Heat capacity (KW/oK)
369. QN2 = CN2 * (TH1 - TH2) 'Q-N2 (kW)
370. 'Air Flow rate needed to Cool N2
371. Cells(19, 16) = AIRTEMIN

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372. TC1 = 25 + 273
373. AIRINTK1 = 25 + 273
374. SCAIR = AIRSPECIFICHEAT(AIRINTK1)
375. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
376. FLAG = 2
377. U = 0.02
378. CHOT = CN2: Q = QN2: SCHOT = SCN2: SCCOLD = SCAIR
379. Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN
GER
380. 'DATA
381. AIRFR = HFR
382. Cells(17, 16) = N2ITMTEMP 'N2 Temperature IN (oC)
383. Cells(18, 16) = TH2 - 273 'N2 Temperature OUT (oC)
384. Cells(19, 16) = 25 'AIR Temperature IN (oC)
385. Cells(20, 16) = TC2 - 273 'AIR Temperature OUT(oC)
386. Cells(23, 16) = NTU 'Number of Elements (No)
387. Cells(24, 16) = AREAHEX 'Shell Area (m^2)
388. Cells(25, 16) = EPS * 100 'Effectiveness (%)
389. Cells(26, 16) = QEFF 'Heat Transfer Rate (KW)
390. Cells(27, 16) = AIRFR 'Air Flow Rate (Kg/hr)
391. Cells(28, 16) = COMPOP 'Condenser inside Pressure (Atm.)
392. '===== COMPRESSOR-3 ===== NH3TOTAL
393. '...INPUT
394. COMPIP = Cells(21, 11) 'Compressor Inlet Pressure (atm.)
395. COMPOP = Cells(22, 11) 'Compressor Outlet Pressure (atm.)
396. Cells(23, 11) = CIT 'Gas Temperature (oC)
397. COMETREFF = Cells(24, 11) 'Compressor Entropy Efficiency (%)
398. SPHASVOL = Cells(25, 11) 'Single Phase Voltage (Volts)
399. MOTOREFF1 = Cells(26, 11) 'Single Phase Motor Efficiency (%)
400. THREPASEVOL = Cells(27, 11) '3 Phase Voltage (Volts)
401. MOTOREFF3 = Cells(28, 11) '3 Phase Motor Efficiency (%)
402. '...Chemical Calculation
403. TK = CIT + 273 'Inlet Gas Temperature (oK)
404. NH3SPECHEAT = NH3SPECHEAT(TK) 'NH3 Specific Heat (kJ/Kg.K)kJ/kg.K (>1atm)
405. NH3TEMP = CIT
406. GAMMA = NH3GAMMA(NH3TEMP) 'GAMMA=Cp/Cv
407. RHONH3 = NH3DENSITY(NH3TEMP) 'NH3 Density (Kg/m^3)
408. NH3VOLD = NH3KG / RHONH3 'NH3 Volume m^3/day
409. NH3VOLM = (NH3VOLD / 24) / 60 'NH3 Volume m^3/min
410. NH3VOLIT = NH3VOLM * 1000 'NH3 Volume L/min
411. Cells(20, 11) = NH3VOLIT 'NH3 Volume L/min,<=====
412. NH3MOL = NH3KG / NH3MW 'NH3 Mols
413. ENTCC = NH3MOL * R * Logn(COMPOP / COMPIP)
414. GASTEMPC = NH3TEMP: GASVOL = NH3VOLIT
415.
416. RMW1 = 17
417. RMWMIXZ = 17
418. MASSMIXCP = 1.13
419. STGE = 5
420. ISENEFF = 0.75
421. MECHANICEFF = 0.95
422. OUTADIATEMP = ((GASTEMPC + 273) * ((COMPOP / COMPIP) ^ ((GAMMA - 1) / GAMMA))) - 273 ' OUTLET ADIABATIC TEMPERATURE
423. DRMOTWATT = ((OUTADIATEMP + 273) - (GASTEMPC + 273)) * 2.22 * (NH3KG / 86400) / ISENEFF 'KW
424. Cells(30, 11) = OUTADIATEMP
425. Cells(31, 11) = DRMOTWATT
426. Cells(32, 11) = DRMOTHP
427. Cells(33, 11) = CURRENT1
428. Cells(34, 11) = CURRENT3
429.
430. '===== CONDENSER-2 (EXCHANGER) CALCULATION =====
431. TL1 = Cells(34, 16)
432. TOD1 = Cells(35, 16)
433. T1HC = OUTADIATEMP
434. Cells(30, 11) = T1HC
435. T1H = T1HC + 273

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436. T2HC = Cells(31, 16)
437. T2H = T2HC + 273
438. '...NH3
439. TK = T1H
440. CCNH3 = NH3SPECHEAT(TK)
441. CNH3 = ((NH3TOTUREA / 24) / 3600) * CCNH3
442. QNH3 = CNH3 * (T1H - T2H)
443. '...AIR
444. T1C = 25 + 273
445. AIRINTK1 = T1C
446. CCAIR2 = AIRSPECIFICHEAT(AIRINTK1)
447. AIRFR2 = 1
448. 50 CAIR2 = ((AIRFR2 / 24) / 3600) * CCAIR2
449. T2C = QNH3 / CAIR2 + T1C 'Air Temperature OUT (K)
450. QAIR1 = CAIR2 * (T2C - T1C)
451. If T1H - T2C >= 0 Then
452. GoTo 60
453. Else
454. AIRFR2 = AIRFR2 + 0.1
455. GoTo 50
456. 60 End If
457. P1 = (T2C - T1C) / (T1H - T1C)
458. R1 = (T1H - T2H) / (T2C - T1C)
459. DELTAA = T1H - T2C
460. DELTAB = T2H - T1C
461. FCORF = 1
462. LMTD = (DELTAA - DELTAB) / Logn(DELTAA / DELTAB) ' (K)
463. COLD = CAIR2: CHOT = CNH3: CFLUIDH = CNH3: TL = TL1: TOD = TOD1: AX1 = 1.2
464. '...DATA OUT
465. Cells(30, 16) = OUTADIATEMP
466. Cells(33, 16) = T2C - 273 'Air Temperature OUT (oC)
467. Cells(36, 16) = NELEM 'Number of Elements (No)
468. Cells(37, 16) = AEX 'Shell Area (m^2)
469. Cells(38, 16) = EPS * 100 'Effectiveness (%)
470. Cells(39, 16) = QEFF 'Heat Transfer Rate (KW)
471. Cells(40, 16) = AIRFR2 'Air Flow Rate (Kg/hr)
472. Cells(41, 16) = COMPOP 'Condenser inside Pressure (Atm.)
473. Cells(13, 4) = H2SOFC
474. '=====
475. ' NH3 --> POWER
476. '=====
477. NH3HHV = NH3EXTRA * 2.604 'High Heating Value (kw)
478. NH3LHV = NH3EXTRA * 2.15 'Low Heating Value (kw)
479. Cells(53, 3) = NH3HHV 'High Heating Value (kw)
480. Cells(54, 3) = NH3LHV 'High Heating Value (kw)
481. '=====
482. ' Cell Heat Losses
483. '=====
484. '----- HEAT IN -----
485. '...N2
486. N2ITK = CITK
487. CN2 = NITROSPCHEAT(N2ITK) 'kJ/kg.K
488. QN2IN = ((N2TOTAVAILABLE / 24) / 3600) * CN2 * N2ITK '(kw)
489. '...H2
490. H2TK = CITK
491. CH2 = HYDROGENSPECHEAT(H2TK) 'kJ/kg.K (T=K)
492. QH2IN = ((H2TOTAVAILABLE / 24) / 3600) * CH2 * H2TK '(kw)
493. 'Total Heat IN
494. QTOTIN = QN2IN + QH2IN + CELLPPOWER '(kw)
495. '----- HEAT OUT -----
496. '...NH3
497. TK = CITK
498. CNH3 = NH3SPECIFICHEAT(TK) 'kJ/kg.K (1atm)
499. QNH3OUT = ((NH3TOTAL / 24) / 3600) * CNH3 * TK '(kw)
500. '...H2

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501. H2TK = CITK
502. CH2 = HYDROGENSPECHEAT(H2TK) 'kJ/kg.K (T=K)
503. QH2IN = ((H2SOFC / 24) / 3600) * CH2 * H2TK '(kW)
504. 'Total Heat OUT
505. QTOTOUT = QNH3OUT + QH2IN '(kW)
506. '----- HEAT LOSSES -----
507. QLOSSES = QTOTIN - QTOTOUT
508. 'Cells OUTPUT
509. Cells(36, 11) = QTOTIN
510. Cells(37, 11) = QTOTOUT
511. Cells(38, 11) = QLOSSES
512. '===== COMPRESSOR-4 ===== NH3 EXTRA
513. '...INPUT
514. COMPIP = Cells(42, 11) 'Compressor Inlet Pressure (atm.)
515. COMPOP = Cells(43, 11) 'Compressor Outlet Pressure (atm.)
516. Cells(44, 11) = CIT 'Gas Temperature (oC)
517. COMETREFF = Cells(45, 11) 'Compressor Entropy Efficiency (%)
518. SPHASVOL = Cells(46, 11) 'Single Phase Voltage (Volts)
519. MOTOREFF1 = Cells(47, 11) 'Single Phase Motor Efficiency (%)
520. THREPASEVOL = Cells(48, 11) '3 Phase Voltage (Volts)
521. MOTOREFF3 = Cells(49, 11) '3 Phase Motor Efficiency (%)
522. '...Chemical Calculation
523. TK = CIT + 273 'Inlet Gas Temperature (oK)
524. NH3SPECHEAT = NH3SPECHEAT(TK) 'NH3 Specific Heat (kJ/Kg.K)kJ/kg.K (>1atm)
525. NH3TEMP = CIT
526. GAMMA = NH3GAMMA(NH3TEMP) 'GAMMA=Cp/Cv
527. RHONH3 = NH3DENSITY(NH3TEMP) 'NH3 Density (Kg/m^3)
528. NH3KGX = NH3EXTRA + NH3TOTUREA 'NH3 Required for Urea (Kg/day)
529. NH3VOLD = NH3KGX / RHONH3 'NH3 Volume m^3/day
530. NH3VOLM = (NH3VOLD / 24) / 60 'NH3 Volume m^3/min
531. NH3VOLIT = NH3VOLM * 1000 'NH3 Volume L/min
532. Cells(41, 11) = NH3VOLIT 'NH3 Volume L/min,<=====
533. NH3MOL = NH3KG / NH3MW 'NH3 MoIs
534. ENTCC = NH3MOL * R * Logn(COMPOP / COMPIP)
535. GASTEMPC = NH3TEMP: GASVOL = NH3VOLIT
536. OUTADIATEMP = ((GASTEMPC + 273) * ((COMPOP / COMPIP) ^ ((GAMMA - 1) / GAMMA))) - 273 ' OUTLET ADIABATIC TEMPERATURE
537. OUTADIATEMPX = OUTADIATEMP + 273
538. DRMOTWATT = (OUTADIATEMPX - (GASTEMPC + 273)) * 2.22 * (NH3KGX / 86400) / 0.75 'KW
539. Cells(51, 11) = OUTADIATEMP
540. Cells(52, 11) = DRMOTWATT
541. Cells(53, 11) = DRMOTHP
542. Cells(54, 11) = CURRENT1
543. Cells(55, 11) = CURRENT3
544. '===== CONDENSER-3 (EXCHANGER) CALCULATION =====
545. COMPIP = COMPOP
546. TL1 = Cells(49, 16) 'TUBE LENGTH (m)
547. TOD1 = Cells(50, 16) 'TUBE DIAMETER (m)
548. T1H = OUTADIATEMP + 273 'NH3 TEMPERATURE IN (K)
549. T2H = CIT + 273
550. '...NH3
551. TK = T1H
552. SCNH3 = NH3SPECHEAT(TK)
553. CNH3 = ((NH3KGX / 24) / 3600) * SCNH3
554. QNH3 = CNH3 * (TH1 - TH2)
555. '...AIR
556. TC1 = 25 + 273
557. AIRINTK1 = TC1
558. SCAIR2 = AIRSPECIFICHEAT(AIRINTK1)
559. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
560. FLAG = 2
561. U = 0.02
562.
563. CHOT = CNH3: Q = QNH3: SCHOT = SCNH3: SCCOLD = SCAIR2
564. Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN

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565. '...DATA OUT
566. AIRFR2 = HFR
567. Cells(44, 16) = COMPIP 'Condenser inlet Pressure (atm)
568. Cells(45, 16) = OUTADIATEMP 'Inlet NH3 Temperature (oC)
569. Cells(46, 16) = TH2 - 273 'Outlet NH3 Temperature (0C)
570. Cells(47, 16) = 25 'Inlet Air Temperature (0C)
571. Cells(48, 16) = TC2 - 273 'Outlet Air Temperature (0C)
572. Cells(51, 16) = NTU 'Number of Elements (No)
573. Cells(52, 16) = AREAHEX 'Shell Area (m^2)
574. Cells(53, 16) = EPS * 100 'Effectiveness (%)
575. Cells(54, 16) = QEFF 'Heat Transfer Rate (KW)
576. Cells(55, 16) = AIRFR2 'Air Flow Rate (Kg/hr)
577. 70 End Sub
578. Static Function Logn(X)
579. Logn = Log(X) / Log(2.718282)
580. End Function
581. Private Static Sub DELTAH(A, B, N, INTEGRALH)
582. H = (B - A) / N
583. T = A
584. SUMM = DELCP(T): C = 2
585. For K = 1 To N - 1
586. C = 6 - C ' Rem GENERATES COEFFICIENTS 4,2,4,2, ...
587. T = A + K * H
588. SUMM = SUMM + C * DELCP(T)
589. Next K
590. SUMM = Sum + DELCP(T)
591. INTEGRALH = (H / 3) * SUMM
592. End Sub
593. Private Static Function DELCP(T)
594. DELCP = -55.169 + 49.856 * 10 ^ -3 * T - 4.05 * 10 ^ 5 * T ^ -2 - 1.976 * 10 ^ -6 * T ^ 2
595. End Function
596. Private Static Function DELCPT(T)
597. DELCPT = (-55.169 + 49.856 * 10 ^ -3 * T - 4.05 * 10 ^ 5 * T ^ -2 - 1.976 * 10 ^ -6 * T ^ 2) ' / T
598. End Function
599. Private Static Function NH3SPECIFICHEAT(TK) 'kJ/kg.K (1atm)
600. A = 1.0948345: B = 0.002555016: C = 27119.844
601. NH3SPECIFICHEAT = A + B * GASTK + C / (TK) ^ 2
602. End Function
603. Private Static Function NH3SPECHEAT(TK) 'kJ/kg.K (>1atm)
604. A = 2.200434: B = -0.001750475: C = 0.000026445871: D = -0.000000741651: E = 7.330493E-11
605. NH3SPECHEAT = A + B * TK + C * TK ^ 2 + D * TK ^ 3 + E * TK ^ 4
606. End Function
607. Private Static Function HYDROGENSPECHEAT(H2TK) 'T=oK kJ/kg.K
608. ZA = 8.3580785: ZB = 0.046774926: ZC = -0.00014346423: ZD = 0.00000023506381: ZE = -2.3076196E-10: ZF = 1.4608608E-13
609. ZG = -6.1673082E-17: ZH = 1.7508367E-20: ZI = -3.2962768E-24: ZJ = 3.9405226E-28: ZK = -2.7046605E-32: ZL = 8.1083083E-37
610. HYDROGENSPECHEAT = ZA + ZB * H2TK + ZC * H2TK ^ 2 + ZD * H2TK ^ 3 + ZE * H2TK ^ 4 + ZF * H2TK ^ 5 + ZG * H2TK ^ 6 + ZH * H2TK ^ 7 + ZI * H2TK ^
8 + ZJ * H2TK ^ 9 + ZK * H2TK ^ 10 + ZL * H2TK ^ 11
611. End Function
612. Private Static Function NITROSPCHEAT(N2ITK) 'kJ/kg.K
613. SA = 1.100752
614. SB = -0.00053474045
615. SC = 0.0000013971884
616. SD = -1.2555363E-09
617. se = 6.0109266E-13
618. SF = -1.6836213E-16
619. SG = 2.7735985E-20
620. SH = -2.5125233E-24
621. SI = 1.0066147E-28
622. SJ = -5.1950017E-34
623. NITROSPCHEAT = SA + SB * N2ITK + SC * N2ITK ^ 2 + SD * N2ITK ^ 3 + se * N2ITK ^ 4 + SF * N2ITK ^ 5 + SG * N2ITK ^ 6 + SH * N2ITK ^ 7 + SI * N2I
TK ^ 8 + SJ * N2ITK ^ 9
624. End Function
625. Private Static Function AIRSPECIFICHEAT(AIRINTK) 'T=oK
626. TA = 1.0828694: TB = -0.00063119116: TC = 0.0000016253087: TD = -1.3949526E-09: TE = 5.3826153E-13: TF = -7.9021928E-17
627. AIRSPECIFICHEAT = TA + TB * AIRINTK + TC * AIRINTK ^ 2 + TD * AIRINTK ^ 3 + TE * AIRINTK ^ 4 + TF * AIRINTK ^ 5

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628. End Function
629. Private Static Sub HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'H
    EAT EXCHANGER
630.     AREAHEX = 3.14 * TOD * TL
631.     LMTD = Q / (U * AREAHEX)
632.     'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
633.     '----- HEATING -----
634.     If FLAG = 1 Then
635.         DELTAA = TH1 - TC2
636.         LMTD = Q / (U * AREAHEX)
637.         X1 = TH1
638. 300 S1 = DELTAA / (LMTD - Logn(DELTAA))
639.         S2 = X1 / (LMTD - Logn(X1))
640.         If S2 >= S1 Then
641.             GoTo 400
642.         Else
643.             X1 = X1 - 0.1
644.             GoTo 300
645. 400 End If
646.         DELTAB = X1
647.         TH2 = DELTAB - TC1
648.         GoTo 700
649.     End If
650.     '-----
651.     '----- COOLING -----
652.     If FLAG = 2 Then
653.         'DELTAA = TH1 - TC2
654.         DELTAB = TH2 - TC1
655.         LMTD = Q / (U * AREAHEX)
656.         X1 = 2
657. 500 S1 = Logn(X1) - X1 / LMTD
658.         S2 = Logn(DELTAB) - DELTAB / LMTD
659.         If S1 >= S2 Then
660.             GoTo 600
661.         Else
662.             X1 = X1 + 0.1
663.             GoTo 500
664. 600 End If
665.         DELTAA = X1
666.         TC2 = TH1 - DELTAA
667.     End If
668.     '-----
669. 700 P = (TC2 - TC1) / (TH1 - TC1)
670.         R = (TH1 - TH2) / (TC2 - TC1)
671.         If R > 1 Then
672.             R1 = 1 / R
673.             P1 = P * R
674.         Else
675.             P1 = P
676.             R1 = R
677.         End If
678.         A1 = (((R1) ^ 2 + 1) ^ 0.5) / (1 - R1)
679.         A2 = Logn((1 - R1 * P1) / Abs(1 - P1))
680.         A3 = 2 - P1 * (1 + R1 - (1 + (R1) ^ 2)) ^ 0.5 'up
681.         A4 = Abs(2 - P1 * (1 + R1 + (1 + (R1) ^ 2)) ^ 0.5) 'down
682.         A5 = Logn(A3 / A4)
683.         FCORF = (A1 * A2) / A5
684.         If Abs(FCORF) > 1 Then
685.             FCORF = 1
686.         End If
687.         LMTD = Q / (U * AREAHEX * FCORF)
688.         CHOT = Q / (TH1 - TH2)
689.         HFR = CHOT * 24 * 3600 / SCHOT
690.     'EFFECTIVENESS
691.     If CCOLD > CHOT Then

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692.   CMIN = CHOT
693.   C1 = CHOT
694.   EPS = (C1 * (TC2 - TC1)) / (CMIN * (TH1 - TC1))
695.   GoTo 800
696.   Else
697.   CMIN = CCOLD
698.   C1 = CCOLD
699.   EPS = (C1 * (TH1 - TH2)) / (CMIN * (TH1 - TC1))
700. 800 End If
701.   QEFF = EPS * CMIN * (TH1 - TC1)
702. 'Number of ELEMENT
703.   NTU = U * AREAHEX / CMIN
704.   If NTU <= 1 Then
705.   NTU = 1
706.   Else
707.   End If
708. End Sub
709. Private Static Function FCORF1(P, R)
710. S1 = (2 - P * (1 + R - (1 + R ^ 2) ^ 0.5)) / (2 - P * (1 + R + (1 + R ^ 2) ^ 0.5))
711.   S2 = (1 - R * P) / (1 - P)
712.   S3 = ((1 + R ^ 2) ^ 0.5) / (1 - R)
713.   FCORF1 = S3 * Logn(S2) * (Logn(S1)) ^ -1
714. End Function
715. Private Static Function NH3DENSITY(NH3TEMPC) ' T=oC
716. Dim F As Double
717. A = 0.76249107: B = -0.0030065503: C = 0.000012095274: D = -0.00000038570889: E = 7.2102508E-11: F = -5.5332429E-14
718. NH3DENSITY = A + B * NH3TEMPC + C * NH3TEMPC ^ 2 + D * NH3TEMPC ^ 3 + E * NH3TEMPC ^ 4 + F * NH3TEMPC ^ 5
719. End Function
720. Private Static Function NH3GAMMA(NH3TEMPC) ' T=oC
721. A = 1.3320734: B = -0.00049999747: C = 0.0000010911546: D = -0.00000002975822: E = 3.4313946E-12
722. NH3GAMMA = A + B * NH3TEMPC + C * NH3TEMPC ^ 2 + D * NH3TEMPC ^ 3 + E * NH3TEMPC ^ 4
723. End Function
724. Private Static Sub COMPRESSOR(GASTEMP, COMPOP, COMPPI, GAMMA, GASVOL, OUTADIATEMP, COMETREFF, WATT, ENTCC, DRMOTWATT, DRMOTHP, MOTOREFF1, MOTO
REFF3, SPHASVOL, THREPASEVOL, CURRENT1, CURRENT3, BETA)
725. End Sub

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Heat balance results for CCS (AD process)

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1. Sub Sheet11_Button1_Click()
2.
3.
4. '-----
5. ' HEAT BALANCE
6. '-----
7. '===== OUTPUT and INPUT FROM DARK
8.   DFBTANK = ActiveWorkbook.Worksheets("DFB-ADB").Cells(100, 4) 'Energy IN DARK CSTR -(kW)
9.   ADBTANK = ActiveWorkbook.Worksheets("DFB-ADB").Cells(101, 4) 'Energy IN ADB CSTR -(kW)
10.  WESTANK1 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(102, 4) 'Energy IN ADB TANK1 -(kW)
11.  WESTANK2 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(103, 4) 'Energy IN ADB TANK2 -(kW)
12.  WESTANK2XX = ActiveWorkbook.Worksheets("SOFC").Cells(35, 11) '
13.  WESTANK2BB = ActiveWorkbook.Worksheets("SOFC").Cells(52, 4) '
14.  WESTANK2BB123 = ActiveWorkbook.Worksheets("SOFC").Cells(53, 4) '
15.  WESTANK2BBTTT = ActiveWorkbook.Worksheets("SOFC").Cells(28, 11) '
16.  AASS = ActiveWorkbook.Worksheets("EMS").Cells(43, 11) '
17. '===== INPUT FROM ADB
18.
19. '===== SOFC TEMPERATURE
20.  SOFCTEMP = ActiveWorkbook.Worksheets("SOFC").Cells(13, 4) 'SOFC Cell Temperature (oC)
21. '===== INPUT DATA FOR TOTAL AIR REQUIRED FOR THE COMPRESSOR
22.  AIRADB = ActiveWorkbook.Worksheets("DFB-ADB").Cells(85, 18) ' AIR REQUIRED FOR ADB (Kg/day)
23.  AIRSOFC = ActiveWorkbook.Worksheets("SOFC").Cells(10, 4) ' AIR REQUIRED FOR SOFC cell (Kg/day)
24.  AIRSOFEC = ActiveWorkbook.Worksheets("SOFEC").Cells(26, 16) ' AIR REQUIRED FOR SOFEC HECH (Kg/day)
25.  AIRITM = ActiveWorkbook.Worksheets("ITM").Cells(5, 4) ' AIR REQUIRED FOR (ITM)HE (Kg/day)
26.  AIRSSAS1 = ActiveWorkbook.Worksheets("SSAS").Cells(27, 16) ' AIR REQUIRED FOR SSAS HE (Kg/day)
27.  AIRSSAS2 = ActiveWorkbook.Worksheets("SSAS").Cells(14, 16) ' AIR REQUIRED FOR SSAS HE (Kg/day)

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28.    AIREMS = ActiveWorkbook.Worksheets("EMS").Cells(32, 11)    ' AIR REQUIRED FOR EMS Condenser(Kg/day)
29.    AIRTEMP = ActiveWorkbook.Worksheets("ITM").Cells(8, 4)    ' AIR TEMPERATURE from (ITM) (oC)
30.    '===== ENERGY IN COMPRESSORS & PUMPMS(kw)
31.    COM3 = ActiveWorkbook.Worksheets("SSAS").Cells(31, 11)    'Compressor No3[SSAS] (kW)-
32.    COM4 = ActiveWorkbook.Worksheets("SSAS").Cells(52, 11)    'Compressor No4[SSAS] (kW)-
33.    COM5 = ActiveWorkbook.Worksheets("SOFC").Cells(32, 4)    'Compressor No5[SOFC] (kW)-
34.    COM6 = ActiveWorkbook.Worksheets("SOFC").Cells(49, 16)    'Compressor No6[SOFC] (kW)-
35.    COM8 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(117, 4)  'Hydrolic Compressor (KW)-
36.    '===== SLUDGE PUMPS =====
37.    SP1 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(68, 4)    'SLURY PUMP DARK REACTOR (W)-
38.    SP2 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(74, 4)    'SLURY PUMP DARK REACTOR (kW)-
39.    SP3 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(108, 4)   'SLURY PUMP DIGESTER (kW)-
40.    SP4 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(116, 4)   'SLURY PUMP DIGESTER (kW)-
41.    '===== ENERGY IN HEAT EXCHANGER & CONDENSER(kw)
42.    HE1 = ActiveWorkbook.Worksheets("ITM").Cells(38, 4)    'Heat Exchanger No1 [ITM] (KW)-
43.    HE2 = ActiveWorkbook.Worksheets("EMS").Cells(12, 16)    'Heat Exchanger No2 [EMS] (KW)+
44.    HE3 = ActiveWorkbook.Worksheets("EMS").Cells(24, 16)    'Heat Exchanger No3 [EMS] (KW)-
45.    HE4 = ActiveWorkbook.Worksheets("SOFC").Cells(13, 16)    'Heat Exchanger No4 [ITM] (KW)+
46.    HE5 = ActiveWorkbook.Worksheets("SOFC").Cells(26, 16)    'Heat Exchanger No5 [SOFC] (KW)+
47.    HE6 = ActiveWorkbook.Worksheets("SSAS").Cells(13, 16)    'N2 Heat Exchanger No6 [SSAS](KW)+
48.    HE7 = ActiveWorkbook.Worksheets("SSAS").Cells(26, 16)    'H2 Heat Exchanger No7 [SSAS](KW)+
49.    HE8 = ActiveWorkbook.Worksheets("SOFC").Cells(34, 11)    'Heat Exchanger BOX 8 [SOFC] (KW)-
50.    HE9 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(97, 4)   'Heat Exchanger No9 [INNOCULUM] (KW)-
51.    HE10 = ActiveWorkbook.Worksheets("SOFC").Cells(51, 4)    'Heat Exchanger BOX 8 [SOFC] (KW)-
52.    'Condenser
53.    COND1 = ActiveWorkbook.Worksheets("DFB-ADB").Cells(84, 11) 'Energy OUT DARK Condenser (kW)+
54.    COND3 = ActiveWorkbook.Worksheets("EMS").Cells(30, 11)    'Heat Condenser No1 [EMS](KW)+
55.    COND5 = ActiveWorkbook.Worksheets("SSAS").Cells(54, 16)    'Heat Condenser No5 [SSAS](KW)+
56.    'Membranes Heat Loss
57.    HLITM = ActiveWorkbook.Worksheets("ITM").Cells(41, 4)    'Heat Loss from ITM Cell (kW)
58.    HLEMS = ActiveWorkbook.Worksheets("EMS").Cells(29, 16)    'Heat Loss from ITM Cell (kW)
59.    HLSOFEC = ActiveWorkbook.Worksheets("SOFC").Cells(29, 11) 'Heat Loss from SOFEC Cell (kW)
60.    HLSSAS = ActiveWorkbook.Worksheets("SSAS").Cells(38, 11)  'Heat Loss from SSAS Cell (kW)
61.    HLSOFC = ActiveWorkbook.Worksheets("SOFC").Cells(40, 11)  'Heat Loss from SOFC Cell (kW)
62.    HLSOFCE4 = ActiveWorkbook.Worksheets("SOFC").Cells(73, 2)  'Heat Loss from SOFC Cell (kW)
63.
64.    'CO2 CALCULATIONS
65.    'CO2
66.    CO2SOFEC = ActiveWorkbook.Worksheets("SOFC").Cells(6, 11)    'CO2 From SOFEC(kg/hr)
67.    CO2SOFECTEMP = ActiveWorkbook.Worksheets("SOFC").Cells(15, 4) 'CO2 TEMPERATURE From Dark oC
68.    CO2PRESIN = ActiveWorkbook.Worksheets("SOFC").Cells(9, 4)    'CO2 Pressure atm.
69.    H2OHEXRECY = ActiveWorkbook.Worksheets("SOFC").Cells(15, 17)
70.    SSASAIRFLOW = ActiveWorkbook.Worksheets("SSAS").Cells(55, 16)
71.    SSASAIRFLOW1 = ActiveWorkbook.Worksheets("SSAS").Cells(40, 16)
72.    SOFECAIRFLOW1 = ActiveWorkbook.Worksheets("SOFC").Cells(9, 11)
73.    SOFECAIRFLOW1PO = ActiveWorkbook.Worksheets("HEAT BALANCE").Cells(87, 16)
74.    'CO2 Calculations
75.    R = 8.314    'J/K.mol
76.    CO2MW = 44    'Molecular Weight
77.    'CO2 Total Flowrate
78.    CO2TOTAL = CO2SOFEC
79.    'MIXED CO2 Temperature
80.    CO2MIXTEMP = CO2SOFECTEMP    'Mixed CO2 Temperature
81.    '===== COMPRESSORE FOR CO2 COM 10 =====
82.    Cells(67, 16) = CO2PRESIN    'Inlet Pressure atm
83.    CO2PRESOUT9 = Cells(68, 16) 'OUTLET Pressure atm
84.    Cells(69, 16) = CO2MIXTEMP    'Inlet Temperature
85.    'CALCULATIONS
86.    COMPIP = CO2PRESIN    'Compressor Inlet Pressure (atm.)
87.    COMPOP = 100    'Compressor Outlet Pressure (atm.)
88.    COMETREFF = Cells(70, 16)    'Compressor Entropy Efficiency (%)
89.    SPHASVOL = Cells(71, 16)    'Single Phase Voltage (Volts)
90.    MOTOREFF1 = Cells(72, 16)    'Single Phase Motor Efficiency (%)
91.    THREPASEVOL = Cells(73, 16)    '3 Phase Voltage (Volts)
92.    MOTOREFF3 = Cells(74, 16)    '3 Phase Motor Efficiency (%)

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93. 'COMPRESSOR DATA
94. GASTK = CO2MIXTEMP + 273 'Inlet Gas Temperature (oK)
95. CO2SPCHEAT = CO2SPEHEAT(GASTK) 'CO2 SPECIFIC HEAT ' Cp of CO2 kJ/Kg K 'NH3 Specific Heat (kJ/Kg.K)kJ/kg.K (>1atm)
96. T = CO2MIXTEMP
97. RHOCO2 = CO2DENSITY(T) 'NH3 Density (kg/m^3)
98. GAMMA = 1.208 ' 1.189 ' 'GAMMA=Cp/Cv
99. CO2VOLD = CO2TOTAL / RHOCO2 'CO2 Volume m^3/day
100. CO2VOLM = (CO2VOLD / 24) / 60 'CO2 Volume m^3/min
101. CO2VOLIT = CO2VOLM * 1000 'CO2 Volume L/min
102. Cells(66, 16) = CO2VOLIT 'CO2TOTAL 'CO2 Volume L/min,<=====
103. CO2MOL = CO2TOTAL / CO2MW 'CO2 Mol
104. OUTADIATEMP = ((CO2MIXTEMP + 273) * ((COMPOP / COMP) ^ ((GAMMA - 1) / GAMMA))) - 273 ' OUTLET ADIABATIC TEMPERATURE
105. DRMOTWATT = ((OUTADIATEMP + 273) - (CO2MIXTEMP + 273)) * CO2SPCHEAT * (CO2TOTAL / 86400) / (MOTOREFF1 / 100) 'KW
106. Cells(65, 21) = OUTADIATEMP
107. Cells(66, 21) = DRMOTWATT
108. Cells(67, 21) = DRMOTHP
109.
110. COM10 = DRMOTWATT / 1000
111. '----- CO2 COOLING Heat EXCHANGER N011
112. TL = Cells(81, 16)
113. TOD = Cells(82, 16)
114. 'CO2
115. TH1 = OUTADIATEMP + 273
116. TH2 = 25.1 + 273
117. GASTK = TH2
118. SCCO2 = CO2SPEHEAT(GASTK)
119. CCO2 = ((CO2TOTAL / 24) / 3600) * SCCO2 'O2 Heat capacity (KW/oK)
120. QO2 = CCO2 * (TH1 - TH2)
121. 'Air Flow rate needed to Cool CO2
122. Cells(78, 16) = 25 'AIR TEMPERATURE IN °C
123. TC1 = 25 + 273
124. AIRINTK1 = TC1
125. AIRINTK1 = 25.1 + 273
126. SCAIR = AIRSPECIFICHEAT(AIRINTK1)
127. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
128. FLAG = 2
129. U = 0.02
130. CHOT = CCO2: Q = QO2: SCHOT = SCCO2: SCCOLD = SCAIR
131. Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN
GER
132. 'OUTPUT
133. AIRCO2 = HFR
134. Cells(77, 16) = OUTADIATEMP
135. Cells(78, 16) = TH2 - 273
136. Cells(79, 16) = 25 'AIR TEMPERATURE IN °C
137. Cells(80, 16) = TC2 - 273 'AIR TEMPERATURE IN °C
138. Cells(83, 16) = NTU
139. Cells(84, 16) = AREAHEX
140. Cells(85, 16) = EPS
141. Cells(86, 16) = QEFF
142. Cells(87, 16) = HFR
143. HE11 = QEFF
144. 'Extra CO2'
145. '=====
146. TL = Cells(94, 16)
147. TOD = Cells(95, 16)
148. 'CO2
149. TH1 = CO2MIXTEMP + 273
150. TH2 = 25.1 + 273
151. GASTK = TH1
152. SCCO2 = CO2SPEHEAT(GASTK)
153. CCO2 = ((CO2TOTAL / 24) / 3600) * SCCO2 'O2 Heat capacity (KW/oK)
154. QO2 = CCO2 * (TH1 - TH2)
155. 'Air Flow rate needed to Cool CO2
156. Cells (91, 16) = 25 'AIR TEMPERATURE IN °C

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157. TC1 = 25 + 273
158. AIRINTK1 = TC1
159. SCAIR = AIRSPECIFICHEAT(AIRINTK1)
160. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
161. FLAG = 2
162. U = 0.02
163. CHOT = CC02: Q = Q02: SCHOT = SCC02: SCCOLD = SCAIR
164. Call HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'HEAT EXCHAN
GER
165. 'OUTPUT
166. AIRCO2 = HFR
167. Cells(90, 16) = TH1 - 273
168. Cells(91, 16) = TH2 - 273
169. Cells(92, 16) = 25 'AIR TEMPERATURE IN oC
170. Cells(93, 16) = TC2 - 273 'AIR TEMPERATURE IN oC
171. Cells(96, 16) = NTU
172. Cells(97, 16) = AREAHEX
173. Cells(98, 16) = EPS
174. Cells(99, 16) = QEFF
175. Cells(100, 16) = HFR
176. HE11 = QEFF
177. '=====
178. 'Injection'
179. Depth = Cells(104, 16)
180. MASSCO2KG = ((CO2TOTAL / 24) / 3600) 'kg.s-1
181. VOLWAT = MASSCO2KG / 0.472 ' m3.s-1 (volume of CO2gas)
182. VOLMATE1 = MASSCO2KG / 818 'm3.s-1 (volume of CO2Liquid)
183. 'Assuming pump diameter =0.1 m'
184. PIP1 = Cells(101, 16)
185. AREAPUMP12 = (3.14) * (PIP1 * PIP1) / 4
186. VOLPUMP = VOLMATE1 / AREAPUMP12 'Velocity m/s'
187. 'k = 1.35
188. VISCOS = 0.0989 / 1000000 '(m2/s)
189. RYNOL = (PIP1 * VOLPUMP) / VISCOS
190. FRIC = 0.25 / Log((1.8 / (3.7 * PIP1)) + (5.7 / RYNOL)) ^ 2 '
191. PIPELENGTH = 10 + Depth ' Length of pipe (m)'
192. KPIPE = FRIC * PIPELENGTH / PIP1
193. KFIT = 1.8 + KPIPE
194. HTE1 = KFIT * (VOLPUMP * VOLPUMP) / (19.6)
195. HESDF2 = HTE1 + Depth
196. PUMPEFF = Cells(102, 16)
197. POWEPUM = (HESDF2 * 9.81 * 818 * VOLMATE1) / PUMPEFF
198. Cells(103, 16) = POWEPUM / 1000
199. PRESSURE1 = MASSCO2KG / AREAPUMP12 'kg/m2.s
200. DELTAPRESSURE = 818 * 9.81 * Depth * 0.0000987
201. CO2PRESOUT92 = DELTAPRESSURE - CO2PRESOUT9
202. Cells(105, 16) = CO2PRESOUT92 'atm
203. '=====
204. ' CALCULATIONS
205. '=====
206. '===== ENERGY OUT (kW)
207. GASTURB = ActiveWorkbook.Worksheets("SOFC").Cells(57, 16) 'Steam Turbine [SOFC] (kW)+
208. '=====
209. 'POWER and Voltage
210. EMSPOWER = ActiveWorkbook.Worksheets("EMS").Cells(18, 11) 'POWER IN OF EMS(kW)-
211. SOFECPOWER = ActiveWorkbook.Worksheets("SOFEC").Cells(25, 11) 'POWER IN OF SOFEC (kW)-
212. ITMPOWER = ActiveWorkbook.Worksheets("ITM").Cells(26, 11) 'POWER OUT OF ITM (kW)+
213. SOFCPOWER = ActiveWorkbook.Worksheets("SOFC").Cells(22, 11) 'POWER OUT OF SOFC (kW)+
214. NH3HHV = ActiveWorkbook.Worksheets("SSAS").Cells(53, 3) 'NH3 Equivalent Power HHV of NH3(KW)+
215. NH3LHV = ActiveWorkbook.Worksheets("SSAS").Cells(54, 3) 'NH3 Equivalent Power LHV of NH3(KW)+
216. SSASPOWER = ActiveWorkbook.Worksheets("SSAS").Cells(49, 3)
217. '=====
218. ' IMPELLERS
219. IMPADB = ActiveWorkbook.Worksheets("DFB-ADB").Cells(48, 19) 'IMPELLER BIO TEACTOR (HP)
220. IMPINOC = ActiveWorkbook.Worksheets("DFB-ADB").Cells(65, 12) 'IMPELLER BIO TEACTOR (HP)

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221.  IMPMIX = ActiveWorkbook.Worksheets("DFB-ADB").Cells(8, 23)    'IMPELER MIXING TANK
222.  CB1W = ActiveWorkbook.Worksheets("DFB-ADB").Cells(85, 4)    'BLOWER BIO REACTOR (WATT)
223.  CB1 = CB1W                                                    'BLOWER BIO REACTOR (KW)
224.  '=====
225.  ' TOTAL AIR REQUIRED PUMPING)
226.  COOLAIR = 25
227.  AIRSSAS = AIRSSAS1 + AIRSSAS2 + AIRSSAS3 + SSASAIRFLOW
228.  TOTAIR = AIRSOFC + AIRITM + AIRSSAS + AIREMS + AIRDARK + AIRADB + AIRCO2    'TOTAL AIR REQUIRED for the SYSTEM (Kg/day)
229.  'Air Density
230.  COOLAIR = AIRTEMP
231.  AIRDEN = AIRDENSITY(AIRTEMP)    'Air Density(Kg/m^3)
232.  'Volumetric Flow
233.  AIRVOL1 = TOTAIR / AIRDEN    'Air Volume (m^3/day)
234.  AIRVOL2 = AIRVOL1 * 1000    'Air Volume (Lt/day)
235.  AIRVOL = (AIRVOL2 / 24) / 60    'Air Volume (Lt/min)
236.  'Compressor DATA IN
237.  Cells(42, 4) = AIRADB    '(Kg/day)
238.  Cells(43, 4) = AIRDARK    '(Kg/day)
239.  Cells(44, 4) = AIREMS    '(Kg/day)
240.  Cells(45, 4) = AIRSOFC    '(Kg/day)
241.  Cells(46, 4) = AIRITM    '(Kg/day)
242.  Cells(47, 4) = AIRSOFEC    '(Kg/day)
243.  Cells(48, 4) = AIRSSAS    '(Kg/day)
244.  Cells(49, 4) = AIRVOL    'Air Volume (Lt/min)
245.  COMPIP = Cells(50, 4)    'Compressor Inlet Pressure (Atm)
246.  COMPOP = Cells(51, 4)    'Compressor Outlet Pressure (Atm)
247.  COMPIT = Cells(52, 4)    'Compressor Inlet Temperature (oC)
248.  COMETREFF = Cells(53, 4)    'Compressor ENTROPY Efficiency (%)
249.  MOTOREFF1 = Cells(47, 11)    'Motor Efficiency 1-Phase (%)
250.  SPHASVOL = Cells(48, 11)    'Single Phase Voltage (Volt)
251.  MOTOREFF3 = Cells(50, 11)    'Motor Efficiency 3-Phase (%)
252.  THREPASEVOL = Cells(51, 11)    '3-Phase Voltage (Volt)
253.  ' CONSTANT
254.  RAIR = 408.97 'J/Kg.K
255.  GAMMA = 2.0339 'Constant for Diatomic gas compression adiabatic temperature rise
256.  ENTCC = AIRDEN * RAIR 'Entropy Change Constant (J/K.M^3)
257.  '
258.  '===== Compressor-1 Calculations =====
259.  GSTEMPC = COMPIT: GASVOL = AIRVOL
260.  GSTEMPC = COMPIT: GASVOL = AIRVOL
261.  OUTADIATEMP = ((GSTEMPC + 273) * ((COMPOP / COMPIP) ^ ((1.4 - 1) / 1.4))) - 273 ' OUTLET ADIABATIC TEMPERATURE
262.  DRMOTWATT = (((OUTADIATEMP + 273) - (GSTEMPC + 273)) * 1.15 * (TOTAIR / 86400)) / (75 / 100) 'KW
263.  '..... DATA OUTPUT ....
264.  Cells(42, 11) = OUTADIATEMP
265.  Cells(43, 11) = COOLAIR
266.  Cells(44, 11) = COOLSYS
267.  Cells(45, 11) = OUTADIATEMP
268.  Cells(45, 11) = DRMOTWATT
269.  Cells(46, 11) = DRMOTHP
270.  Cells(49, 11) = CURRENT1
271.  Cells(52, 11) = CURRENT3
272.  '===== Energy =====
273.  COM9 = DRMOTWATT 'Air Compressor
274.  TOTALINKW = COM1 + COM2 + COM3 + COM4 + COM5 + COM6 + COM7 + COM8 + COM9 + SP1 + SP2 + SP3 + SP8 + CB1 'kw
275.  ' DATA OUTPUT
276.  '=====
277.  '          ENERGY IN
278.  '=====
279.  'ENERGY IN for Compressors
280.  TOTALCOM = COM1 + COM2 + COM3 + COM4 + COM5 + COM6 + COM7 + COM8 + COM10 + COOLSYS 'Compressors
281.  Cells(56, 3) = COM1    'Compressor No1[MFI(ZM)](kw)
282.  Cells(57, 3) = COM2    'Compressor No1[SOFEC](kw)
283.  Cells(58, 3) = COM3    'Compressor No3[SSAS] (kw)
284.  Cells(59, 3) = COM4    'Compressor No4[SSAS] (kw)
285.  Cells(60, 3) = COM5    'Compressor No5[SOFEC] (kw)

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286. Cells(61, 3) = COM6 'Compressor No6[SOFC] (kW)
287. Cells(62, 3) = COM7 'Compressor No7[SOFC] (kW)
288. Cells(63, 3) = COM8 'Compressor No7[ADB] CAKING (kW)
289. Cells(64, 3) = COM9 'Compressor No9 [For Total AIR required [ENERGY (kW)]
290. Cells(65, 3) = TOTALCOM 'TOTAL Compressors
291. 'ENERGY IN for PUMPS & Fan
292. Cells(67, 3) = SP1 'Sludge Pump[DARK.REACTOR] (kW)
293. Cells(68, 3) = SP2 'Sludge Pump[DARK.REACTOR] (kW)
294. Cells(69, 3) = SP3 'For Digester Sludge (kW)
295. Cells(70, 3) = SP4 'For Digester Sludge (kW)
296. Cells(72, 3) = CB1 'Centrifugal fan[BIOREACTOR] (kW)
297. TOTALF = SP1 / 1000 + SP2 / 1000 + SP3 + SP4 + CB1
298. Cells(73, 3) = TOTALF 'Total (kW)
299. 'ENERGY IN for Heat-Exchangers
300. Cells(75, 3) = HE1
301. Cells(76, 3) = HE3
302. Cells(77, 3) = HE5
303. Cells(78, 3) = HE8
304. Cells(79, 3) = HE9
305. Cells(80, 3) = HE10
306. TOTALHEXIN = HE1 + HE3 + HE5 + HE8 + HE9 + HE10 + HE4
307. Cells(81, 3) = TOTALHEXIN
308. 'ENERGY IN FOR IMPELLER
309. IMPDFBW = IMPDFB * 0.745 'Dark Impeller (kW)
310. IMPADBW = IMPADB * 0.745 'BIO Impeller (kW)
311. IMPINOCW = IMPINOC * 0.745 'Inoculum Impeller (kW)
312. IMPMIXT = IMPMIX * 0.745 'Mixing Tank (kW)
313. TOTALIMP = IMPDFBW + IMPADBW + IMPINOCW + IMPMIXT
314. 'Cells
315. Cells(83, 3) = IMPDFBW 'Dark Impeller (kW)
316. Cells(84, 3) = IMPADBW 'BIO Impeller (kW)
317. Cells(85, 3) = IMPINOCW 'Inoculum Impeller (kW)
318. Cells(86, 3) = IMPMIXT 'Mixer Impeller (kW)
319. Cells(87, 3) = TOTALIMP
320. 'ENERGY IN FOR WASTE TANKS
321. TOTALTANKS = DFBTANK + ADBTANK + WESTANK1 + WESTANK2
322. Cells(89, 3) = DFBTANK 'Energy IN DARK CSTR -(kW)
323. Cells(90, 3) = ADBTANK 'Energy IN ADB CSTR -(kW)
324. Cells(91, 3) = WESTANK1 'Energy IN ADB TANK1 -(kW)
325. Cells(92, 3) = WESTANK2 'Energy IN ADB TANK2 -(kW)
326. Cells(93, 3) = TOTALTANKS
327. 'Membranes Heat Loss
328. TOTALHLMEMB = HLMFI + HLITM + HLEMS + HLSOFEC + HLSSAS + HLSOFC 'Total MEMBRANE HEAT LOSS (kW)
329. Cells(95, 3) = HLMFI 'Heat Loss from MFI Cell (kW)
330. Cells(96, 3) = HLITM 'Heat Loss from ITM Cell (kW)
331. Cells(97, 3) = HLEMS 'Heat Loss from EMS Cell (kW)
332. Cells(98, 3) = HLSOFEC 'Heat Loss from SOFEC Cell (kW)
333. Cells(99, 3) = HLSSAS 'Heat Loss from SSAS Cell (kW)
334. Cells(100, 3) = HLSOFC 'Heat Loss from SOFC Cell (kW)
335. Cells(101, 3) = TOTALHLMEMB 'Total MEMBRANE HEAT LOSS (kW)
336. '
337. '=====
338. ' ENERGY OUT
339. '=====
340. '...ENERGY OUT of Turbines
341. TOTALOUTTURBKW = STEATURB + GASTURB '+ GASTURB2
342. Cells(54, 11) = STEATURB
343. Cells(55, 11) = GASTURB
344. Cells(43, 15) = GASTURB2
345. Cells(56, 11) = TOTALOUTTURBKW
346. '...ENERGY OUT for Heat-Exchangers and Condensers
347. 'HEAT-EXCHANGERS
348. Cells(58, 11) = HE2
349. Cells(59, 11) = HE4
350. Cells(60, 11) = HE6

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351. Cells(61, 11) = HE7
352. 'Condensers
353. Cells(62, 11) = COND1
354. Cells(63, 11) = COND2
355. Cells(64, 11) = COND3
356. Cells(65, 11) = COND4
357. Cells(66, 11) = COND5
358. TOTALHEXCONOUT = HE6 + HE7 + COND3 + COND4 + COND1 + COND2 + COND5 + HE11 + HE2
359. Cells(67, 11) = TOTALHEXCONOUT
360. BCV = 0.1 * TOTALHEXCONOUT
361. 'TOTAL PRODUCED
362. TOTAPRO = TOTALOUTTURBKW + TOTALHEXCONOUT 'Total Produced (kW)
363. Cells(68, 11) = TOTAPRO '(A+B)
364. 'Total Balance (1)
365. ENERGYIN = TOTALCOM + ((SP1 + SP2)) + CB1 + SP4 + TOTALHEXIN + TOTALIMP + TOTALTANKS + TOTALHLMEMB 'Total IN from compressor + .....
366. TOTALGIVEN = TOTAPRO - ENERGYIN 'ENERGY BALANCE (1)OUT
367. Cells(70, 11) = ENERGYIN 'Energy Consumed (kW)
368. Cells(71, 11) = TOTAPRO 'Energy Produced(kW)
369. Cells(72, 11) = TOTALGIVEN 'ENERGY BALANCE (1)
370. 'TOTAL OUT
371. TOTALOUTHEXTURB = TOTALOUTTURBKW + TOTALHEXCONOUT
372. Cells(69, 11) = TOTALOUTHEXTURB '(A+B)
373. '=====
374. ' Cell Voltages to Power + NH3 + UREA
375. '=====
376. MSTEAMTOT = ((H2OHEXRECY + WESTANK2XX + (WESTANK2BB - WESTANK2BB123)) / 86400) * (1000 - WESTANK2BBTBT) * 4.18
377. Cells(70, 21) = MSTEAMTOT
378. 'Total Energy from Voltage
379. TOTALVOLTAGE = -SOFCEPOWER - EMSPower + ITMPOWER + SOFCPOWER - SSASPOWER 'Total Voltage Power (kW)(2)
380. 'Energy From NH3
381. NH3HHV = NH3HHV 'Energy from NH3 (kW) (4)
382. 'TOTAL ENERGY WITHOUT NH3
383. TOTENER3 = TOTALGIVEN + TOTALVOLTAGE - CO2CONPW - DRMOTWATT - MSTEAMTOT - QEFF - BCV - AASS - (POWEPUM / 1000) '(1) +(2)-(3)
384. 'TOTAL ENERGY WITHOUT NH3
385. TOTENERWNH3 = NH3HHV + TOTENER3 'Total Energy with NH3 (1) +(2)-(3) +(4)
386. 'Cells
387. Cells(65, 6) = EMSPower 'Voltage in Kw from EMS
388. Cells(66, 6) = SOFCEPOWER 'Voltage in Kw from SOFEC
389. Cells(67, 6) = ITMPOWER 'Voltage in Kw from ITM
390. Cells(68, 6) = SOFCPOWER 'Voltage in Kw from SOFC
391. Cells(69, 6) = TOTALVOLTAGE 'Energy OUT From Voltages (kW)
392. Cells(71, 6) = NH3HHV 'ENERGY IN from NH3
393. Cells(72, 6) = TOTENER3 'ENERGY BALANCE (2)
394. Cells(73, 6) = TOTENERWNH3 'ENERGY BALANCE (3)
395. End Sub
396. Static Function Logn(X)
397. Logn = Log(X) / Log(2.718282)
398. End Function
399. Private Static Function AIRDENSITY(AIRTEMP)
400. A1 = 1.2910739
401. B1 = 279.63468
402. C1 = 0.0036989433
403. D1 = 1.0050404
404. AIRDENSITY = (A1 * B1 + C1 * AIRTEMP ^ D1) / (B1 + AIRTEMP ^ D1) 'Air Density (Kg/m^3) oC
405. End Function
406. Private Static Sub COMPRESSOR(GASTEMPC, COMPOP, COMPIP, GAMMA, GASVOL, OUTADIATEMP, COOLSYS, COMETREFF, WATT, ENTCC, DRMOTWATT, DRMOTHP, MOTORE
FF1, MOTOREFF3, SPHASVOL, THREPASEVOL, CURRENT1, CURRENT3)
407. A1 = 1000
408. A2 = 60
409. End Sub
410. Private Static Function CO2SPEHEAT(GASTK) 'CO2 SPECIFIC HEAT ' Cp of CO2 kJ/Kg K)
411. Z1 = 0.51476288
412. Z2 = 5820.1918
413. Z3 = 1.4877831
414. Z4 = 1.404349

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415. CO2SPEHEAT = (Z1 * Z2 + Z3 * GASTK ^ Z4) / (Z2 + GASTK ^ Z4)
416. End Function
417. Private Static Function AIRSPECIFICHEAT(AIRTK) 'AIRSPECIFICHEAT (kJ/kg.K)
418. TA = 1.0828694: TB = -0.00063119116: TC = 0.0000016253087: TD = -1.3949526E-09: TE = 5.3826153E-13: TF = -7.9021928E-17
419. AIRSPECIFICHEAT = TA + TB * AIRTK + TC * AIRTK ^ 2 + TD * AIRTK ^ 3 + TE * AIRTK ^ 4 + TF * AIRTK ^ 5
420. End Function
421. Private Static Function WATERSPECIFICHEAT(H2OTEMP) 'WATER SPECIFIC HEAT (kJ/kg.K)
422. WATERSPECIFICHEAT = 1.224986 + 0.0014072339 * H2OTEMP - 0.0000039722778 * H2OTEMP ^ 2 + 5.3431749E-11 * H2OTEMP ^ 3 + -2.7473115E-
15 * H2OTEMP ^ 4
423. End Function
424. Private Static Function CO2DENSITY(T) 'T=oC,Kg/m^3
425. A = 0.50649907: B = 0.0019289299: C = 1.0174749
426. CO2DENSITY = (A + B * T) ^ (-1 / C)
427. End Function
428. Private Static Sub HEX(FLAG, TH1, TH2, TC1, TC2, CCOLD, CHOT, Q, SCHOT, SCCOLD, TL, TOD, FCORF, LMTD, AREAHEX, HFR, U, NTU, EPS, QEFF, P, R) 'H
EAT EXCHANGER
429. AREAHEX = 3.14 * TOD * TL
430. 'DELTAB = TH2 - TC1
431. LMTD = Q / (U * AREAHEX)
432. 'FLAG=1 for HEATING and FLAG=2 for COOLING, FLAG=3 All Temperature are Known.
433. '----- HEATING -----
434. If FLAG = 1 Then
435. DELTAA = TH1 - TC2
436. 'DELTAB = TH2 - TC1
437. LMTD = Q / (U * AREAHEX)
438. X1 = 1
439. 300 S1 = DELTAA / (LMTD - Logn(DELTAA))
440. S2 = X1 / (LMTD - Logn(X1))
441. If S2 >= S1 Then
442. GoTo 400
443. Else
444. X1 = X1 + 0.1
445. GoTo 300
446. 400 End If
447. DELTAB = X1
448. TH2 = DELTAB + TC1
449. GoTo 700
450. End If
451. '-----
452. '----- COOLING -----
453. If FLAG = 2 Then
454. 'DELTAA = TH1 - TC2
455. DELTAB = TH2 - TC1
456. LMTD = Q / (U * AREAHEX)
457. X1 = 2
458. 500 S1 = Logn(X1) - X1 / LMTD
459. S2 = Logn(DELTAB) - DELTAB / LMTD
460. If S1 >= S2 Then
461. GoTo 600
462. Else
463. X1 = X1 + 0.1
464. GoTo 500
465. 600 End If
466. DELTAA = X1
467. TC2 = TH1 - DELTAA
468. End If
469. '-----
470. 700 P = (TC2 - TC1) / (TH1 - TC1)
471. R = (TH1 - TH2) / (TC2 - TC1)
472. If R > 1 Then
473. R1 = 1 / R
474. P1 = P * R
475. Else
476. P1 = P
477. R1 = R

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478. End If
479. A1 = (((R1) ^ 2 + 1) ^ 0.5) / (1 - R1)
480. A2 = Logn((1 - R1 * P1) / Abs(1 - P1))
481. A3 = 2 - P1 * (1 + R1 - (1 + (R1) ^ 2)) ^ 0.5 'up
482. A4 = Abs(2 - P1 * (1 + R1 + (1 + (R1) ^ 2)) ^ 0.5) 'down
483. A5 = Logn(A3 / A4)
484. FCORF = (A1 * A2) / A5
485. If Abs(FCORF) > 1 Then
486. FCORF = 1
487. End If
488. If FLAG = 1 Then
489. LMTD = Q / (U * AREAHEX * FCORF)
490. CHOT = Q / (TH1 - TH2)
491. HFR = CHOT * 24 * 3600 / SCHOT
492. GoTo 800
493. End If
494. If FLAG = 2 Then
495. LMTD = Q / (U * AREAHEX * FCORF)
496. CCOLD = Q / (TH1 - TH2)
497. HFR = CCOLD * 24 * 3600 / SCHOT
498. End If
499. 'EFFECTIVENESS
500. 800 If CCOLD > CHOT Then
501. CMIN = CHOT
502. C1 = CHOT
503. EPS = (C1 * (TC2 - TC1)) / (CMIN * (TH1 - TC1))
504. GoTo 900
505. Else
506. CMIN = CCOLD
507. C1 = CCOLD
508. EPS = (C1 * (TH1 - TH2)) / (CMIN * (TH1 - TC1))
509. 900 End If
510. QEFF = EPS * CMIN * (TH1 - TC1)
511. 'Number of ELEMENT
512. NTU = U * AREAHEX / CMIN
513. If NTU <= 1 Then
514. NTU = 1
515. Else
516. End If
517. End Sub

```

Appendix B: Inventory Processes for the LCA

A sample of inventory processes along with the input and output data (parameters) used in the LCA is shown in Table B.1- B.6.

B.1 Input and output parameters and values

B.1.1 Ammonia/ammonia+urea production through AD-only process

Table B.1: Input parameters of AD-only process for ammonia/ammonia+urea production.

Input Parameters	Values	Distribution	SD2 or ZSD	Min	Max	Comments
Use_Wind	0	Undefined				Switch to select wind(0=off and 1=on)
Use_Solar	1	Undefined				Switch to select wind(0=off and 1=on)
Use_Allocation	1	Undefined				Switch (0 or 1)
Mass_Allocation	1	Undefined				Switch (0 or 1)
Avoided_Products	1	Undefined				Switch (0 or 1)
_Cells_EMS	66	Lognormal	2.05			(4,1,1,5,na) Number of cells for EMS
_Cells_SSAS	531	Lognormal	2.05			(4,1,1,5,na) Number of cells for SSAS
_Cells_SSAS_no_SOFC	535	Lognormal	2.05			(4,1,1,5,na) Number of cells for SSAS without SOFC
_dELEC_Gross_Demand_No_Urea	21,136.449	Lognormal	1.56			(4,1,1,4,na) kW
_dELEC_Gross_Demand_Urea	191,075.457	Lognormal	1.56			(4,1,1,4,na) kW (Net demand ** without SOFC)
_dELEC_Supply_SOFC	46.547	Lognormal	1.56			(4,1,1,4,na) kW
_dELEC_Net_Demand_CCS	22,103.570	Lognormal	1.56			(4,1,1,4,na) kW
_dELEC_Net_Demand_no_injection	22,087.561	Lognormal	1.56			(4,1,1,4,na) kW
_dELEC_injection_Per_kgCO2	0.00028	Lognormal	1.56			(4,1,1,4,na) kW
_dELEC_Gross_No_Injection	13,491.426	Lognormal	1.56			(4,1,1,4,na) kW
_dFlow_Rate	20,000	Lognormal	1.11			(3,1,1,1,na) kg/day Daily flow rate (Feedstock without dilution water)
_dMass_CH ₄	16,643.806	Lognormal	1.56			(4,1,1,4,na) kg/day (Methane flow rate)
_dMass_CO ₂	56,143.234	Lognormal	1.56			(4,1,1,4,na) kg/day (CO ₂ flow rate)
_dMass_Compost	154.762	Lognormal	1.56			(4,1,1,4,na) kg/day
_dMass_N_Load	85.8	Lognormal	1.11			(3,1,1,1,na) kg/N-Feedstock
_dMass_NaOH	0	Lognormal	1.56			(4,1,1,4,na) kg/day of NaOH added for pH balance
_dMass_NH ₃ No_Urea_No_SOFC	47,211.097	Lognormal	2.05			(4,1,1,5,na) kg/day
_dMass_NH ₃ No_Urea_w_SOFC	46,863.125	Lognormal	2.05			(4,1,1,5,na) kg/day (Daily flow rate of ammonia without urea production)
_dMass_NH ₃ Urea_No_SOFC	3,827.689	Lognormal	2.05			(4,1,1,5,na) kg/day
_dMass_NH ₃ Urea_SOFC	3,479.717	Lognormal	2.05			(4,1,1,5,na) kg/day (Daily Flow Rate of Ammonia)
_dMass_Sulfur	4.096	Lognormal	2.05			(4,1,1,5,na) kg/day
_dMass_Urea	76,473.975	Lognormal	1.56			(4,1,1,4,na) kg/day (Daily flow rate of urea with the SOFC)
_Frac_of_F2H	0.5	Lognormal	1.11			(3,1,1,1,na) % (Fraction of FW/HW (One-to-One=0.5))
_Tubes_ITM	2991	Lognormal	2.05			(4,1,1,5,na) Number of tubes for ITM

_Tubes_MFI	0	Lognormal	2.05			(4,1,1,1,5,na) Number of tubes for MFI
_Tubes_SOFECC	60,409	Lognormal	2.05			(4,1,1,1,5,na) Number of tubes for SOFECC
Array_Incidence	0.2862	Lognormal	1.56			(4,1,1,1,4,na) kW/m ² (Solar array)
CH ₄ _Leak_Rate	0.015	Uniform		0.01	0.03	%
CO ₂ _Loss_Rate	0.01	Uniform		0.01	0.03	%
d_FoodWaste	24.9	Uniform		22.4	27.4	Distance travelled from collection facility to the plant (km) (+_10% Assumption)
d_HumanWaste	45.4	Uniform		40.9	50	Distance travelled from collection facility to the plant (km) (+_10% Assumption)
DI_Water_SOFECC_feed	37,447.94	Lognormal	2.05			(4,1,1,1,5,na) kg/day (Daily DI water required for SOFECC)
Feedstock_Dilution_Water	2.5	Lognormal	1.11			(3,1,1,1,1,na) Ratio of water to FW (For the bioreactors)
H ₂ O_Urea_out	22,175.718	Lognormal	1.56			(4,1,1,1,4,na) kg/day of water from urea production
N ₂ O_Conv_Rate	0.005	Lognormal	1.11			(3,1,1,1,1,na) %
NH ₃ _Loss_Rate	0.005	Uniform		0.001	0.02	%

B.1.1.1 Calculated parameters for AD-only process

Table B.2: Calculated parameters of AD-only process for ammonia/ammonia+urea production.

m_FoodWaste	$(_dFlow_Rate)*(_Frac_of_F2H)=1E4$
m_HumanWaste	$(_dFlow_Rate)*(1-_Frac_of_F2H)=1E4$
tkm_FoodWaste	$(m_FoodWaste/1000)*d_FoodWaste=249$
tkm_HumanWaste	$(m_HumanWaste/1000)*d_HumanWaste=454$

B.1.2 Ammonia/ammonia+urea production through two-stage DF+AD

Table B.3: Input parameters of a two-stage DF+AD process for ammonia/ammonia+urea production.

Input Parameters	Values	Distribution	SD2 or 2SD	Min	Max	Comments
Use_Wind	0	Undefined				Switch to select wind(0=off and 1=on)
Use_Solar	1	Undefined				Switch to select wind(0=off and 1=on)
Use_Allocation	1	Undefined				Switch (0 or 1)
Mass_Allocation	1	Undefined				Switch (0 or 1)
Avoided_Products	1	Undefined				Switch (0 or 1)
_Cells_EMS	58	Lognormal	2.05			(4,1,1,1,5,na) Number of cells for EMS
_Cells_SSAS	509	Lognormal	2.05			(4,1,1,1,5,na) Number of cells for SSAS
_Cells_SSAS_no_SOFC	509	Lognormal	2.05			(4,1,1,1,5,na) Number of cells for SSAS without SOFC
_dELEC_Gross_Demand_No_Urea	13,228.78	Lognormal	1.56			(2,2,1,1,4,na) kW
_dELEC_Gross_Demand_Urea	187,705.780	Lognormal	1.56			(2,2,1,1,4,na) kW (Net demand ** without SOFC)
_dELEC_Net_Demand_CCSS	13,507.988	Lognormal	1.56			(2,2,1,1,4,na) kW
_dELEC_Supply_SOFC	0.30	Lognormal	1.56			(2,2,1,1,4,na) kW
_dELEC_Net_Demand_no_injection	13,491.42625	Lognormal	1.56			(2,2,1,1,4,na) kW
_dELEC_injection_Per_kgCO2	0.000285237	Lognormal	1.56			(2,2,1,1,4,na) kW
_dELEC_Gross_No_Injection	13,491.42625	Lognormal	1.56			(2,2,1,1,4,na) kW

_dFlow_Rate	20,000	Lognormal	1.11			(3,1,1,1,1,na) kg/day Daily flow rate (Feedstock without dilution water)
_dMass_CH ₄	14,794.494	Lognormal	1.56			(4,1,1,1,4,na) kg/day (Methane flow rate)
_dMass_CO ₂	49,905.097	Lognormal	1.56			(4,1,1,1,4,na) kg/day (CO ₂ flow rate)
_dMass_Compost	127.138	Lognormal	1.56			(4,1,1,1,4,na) kg/day
_dMass_N_Load	85.8	Lognormal	1.11			(3,1,1,1,1,na) kg/N-Feedstock
_dMass_NaOH	0.371	Lognormal	1.56			(4,1,1,1,4,na) kg/day of NaOH added for pH balance
_dMass_NH ₃ _No_Urea_No_SOFC	44918.621	Lognormal	2.05			(4,1,1,1,5,na) kg/day
_dMass_NH ₃ _No_Urea_w_SOFC	44916.730	Lognormal	2.05			(4,1,1,1,5,na) kg/day (Daily flow rate of ammonia without urea production)
_dMass_NH ₃ _Urea_no_SOFC	24.96	Lognormal	2.05			(4,1,1,1,5,na) kg/day
_dMass_NH ₃ _Urea_SOFC	22.693	Lognormal	2.05			(4,1,1,1,5,na) kg/day (Daily flow rate of ammonia)
_dMass_Sulfur	3.641	Lognormal	2.05			(4,1,1,1,5,na) kg/day
_dMass_Urea	79,136.165	Lognormal	1.56			(4,1,1,1,4,na) kg/day (Daily flow rate of urea with the SOFC)
_Frac_of_F2H	0.5	Lognormal	1.11			(3,1,1,1,1,na) % (Fraction of FW/HW (One-to-One=0.5))
_Tubes_ITM	2781	Lognormal	2.05			(4,1,1,1,5,na) Number of tubes for ITM
_Tubes_MFI	1739	Lognormal	2.05			(4,1,1,1,5,na) Number of tubes for MFI
_Tubes_SOFEFC	67,960	Lognormal	2.05			(4,1,1,1,5,na) Number of tubes for SOFEFC
Array_Incidence	0.2862	Lognormal	1.56			(4,1,1,1,4,na) kW/m ² (Solar array)
CH ₄ _Leak_Rate	0.015	Uniform		0.01	0.03	%
CO ₂ _Loss_Rate	0.01	Uniform		0.01	0.03	%
d_FoodWaste	24.9	Uniform		22.4	27.4	Distance travelled from collection facility to the plant (km) (+_10% Assumption)
d_HumanWaste	45.4	Uniform		40.9	50	Distance travelled from collection facility to the plant (km) (+_10% Assumption)
DI_Water_SOFEFC_feed	33,286.992	Lognormal	2.05			(4,1,1,1,5,na) kg/day (Daily DI water required for SOFEFC)
Feedstock_Dilution_Water	2.5	Lognormal	1.11			(3,1,1,1,1,na) Ratio of water to FW (For the bioreactors)
H ₂ O_Urea_out	23,730.334	Lognormal	1.56			(4,1,1,1,4,na) kg/day of water from urea production
N ₂ O_Conv_Rate	0.005	Lognormal	1.11			(3,1,1,1,1,na) %
NH ₃ _Loss_Rate	0.01	Uniform		0.001	0.02	%

B.1.2.1 Calculated parameters for two-stage DF+AD process

Table B.4: Calculated parameters of a two-stage DF+AD process for ammonia/ammonia+urea production.

m_FoodWaste	(_dFlow_Rate)*(_Frac_of_F2H)=1E4
m_HumanWaste	(_dFlow_Rate)*(1-_Frac_of_F2H)=1E4
tkm_FoodWaste	(m_FoodWaste/1000)*d_FoodWaste=249
tkm_HumanWaste	(m_HumanWaste/1000)*d_HumanWaste=454

B.2 Inventory processes

Table B.5: CCS without SOFC using solar PV.

Input Parameters	Value	Unit
Use_SOFC	1	
Make_Urea	1	
Calculated parameters	Expression	
_dMass_NH3	$((_dMass_NH3_Urea_SOFC)*Make_Urea+Use_SOFC+_dMass_NH3_No_Urea_w_SOFC*(1-Make_Urea)*Use_SOFC+_dMass_NH3_Urea_no_SOFC*Make_Urea*(1-Use_SOFC)+_dMass_NH3_No_Urea_No_SOFC*(1-Make_Urea)*(1-Use_SOFC))*(1-NH3_Loss_Rate)$	
_Mass_NaOH	$_dMass_NaOH/_dMass_NH3$	
_dELEC_Net_No_Urea	$_dELEC_Gross_Demand_No_Urea-_dELEC_Supply_SOFC*Use_SOFC$	kW
_dELEC_Net_Urea	$_dELEC_Gross_Demand_Urea-_dELEC_Supply_SOFC*Use_SOFC$	kW
_ELEC_W_Urea	$Iff(_dELEC_Net_Urea<0,0,_dELEC_Net_Urea)/24/_dMass_NH3$	kWh
_ELEC_No_Urea	$Iff(_dELEC_Net_No_Urea<0,0,_dELEC_Net_No_Urea)/24/_dMass_NH3$	
_ELEC_From_SOFC	$_dELEC_Supply_SOFC/24/_dMass_NH3*Use_SOFC$	kWh
Share_mass_NH3	$_dMass_NH3/(_dMass_NH3+_dMass_Urea)*100$	
Share_NH3	$iff(Use_Allocation=0,100,iff(Mass_Allocation=1,Share_mass_NH3,iff(Avoided_Products=1,100,0)))$	
Share_Urea	$100-(Share_NH3)$	

Outputs to Technosphere, Avoided products	Amount	Unit
_Urea, as N {GLO} market for Cut-off, U Modified_no_Capital_Goods	$(_dMass_Urea*Make_Urea*0.467)/_dMass_NH3=0$	kg
Compost {RoW} treatment of biowaste, industrial composting Cut-off, U	$(_dMass_Compost)/(_dMass_NH3)=0.00329$	kg
Sulfur {GLO} market for Cut-off, U	$(_dMass_Sulfur)/(_dMass_NH3)=8.72E-5$	kg
Oxygen, liquid {RoW} market for Cut-off, U	$(_dMass_Comp_O2*Use_SOFC+_dMass_Comp_O2_no_SOFC*(1-Use_SOFC))/(_dMass_NH3)=0$	kg
Electricity, medium voltage {WECC, US only} market for Cut-off, U	$(Iff(_dELEC_Net_Urea<0,ABS(_dELEC_Net_Urea),0)*Make_Urea+Iff(_dELEC_Net_No_Urea<0,ABS(_dELEC_Net_No_Urea),0)*(1-Make_Urea))/24/_dMass_NH3=0$	kWh
Inputs from Technosphere	Amount	
Food Waste	$m_FoodWaste/_dMass_NH3=0.213$	kg
Human Waste	$m_HumanWaste/_dMass_NH3=0.213$	kg
Transport, freight, lorry with reefer, cooling {GLO} processing Cut-off, U	$(tkm_FoodWaste+tkm_HumanWaste)/(_dMass_NH3)=0.015$	tkm
Tap water {RoW} tap water production, conventional treatment Cut-off, U	$(Feedstock_Dilution_Water*m_FoodWaste)/_dMass_NH3 - (H2O_Urea_Out/_dMass_NH3)*(Make_Urea)=0.532$	kg
Water, deionised, from tap water, at user {RoW} production Cut-off, U	$DI_Water_SOFC_feed/_dMass_NH3=0.797$	kg
Sodium hydroxide, without water, in 50% solution state {GLO} market for Cut-off, U	$_dMass_NaOH/_dMass_NH3=0$	kg
Electricity, medium voltage {WECC, US only} electricity voltage transformation from high to medium voltage Cut-off, U	$IFF(Use_Solar=1,0,IFF(Use_Wind=1,0,1))*(_ELEC_W_Urea*Make_Urea+(1-Make_Urea)*_ELEC_No_Urea)=0.0196$	kWh
Modified Solar Electricity, low voltage {WECC, US only} electricity production, photovoltaic, 570kWp open ground installation, multi-Si Cut-off, U	$IFF(Use_Solar=1,1,0)*(_ELEC_W_Urea*Make_Urea+(1-Make_Urea)*_ELEC_No_Urea)=0$	kWh
SOFC Co-GEN, using new SOFC, electricity with heat	$(_dELEC_Supply_SOFC/125)*(Use_SOFC)/(_dMass_NH3)=0$	kWh
ITM_Tube_Proxy	$_Tubes_ITM_dMass_NH3=0.0637$	p
SOFC_Cell_Proxy	$_Tubes_SOFC_dMass_NH3=1.45$	p
MFL_tube	$_Tubes_MFL_dMass_NH3=0$	p

SSAS_Cell_Proxy	$(_Cells_SSAS*Use_SOFC+_Cells_SSAS_no_SOFC*(1-Use_SOFC))/_dMass_NH3=0.0114$	p
EMS_Cell_Proxy	$_Cells_EMS/_dMass_NH3=0.00141$	p
_CO2 output streams	$(_dMass_CO2*(1-CO2_Loss_Rate)/_dMass_NH3)*(1-Make_Urea)=1.18$	kg
_CO2 Leakage	$CO2_Loss_Rate*_dMass_CO2/_dMass_NH3*Make_Urea=0$	kg
_CH4 Leakage	$CH4_Leak_Rate*_dMass_CH4/_dMass_NH3=0.00531$	kg
NH3 Leakage	$NH3_Loss_Rate*(_dMass_NH3/(1-NH3_Loss_Rate))/_dMass_NH3=0.00503$	kg
_N2O leakage	$N2O_Conv_Rate*_dMass_N_Load/_dMass_NH3=9.13E-6$	kg
Electricity, high voltage {WECC, US only} electricity production, wind, <1MW turbine, onshore Cut-off, U	$IFF(Use_Wind=1,1,0)*(_ELEC_W_Urea*Make_Urea+(1-Make_Urea)*_ELEC_No_Urea)=0$	kWh
Electricity, medium voltage {WECC, US only} market for Cut-off, U	$_dELEC_Injection_Per_kgCO2*(1-CO2_Loss_Rate)*_dMass_CO2/_dMass_NH3=0.000337$	kWh

Table B.6: Integrated CO₂-to-urea with SOFC using grid.

Outputs to Technosphere, Avoided products	Amount	Unit
_Urea, as N {GLO} market for Cut-off, U, Modified_no_Capital_Goods	$(_dMass_Urea*Make_Urea*0.467)/_dMass_NH3*(Avoided_Products)=10.3$	kg
Compost {RoW} treatment of biowaste, industrial composting Cut-off, U	$(_dMass_Compost)/(_dMass_NH3) =0.0447$	kg
Sulfur {GLO} market for Cut-off, U	$(_dMass_Sulfur)/(_dMass_NH3) =0.00118$	kg
Oxygen, liquid {RoW} market for Cut-off, U	$(_dMass_Comp_O2*Use_SOFC+_dMass_Comp_O2_no_SOFC*(1-Use_SOFC))/(_dMass_NH3)=0$	kg
Electricity, medium voltage {WECC, US only} market for Cut-off, U	$(If(_dELEC_Net_Urea<0,ABS(_dELEC_Net_Urea),0)*Make_Urea+If(_dELEC_Net_No_Urea<0,ABS(_dELEC_Net_No_Urea),0)*(1-Make_Urea))/24/_dMass_NH3=0$	kWh
Inputs from Technosphere	Amount	
Food Waste	$m_FoodWaste/_dMass_NH3=0.289$	kg
Human Waste	$m_HumanWaste/_dMass_NH3=0.289$	kg
Transport, freight, lorry with reefer, cooling {GLO} processing Cut-off, U	$(tkm_FoodWaste+tkm_HumanWaste)/(_dMass_NH3) =0.203$	tkm
Tap water {RoW} tap water production, conventional treatment Cut-off, U	$(Feedstock_Dilution_Water*m_FoodWaste)/_dMass_NH3 - (H2O_Urea_Out/_dMass_NH3)*(Make_Urea)=0.816$	kg
Water, deionised, from tap water, at user {RoW} production Cut-off, U	$DI_Water_SOFC_feed/_dMass_NH3=10.8$	kg
Sodium hydroxide, without water, in 50% solution state {GLO} market for Cut-off, U	$_dMass_NaOH/_dMass_NH3= 0$	kg
Electricity, medium voltage {WECC, US only} electricity voltage transformation from high to medium voltage Cut-off, U	$IFF(Use_Solar=1,0, IFF(Use_Wind=1,0,1))*(_ELEC_W_Urea*Make_Urea+(1-Make_Urea)*_ELEC_No_Urea)=2.3$	kWh
Modified Solar Electricity, low voltage {WECC, US only} electricity production, photovoltaic, 570kWp open ground installation, multi-Si Cut-off, U	$IFF(Use_Solar=1,1,0)*(_ELEC_W_Urea*Make_Urea+(1-Make_Urea)*_ELEC_No_Urea)=0$	kWh
SOFC Co-GEN, using new SOFC, electricity with heat	$(_dELEC_Supply_SOFC/125)*Use_SOFC)/(_dMass_NH3)=0.000108$	kWh
ITM_Tube_Proxy	$_Tubes_ITM/_dMass_NH3=0.864$	p
SOFC_Cel_Proxy	$_Tubes_SOFC/_dMass_NH3=19.6$	p
MFI_tube	$_Tubes_MFI/_dMass_NH3=0$	p
SSAS_Cell_Proxy	$(_Cells_SSAS*Use_SOFC+_Cells_SSAS_no_SOFC*(1-Use_SOFC))/_dMass_NH3=0.153$	p
EMS_Cell_Proxy	$_Cells_EMS/_dMass_NH3=0.0191$	p
_CO2 output streams	$(_dMass_CO2*(1-CO2_Loss_Rate)/_dMass_NH3)*(1-Make_Urea)=0$	kg
_CO2 Leakage	$CO2_Loss_Rate*_dMass_CO2/_dMass_NH3*Make_Urea=0.162$	kg
_CH4 Leakage	$CH4_Leak_Rate*_dMass_CH4/_dMass_NH3=0.0721$	kg
NH3 Leakage	$NH3_Loss_Rate*(_dMass_NH3/(1-NH3_Loss_Rate))/_dMass_NH3=0.00503$	kg

_N2O leakage	N2O_Conv_Rate*dMass_N_Load/dMass_NH3=0.000124	kg
Electricity, high voltage [WECC, US only] electricity production, wind, <1MW turbine, onshore Cut-off, U	IFF(Use_Wind=1,1,0)*(_ELEC_W_Urea*Make_Urea+(1-Make_Urea)*_ELEC_No_Urea)=0	kWh

Appendix C: Contribution Analysis Results for the LCA

Table C.1: Contribution analysis results using IPCC 2013 GWP 100a impact assessment method for different configurations of AD-only process.

Green Ammonia, 20 tonnes/day of waste, 50:50 Food Waste: Human Waste	Integrated CO ₂ -to-Urea and SOFC process with Grid (unallocated)	Integrated CO ₂ -to-Urea and SOFC process (unallocated)	Integrated CO ₂ -to-Urea process (unallocated)	Integrated CO ₂ -to-Urea and SOFC process with Grid (mass allocation)	Integrated CO ₂ -to-Urea and SOFC process (mass allocation)	Integrated CO ₂ -to-Urea process (mass allocation)	Integrated CO ₂ -to-Urea and SOFC process with Grid (avoided product)	Integrated CO ₂ -to-Urea and SOFC process (avoided product)	Integrated CO ₂ -to-Urea process (avoided product)	With SOFC and without CO ₂ Utilization	without CO ₂ Utilization	CCS without SOFC	CCS with SOFC	CCU with SOFC	CCU without SOFC
Unit	kg CO ₂ :eq	kg CO ₂ :eq	kg CO ₂ :eq	kg CO ₂ :eq	kg CO ₂ :eq	kg CO ₂ :eq	kg CO ₂ :eq	kg CO ₂ :eq	kg CO ₂ :eq	kg CO ₂ :eq	kg CO ₂ :eq	kg CO ₂ :eq	kg CO ₂ :eq	kg CO ₂ :eq	kg CO ₂ :eq
Unallocated total	3.43	2.35	2.13	0.15	0.10	0.10	3.43	2.35	2.13	0.17	0.17	0.17	0.17	0.17	0.17
	3.433953	2.346415	2.1331183	0.14802122	0.10114271	0.1007092	-26.852598	-27.940135	-25.400109	0.17040288	0.16914801	0.16934086	0.17059827	0.17042702	0.16917088
Food Waste	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Human Waste	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Transport delivery of waste	0.024955	0.024935	0.022668	0.001074	0.001074	0.00107	0.024955	0.024935	0.022668	0.001851	0.001837	0.001837	0.001851	0.001851	0.001837
Water, Waste Dilution	0.000382	3.82E-04	0.000347182	1.65E-05	1.65E-05	1.64E-05	0.0003819	3.82E-04	0.000347182	2.51E-04	0.000249162	0.000249162	0.000251	2.51E-04	2.49E-04
SOFC Water	0.016579	0.016579	0.015071834	0.000714642	0.000714642	0.000716	0.016579017	0.016579017	0.015071834	0.001231038	0.001221965	0.001221965	0.001231038	0.001231038	0.001221965
NaOH, Dark Fermentation	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Process Electricity, Grid	1.148814	0	0	0.049519	0	0	1.148813		0	0	0	0.000170357	1.72E-04	0	0
Process Electricity, Solar	0	0.061277	0.055719574	0.000E+00	0.00264134	0.0026306	0	0.0612766	0.055719574	0.000502323	0.000499721	0.000522211	0.000526089	0.000526466	0.000522586
Process Electricity, SOFC	3.79E-07	3.79E-07	0.00E+00	1.08E-10	1.08E-10	0	3.79E-07	3.79E-07	0.00E+00	1.92E-10	0.00E+00	0.00E+00	1.92E-10	1.92E-10	0.00E+00
ITM_Tube_Proxy	2.09E-02	2.09E-02	1.90E-02	5.94E-06	5.94E-06	5.94E-06	2.09E-02	2.09E-02	1.90E-02	1.06E-05	1.06E-05	1.06E-05	1.06E-05	1.06E-05	1.06E-05
SOFC_Cell_Proxy	6.62E-07	6.62E-07	6.02E-07	1.88E-10	1.88E-10	1.88E-10	6.62E-07	6.62E-07	6.02E-07	3.35E-10	3.35E-10	3.35E-10	3.35E-10	3.35E-10	3.35E-10
MFI_tube	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SSAS_Cell_Proxy	2.78E-10	2.78E-10	2.55E-10	1.20E-11	1.20E-11	1.20E-11	2.78E-10	2.78E-10	2.55E-10	2.07E-11	2.07E-11	2.07E-11	2.07E-11	2.07E-11	2.07E-11
EMS_Cell_Proxy	6.87E-12	6.87E-12	6.25E-12	2.96E-13	2.96E-13	2.95E-13	6.87E-12	6.87E-12	6.25E-12	5.10E-13	5.07E-13	5.07E-13	5.10E-13	5.10E-13	5.07E-13
_CO2 Leakage	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
_CH4 Leakage	2.210368	2.210368	2.009425	0.095278	0.095278	0.09486	2.210367	2.210367	2.009425	0.164125	0.162916	0.162916	0.164125	0.164125	0.162916
NH3_Leakage	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
_N2O leakage	0.033001	0.033001	0.030000	0.001422	0.001422	0.00141	0.033000	0.033000	0.030000	0.002450	0.002432	0.002432	0.002450	0.002450	0.002432
Urea, as N (RoW) production Cut-off, U	0	0	0	0	0	0	-3.03E+01	-3.03E+01	-27.53322	0	0	0	0	0	0
Compost (RoW) treatment of biowaste, industrial composting Cut-off, U	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Sulfur (GLO) market for Cut-off, U	-0.00027	-2.73E-04	-2.48E-04	-1.18E-05	-1.18E-05	-1.17E-05	-0.000273	-2.73E-04	-2.48E-04	-2.03E-05	-2.01E-05	-2.01E-05	-2.03E-05	-2.03E-05	-2.01E-05
Oxygen, liquid (RoW) market for Cut-off, U	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table C.2: Contribution analysis results using IPCC 2013 GWP 100a impact assessment method for different configurations of a two-stage DF+AD process.

Green Ammonia, 20 tonnes/day of waste, 50:50 Food Waste: Human Waste	Integrated CO ₂ -to-Urea and SOFC process with Grid (unallocated)	Integrated CO ₂ -to-Urea and SOFC process (unallocated)	Integrated CO ₂ -to-Urea process (unallocated)	Integrated CO ₂ -to-Urea and SOFC process with Grid (mass allocation)	Integrated CO ₂ -to-Urea and SOFC process (mass allocation)	Integrated CO ₂ -to-Urea process (mass allocation)	Integrated CO ₂ -to-Urea and SOFC process with Grid (avoided product)	Integrated CO ₂ -to-Urea and SOFC process (avoided product)	Integrated CO ₂ -to-Urea process (avoided product)	With SOFC and without CO ₂ Utilization	without CO ₂ Utilization	CCS without SOFC	CCS with SOFC	CCU with SOFC	CCU without SOFC
Unit	kg CO ₂ eq	kg CO ₂ eq	kg CO ₂ eq	kg CO ₂ eq	kg CO ₂ eq	kg CO ₂ eq	kg CO ₂ eq	kg CO ₂ eq	kg CO ₂ eq	kg CO ₂ eq	kg CO ₂ eq	kg CO ₂ eq	kg CO ₂ eq	kg CO ₂ eq	kg CO ₂ eq
Unallocated total	485.58	321.72	292.48	0.14	0.09	0.09	485.58	321.72	292.48	0.16	0.16	0.16	0.16	0.16	0.16
Food Waste	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Human Waste	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Transport delivery of waste	3.82355	3.82355	3.47600	0.00108	0.00108	0.0010	3.8235	3.82355	3.47600	0.0019	0.0019	0.00193	0.00193	0.00193	0.00190
Water, Waste Dilution	2.63E-02	2.63E-02	2.39E-02	7.47E-06	7.47E-06	7.47E-06	0.02632588	0.026325885	0.02393291	2.62E-04	2.62E-04	2.62E-04	2.62E-04	2.62E-04	2.62E-04
SOFC Water	2.259735	2.259735	2.054329	0.000641337	0.000641337	0.0006413	2.2597348	2.2597348	2.054329	0.00114167	0.00114162	0.001141624	0.001141672	0.001141672	0.001141624
NaOH, Dark Fermentation	2.24E-02	2.24E-02	2.03E-02	6.35E-06	6.35E-06	6.35E-06	0.02238065	0.022380646	0.020346286	1.13E-05	1.13E-05	1.13E-05	1.13E-05	1.13E-05	1.13E-05
Process Electricity, Grid	173.093	0	0	0.04912	0	0	173.09303	0	0	0	0	1.59E-04	1.59E-04	0	0
Process Electricity, Solar	0	9.23261	8.39339	0	0.00262	0.0026	0	9.23261	8.39339	0.0003	0.0003	0.00033	0.00033	0.00033	0.00033
Process Electricity, SOFC	3.79E-07	3.79E-07	0	1.08E-10	1.08E-10	0.00E+00	3.79E-07	3.79E-07	0	1.92E-10	0	0	1.92E-10	1.92E-10	0
ITM_Tube_Proxy	2.09E-02	2.09E-02	1.90E-02	5.94E-06	5.94E-06	5.94E-06	0.02091618	0.020916175	0.019014933	1.06E-05	1.06E-05	1.06E-05	1.06E-05	1.06E-05	1.06E-05
SOFC_Cell_Proxy	6.62E-07	6.62E-07	6.02E-07	1.88E-10	1.88E-10	1.88E-10	6.62E-07	6.62E-07	6.02E-07	3.35E-10	3.35E-10	3.35E-10	3.35E-10	3.35E-10	3.35E-10
MFI_tube	1.56E-05	1.56E-05	1.42E-05	4.42E-09	4.42E-09	4.42E-09	1.56E-05	1.56E-05	1.42E-05	7.87E-09	7.87E-09	7.87E-09	7.87E-09	7.87E-09	7.87E-09
SSAS_Cell_Proxy	4.09E-08	4.09E-08	3.72E-08	1.16E-11	1.16E-11	1.16E-11	4.09E-08	4.09E-08	3.72E-08	2.07E-11	2.07E-11	2.07E-11	2.07E-11	2.07E-11	2.07E-11
EMS_Cell_Proxy	9.26E-10	9.26E-10	8.42E-10	2.63E-13	2.63E-13	2.63E-13	9.26E-10	9.26E-10	8.42E-10	4.68E-13	4.68E-13	4.68E-13	4.68E-13	4.68E-13	4.68E-13
_CO2 Leakage	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
_CH4 Leakage	301.2757	301.2757	2.74E+02	0.085505281	0.085505281	8.55E-02	301.2757	301.2757	273.89029	0.15221165	0.15220524	0.15220524	0.15221165	0.15221165	0.15220524
NH3_Leakage	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
_N2O leakage	5.060298	5.060298	4.6003258	0.001436167	0.001436167	0.0014361	5.0602976	5.0602976	4.6003258	2.56E-03	0.00255648	0.002556475	0.002556583	0.002556583	0.002556475
Urea, as N (RoW) production Cut-off, U	0	0	0	0	0	0	-5186.2723	-5186.272	-4714.849	0	0	0	0	0	0
Compost (RoW) treatment of biowaste, industrial composting Cut-off, U	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Sulfur (GLO) market for Cut-off, U	-3.72E-02	-3.72E-02	-3.38E-02	-1.06E-05	-1.06E-05	-1.06E-05	0.0372151	0.037215056	0.033832276	-1.88E-05	-1.88E-05	-1.88E-05	-1.88E-05	-1.88E-05	-1.88E-05
Oxygen, liquid (RoW) market for Cut-off, U	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table C.3: Contribution analysis results using ReCiPe 2016 Endpoint (H) V1.03 / World (2010) H/A impact assessment method for different configurations of AD-only process.

Without CO ₂ Utilization																						
Damage category	Unit	Total	Without CO ₂ Utilization	Food Waste	Human Waste	Transport, freight, lorry with reefer, cooling	Tap water	Deionized Water	Modified Solar Electricity	SOF C Co-GEN	ITM	SOFC C	SSAS	EMS	CO ₂ leak	CH ₄ leak	NH ₃ leak	N ₂ O leak	Urea	Compost	Sulfur	
Human health	DAL Y	1.71E-06	0	0	0	3.94E-09	1.90E-09	5.51E-09	1.83E-09	0	2.21E-10	7.83E-15	5.41E-16	1.36E-18	0	1.69E-07	1.53E-06	2.60E-09	0	0	-5.44E-11	
Ecosystems	speci es.yr	4.76E-09	0	0	0	9.39E-12	8.38E-12	1.66E-11	4.38E-12	0	2.47E-13	9.40E-18	6.12E-19	2.48E-21	0	5.09E-10	4.20E-09	7.66E-12	0	0	-1.05E-13	
Resources	USD 2013	0.000373	0	0	0	0.000284	1.30E-05	6.63E-05	3.13E-05	0	1.35E-06	5.91E-11	2.64E-12	6.72E-14	0	0	0	0	0	0	-2.26E-05	
With SOFC and without CO ₂ Utilization																						
Damage category	Unit	Total	With SOFC and without CO ₂ utilization	Food Waste	Human Waste	Transport, freight, lorry with reefer, cooling	Tap water	Deionized Water	Modified Solar Electricity	SOF C Co-GEN	ITM	SOFC C	SSAS	EMS	CO ₂ leak	CH ₄ leak	NH ₃ leak	N ₂ O leak	Urea	Compost	Sulfur	
Human health	DAL Y	1.71E-06	0	0	0	3.97E-09	1.91E-09	5.55E-09	1.84E-09	1.11E-14	2.23E-10	7.89E-15	5.41E-16	1.37E-18	0	1.70E-07	1.53E-06	2.62E-09	0	0	-5.48E-11	
Ecosystems	speci es.yr	4.76E-09	0	0	0	9.46E-12	8.44E-12	1.67E-11	4.41E-12	2.05E-17	2.49E-13	9.47E-18	6.12E-19	2.49E-21	0	5.12E-10	4.20E-09	7.71E-12	0	0	-1.06E-13	
Resources	USD 2013	0.000376	0	0	0	0.000286	1.31E-05	6.68E-05	3.14E-05	2.10E-10	1.36E-06	5.96E-11	2.63E-12	6.76E-14	0	0	0	0	0	0	-2.27E-05	
CCS without SOFC																						
Damage category	Unit	Total	CCS without SOFC	Food Waste	Human Waste	Transport, freight, lorry with reefer, cooling	Tap water	Deionized Water	Modified Solar Electricity	SOF C Co-GEN	ITM	SOFC C	SSAS	EMS	CO ₂ leak	CH ₄ leak	NH ₃ leak	N ₂ O leak	Electricity, medium voltage	Compost	Sulfur	
Human health	DAL Y	1.71E-06	0	0	0	3.94E-09	1.90E-09	5.51E-09	1.92E-09	0.00E+00	2.21E-10	7.83E-15	5.41E-16	1.36E-18	0	1.69E-07	1.53E-06	2.60E-09	5.64E-10	0	-5.44E-11	
Ecosystems	speci es.yr	4.76E-09	0	0	0	9.39E-12	8.38E-12	1.66E-11	4.58E-12	0.00E+00	2.47E-13	9.40E-18	6.12E-19	2.48E-21	0	5.09E-10	4.20E-09	7.66E-12	7.31E-13	0	-1.05E-13	
Resources	USD 2013	0.000383	0	0	0	0.000284	1.30E-05	6.63E-05	3.27E-05	0.00E+00	1.35E-06	5.91E-11	2.64E-12	6.72E-14	0	0	0	0	8.80E-06	0	-2.26E-05	
CCS with SOFC																						
Damage category	Unit	Total	CCS with SOFC	Food Waste	Human Waste	Transport, freight, lorry with reefer, cooling	Tap water	Deionized Water	Modified Solar Electricity	SOF C Co-GEN	ITM	SOFC C	SSAS	EMS	CO ₂ leak	CH ₄ leak	NH ₃ leak	N ₂ O leak	Electricity, medium voltage	Compost	Sulfur	
Human health	DAL Y	1.71E-06	0	0	0	3.97E-09	1.91E-09	5.55E-09	1.93E-09	1.11E-14	2.23E-10	7.89E-15	5.41E-16	1.37E-18	0	1.70E-07	1.53E-06	2.62E-09	5.69E-10	0	-5.48E-11	
Ecosystems	speci es.yr	4.76E-09	0	0	0	9.46E-12	8.44E-12	1.67E-11	4.62E-12	2.05E-17	2.49E-13	9.47E-18	6.12E-19	2.49E-21	0	5.12E-10	4.20E-09	7.71E-12	7.36E-13	0	-1.06E-13	
Resources	USD 2013	0.000386	0	0	0	0.000286	1.31E-05	6.68E-05	3.29E-05	2.10E-10	1.36E-06	5.96E-11	2.63E-12	6.76E-14	0	0	0	0	8.87E-06	0	-2.27E-05	
CCU without SOFC																						
Damage category	Unit	Total	CCU without SOFC	Food Waste	Human Waste	Transport, freight, lorry with reefer, cooling	Tap water	Deionized Water	Modified Solar Electricity	SOF C Co-GEN	ITM	SOFC C	SSAS	EMS	CO ₂ leak	CH ₄ leak	NH ₃ leak	N ₂ O leak	Urea	Compost	Sulfur	
Human health	DAL Y	1.71E-06	0	0	0	3.94E-09	1.90E-09	5.51E-09	1.92E-09	0	2.21E-10	7.83E-15	5.41E-16	1.36E-18	0	1.69E-07	1.53E-06	2.60E-09	0	0	-5.44E-11	
Ecosystems	speci es.yr	4.76E-09	0	0	0	9.39E-12	8.38E-12	1.66E-11	4.59E-12	0	2.47E-13	9.40E-18	6.12E-19	2.48E-21	0	5.09E-10	4.20E-09	7.66E-12	0	0	-1.05E-13	
Resources	USD 2013	0.000374	0	0	0	0.000284	1.30E-05	6.63E-05	3.27E-05	0	1.35E-06	5.91E-11	2.64E-12	6.72E-14	0	0	0	0	0	0	-2.26E-05	
CCU with SOFC																						
Damage category	Unit	Total	CCU with SOFC	Food Waste	Human Waste	Transport, freight, lorry with reefer, cooling	Tap water	Deionized Water	Modified Solar Electricity	SOF C Co-GEN	ITM	SOFC C	SSAS	EMS	CO ₂ leak	CH ₄ leak	NH ₃ leak	N ₂ O leak	Urea	Compost	Sulfur	
Human health	DAL Y	1.71E-06	0	0	0	3.97E-09	1.91E-09	5.55E-09	1.93E-09	1.11E-14	2.23E-10	7.89E-15	5.41E-16	1.37E-18	0	1.70E-07	1.53E-06	2.62E-09	0	0	-5.48E-11	
Ecosystems	speci es.yr	4.76E-09	0	0	0	9.46E-12	8.44E-12	1.67E-11	4.62E-12	2.05E-17	2.49E-13	9.47E-18	6.12E-19	2.49E-21	0	5.12E-10	4.20E-09	7.71E-12	0	0	-1.06E-13	
Resources	USD 2013	0.000377	0	0	0	0.000286	1.31E-05	6.68E-05	3.29E-05	2.10E-10	1.36E-06	5.96E-11	2.63E-12	6.76E-14	0	0	0	0	0	0	-2.27E-05	
Integrated CO ₂ -to-Urea process (mass allocation)																						

Damag e categor y	Unit	Total	Integrated CO ₂ -to-Urea process (mass allocation)	Food Waste	Human Waste	Transport, freight, lorry with reefer, cooling	Tap water	Deioniz ed Water	Modified Solar Electricit y	SOF C Co-GEN	ITM	SOFE C	SSAS	EMS	CO ₂ leak	CH ₄ leak	NH ₃ leak	N ₂ O leak	Urea	Compo st	Sulfur
Human health	DAL Y	1.87E-07	0	0	0	2.29E-09	1.25E-10	3.21E-09	9.65E-09	0	1.29E-10	4.56E-15	3.15E-16	7.90E-19	0	9.83E-08	7.20E-08	1.51E-09	0	0	-3.17E-11
Ecosyst ems	speci es.yr	5.38E-10	0	0	0	5.47E-12	5.51E-13	9.66E-12	2.31E-11	0	1.44E-13	5.48E-18	3.56E-19	1.44E-21	0	2.96E-10	1.98E-10	4.46E-12	0	0	-6.12E-14
Resour ces	USD 2013	0.000357	0	0	0	0.000165	8.57E-07	3.86E-05	0.000165	0	7.86E-07	3.44E-11	1.53E-12	3.91E-14	0	0	0	0	0	0	-1.32E-05

Integrated CO₂-to-Urea and SOFC process (mass allocation)

Damag e categor y	Unit	Total	Integrated CO ₂ -to-Urea and SOFC process (mass allocation)	Food Waste	Human Waste	Transport, freight, lorry with reefer, cooling	Tap water	Deioniz ed Water	Modified Solar Electricit y	SOF C Co-GEN	ITM	SOFE C	SSAS	EMS	CO ₂ leak	CH ₄ leak	NH ₃ leak	N ₂ O leak	Urea	Compo st	Sulfur
Human health	DAL Y	1.81E-07	0	0	0	2.30E-09	1.25E-10	3.22E-09	9.69E-09	6.46E-15	1.29E-10	4.58E-15	3.14E-16	7.93E-19	0	9.87E-08	6.57E-08	1.52E-09	0	0	-3.18E-11
Ecosyst ems	speci es.yr	5.22E-10	0	0	0	5.49E-12	5.54E-13	9.71E-12	2.32E-11	1.19E-17	1.44E-13	5.50E-18	3.55E-19	1.45E-21	0	2.97E-10	1.81E-10	4.48E-12	0	0	-6.15E-14
Resour ces	USD 2013	0.000358	0	0	0	0.000166	8.61E-07	3.88E-05	0.000165	1.22E-10	7.89E-07	3.46E-11	1.53E-12	3.93E-14	0	0	0	0	0	0	-1.32E-05

Integrated CO₂-to-Urea and SOFC process with Grid (mass allocation)

Damag e categor y	Unit	Total	Integrated CO ₂ -to-Urea and SOFC process with Grid (mass allocation)	Food Waste	Human Waste	Transport, freight, lorry with reefer, cooling	Tap water	Deioniz ed Water	Electricit y, medium voltage	SOF C Co-GEN	ITM	SOFE C	SSAS	EMS	CO ₂ leak	CH ₄ leak	NH ₃ leak	N ₂ O leak	Urea	Compo st	Sulfur
Human health	DAL Y	3.36E-07	0	0	0	2.30E-09	1.25E-10	3.22E-09	1.64E-07	6.46E-15	1.29E-10	4.58E-15	3.14E-16	7.93E-19	0	9.87E-08	6.57E-08	1.52E-09	0	0	-3.18E-11
Ecosyst ems	speci es.yr	7.11E-10	0	0	0	5.49E-12	5.54E-13	9.71E-12	2.12E-10	1.19E-17	1.44E-13	5.50E-18	3.55E-19	1.45E-21	0	2.97E-10	1.81E-10	4.48E-12	0	0	-6.15E-14
Resour ces	USD 2013	0.002767	0	0	0	0.000166	8.61E-07	3.88E-05	0.002574	1.22E-10	7.89E-07	3.46E-11	1.53E-12	3.93E-14	0	0	0	0	0	0	-1.32E-05

Integrated CO₂-to-Urea process (avoided product)

Damag e categor y	Unit	Total	Integrated CO ₂ -to-Urea process (avoided product)	Food Waste	Human Waste	Transport, freight, lorry with reefer, cooling	Tap water	Deioniz ed Water	Modified Solar Electricit y	SOF C Co-GEN	ITM	SOFE C	SSAS	EMS	CO ₂ leak	CH ₄ leak	NH ₃ leak	N ₂ O leak	Urea	Compo st	Sulfur
Human health	DAL Y	-5.90E-05	0	0	0	4.86E-08	2.64E-09	6.79E-08	2.04E-07	0	2.73E-09	9.65E-14	6.67E-15	1.67E-17	0	2.08E-06	1.53E-06	3.20E-08	-6.30E-05	0	-6.71E-10
Ecosyst ems	speci es.yr	-1.30E-07	0	0	0	1.16E-10	1.17E-11	2.05E-10	4.89E-10	0	3.05E-12	1.16E-16	7.54E-18	3.05E-20	0	6.27E-09	4.20E-09	9.44E-11	-1.41E-07	0	-1.30E-12
Resour ces	USD 2013	4.54767	0	0	0	0.003499	1.82E-05	0.000818	0.003485	0	1.66E-05	7.30E-10	3.25E-11	8.28E-13	0	0	0	0	-4.55523	0	-0.00028

Integrated CO₂-to-Urea and SOFC process (avoided product)

Damag e categor y	Unit	Total	Integrated CO ₂ -to-Urea and SOFC process (avoided product)	Food Waste	Human Waste	Transport, freight, lorry with reefer, cooling	Tap water	Deioniz ed Water	Modified Solar Electricit y	SOF C Co-GEN	ITM	SOFE C	SSAS	EMS	CO ₂ leak	CH ₄ leak	NH ₃ leak	N ₂ O leak	Urea	Compo st	Sulfur
Human health	DAL Y	-6.51E-05	0	0	0	5.34E-08	2.91E-09	7.47E-08	2.25E-07	1.50E-13	3.00E-09	1.06E-13	7.28E-15	1.84E-17	0	2.29E-06	1.53E-06	3.52E-08	-6.93E-05	0	-7.38E-10
Ecosyst ems	speci es.yr	-1.43E-07	0	0	0	1.27E-10	1.28E-11	2.25E-10	5.38E-10	2.76E-16	3.35E-12	1.28E-16	8.24E-18	3.36E-20	0	6.90E-09	4.20E-09	1.04E-10	-1.55E-07	0	-1.43E-12
Resour ces	USD 2013	5.00244	0	0	0	0.003849	2.00E-05	0.000899	0.003832	2.82E-09	1.83E-05	8.02E-10	3.55E-11	9.11E-13	0	0	0	0	-5.01075	0	-0.00031

Integrated CO₂-to-Urea and SOFC process with Grid (avoided product)

Damag e categor y	Unit	Total	Integrated CO ₂ -to-Urea and SOFC process with Grid (avoided product)	Food Waste	Human Waste	Transport, freight, lorry with reefer, cooling	Tap water	Deioniz ed Water	Electricit y, medium voltage	SOF C Co-GEN	ITM	SOFE C	SSAS	EMS	CO ₂ leak	CH ₄ leak	NH ₃ leak	N ₂ O leak	Urea	Compo st	Sulfur
Human health	DAL Y	-6.15E-05	0	0	0	5.34E-08	2.91E-09	7.47E-08	3.80E-06	1.50E-13	3.00E-09	1.06E-13	7.28E-15	1.84E-17	0	2.29E-06	1.53E-06	3.52E-08	-6.93E-05	0	-7.38E-10
Ecosyst ems	speci es.yr	-1.39E-07	0	0	0	1.27E-10	1.28E-11	2.25E-10	4.92E-09	2.76E-16	3.35E-12	1.28E-16	8.24E-18	3.36E-20	0	6.90E-09	4.20E-09	1.04E-10	-1.55E-07	0	-1.43E-12
Resour ces	USD 2013	4.94657	0	0	0	0.003849	2.00E-05	0.000899	0.059705	2.82E-09	1.83E-05	8.02E-10	3.55E-11	9.11E-13	0	0	0	0	-5.01075	0	-0.00031

Integrated CO₂-to-Urea process (per tonne of waste)

Damag e categor y	Unit	Total	Integrated CO ₂ -to-Urea process (per tonne of waste)	Food Waste	Human Waste	Transport, freight, lorry with reefer, cooling	Tap water	Deioniz ed Water	Modified Solar Electricit y	SOF C Co-GEN	ITM	SOFE C	SSAS	EMS	CO ₂ leak	CH ₄ leak	NH ₃ leak	N ₂ O leak	Urea	Compo st	Sulfur
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Damage category	Unit	Total	Integrated CO ₂ -to-Urea and SOFC process (per tonne of waste)	Food Waste	Human Waste	Transport, freight, lorry with reefer, cooling	Tap water	Deionized Water	Modified Solar Electricity	SOF C Co-GEN	ITM	SOFC	SSAS	EMS	CO ₂ leak	CH ₄ leak	NH ₃ leak	N ₂ O leak	Urea	Compost	Sulfur
Human health	DAL Y	3.96E-06	0	0	0	4.86E-08	2.64E-09	6.79E-08	2.04E-07	0	2.73E-09	9.65E-14	6.67E-15	1.67E-17	0	2.08E-06	1.53E-06	3.20E-08	0	0	-6.71E-10
Ecosystems	species.yr	1.14E-08	0	0	0	1.16E-10	1.17E-11	2.05E-10	4.89E-10	0	3.05E-12	1.16E-16	7.54E-18	3.05E-20	0	6.27E-09	4.20E-09	9.44E-11	0	0	-1.30E-12
Resources	USD 2013	0.007558	0	0	0	0.003499	1.82E-05	0.000818	0.003485	0	1.66E-05	7.30E-10	3.25E-11	8.28E-13	0	0	0	0	0	0	-0.00028
Integrated CO ₂ -to-Urea and SOFC process (per tonne of waste)																					
Human health	DAL Y	4.21E-06	0	0	0	5.34E-08	2.91E-09	7.47E-08	2.25E-07	1.50E-13	3.00E-09	1.06E-13	7.28E-15	1.84E-17	0	2.29E-06	1.53E-06	3.52E-08	0	0	-7.38E-10
Ecosystems	species.yr	1.21E-08	0	0	0	1.27E-10	1.28E-11	2.25E-10	5.38E-10	2.76E-16	3.35E-12	1.28E-16	8.24E-18	3.36E-20	0	6.90E-09	4.20E-09	1.04E-10	0	0	-1.43E-12
Resources	USD 2013	0.008313	0	0	0	0.003849	2.00E-05	0.000899	0.003832	2.82E-09	1.83E-05	8.02E-10	3.55E-11	9.11E-13	0	0	0	0	0	0	-0.00031
Integrated CO ₂ -to-Urea and SOFC process with Grid (per tonne of waste)																					
Human health	DAL Y	7.78E-06	0	0	0	5.34E-08	2.91E-09	7.47E-08	3.80E-06	1.50E-13	3.00E-09	1.06E-13	7.28E-15	1.84E-17	0	2.29E-06	1.53E-06	3.52E-08	0	0	-7.38E-10
Ecosystems	species.yr	1.65E-08	0	0	0	1.27E-10	1.28E-11	2.25E-10	4.92E-09	2.76E-16	3.35E-12	1.28E-16	8.24E-18	3.36E-20	0	6.90E-09	4.20E-09	1.04E-10	0	0	-1.43E-12
Resources	USD 2013	0.064185	0	0	0	0.003849	2.00E-05	0.000899	0.059705	2.82E-09	1.83E-05	8.02E-10	3.55E-11	9.11E-13	0	0	0	0	0	0	-0.00031

Table C.4: Contribution analysis results using ReCiPe 2016 Endpoint (H) V1.03 / World (2010) H/A impact assessment method for different configurations of a two-stage DF+AD process.

Without CO ₂ Utilization																						
Damage category	Unit	Total	Without CO ₂ Utilization	Food Waste	Human Waste	Transport, freight, lorry with reefer, cooling	Tap water	Deionized Water	Modified Solar Electricity	SOF C Co-GEN	MFI	ITM	SOFC	SSAS	EMS	CO ₂ leak	CH ₄ leak	NH ₃ leak	N ₂ O leak	Urea	NaOH	S ₂
Human health	DAL Y	1.70E-06	0	0	0	4.14E-09	1.99E-09	5.14E-09	1.21E-09	0	2.77E-14	2.16E-10	7.31E-15	5.41E-16	1.25E-18	0	1.58E-07	1.53E-06	2.73E-09	0	3.24E-11	5.08E-11
Ecosystems	species.yr	4.72E-09	0	0	0	9.87E-12	8.81E-12	1.55E-11	2.88E-12	0	3.91E-17	2.41E-13	8.79E-18	6.12E-19	2.29E-21	0	4.75E-10	4.20E-09	8.05E-12	0	5.63E-14	9.82E-14
Resources	USD 2013	0.000375	0	0	0	0.000298	1.37E-05	6.19E-05	2.06E-05	0	6.00E-10	1.32E-06	5.53E-11	2.64E-12	6.20E-14	0	0	0	0	0	5.91E-07	2.11E-05
With SOFC and without CO ₂ Utilization																						
Damage category	Unit	Total	With SOFC and without CO ₂ Utilization	Food Waste	Human Waste	Transport, freight, lorry with reefer, cooling	Tap water	Deionized Water	Modified Solar Electricity	SOF C Co-GEN	MFI	ITM	SOFC	SSAS	EMS	CO ₂ leak	CH ₄ leak	NH ₃ leak	N ₂ O leak	Compost	NaOH	S ₂
Human health	DAL Y	1.70E-06	0	0	0	4.14E-09	1.99E-09	5.14E-09	1.21E-09	2.77E-14	9.52E-16	2.16E-10	7.31E-15	5.41E-16	1.25E-18	0	1.58E-07	1.53E-06	2.73E-09	0	3.24E-11	5.08E-11
Ecosystems	species.yr	4.72E-09	0	0	0	9.87E-12	8.81E-12	1.55E-11	2.88E-12	3.91E-17	1.75E-18	2.41E-13	8.79E-18	6.12E-19	2.29E-21	0	4.75E-10	4.20E-09	8.05E-12	0	5.63E-14	9.82E-14
Resources	USD 2013	0.000375	0	0	0	0.000298	1.37E-05	6.19E-05	2.06E-05	6.00E-10	1.79E-11	1.32E-06	5.53E-11	2.64E-12	6.20E-14	0	0	0	0	0	5.91E-07	2.11E-05
CCS without SOFC																						
Damage category	Unit	Total	CCS without SOFC	Food Waste	Human Waste	Transport, freight, lorry with reefer, cooling	Tap water	Deionized Water	Modified Solar Electricity	SOF C Co-GEN	MFI	ITM	SOFC	SSAS	EMS	CO ₂ leak	CH ₄ leak	NH ₃ leak	N ₂ O leak	Electricity, medium voltage	NaOH	S ₂
Human health	DAL Y	1.70E-06	0	0	0	4.14E-09	1.99E-09	5.14E-09	1.23E-09	0	2.77E-14	2.16E-10	7.31E-15	5.41E-16	1.25E-18	0	1.58E-07	1.53E-06	2.73E-09	5.27E-10	3.24E-11	5.08E-11

Ecosyst	speci	4.72E-	0	0	0	9.87E-12	8.81E-	1.55E-	2.94E-12	0	3.91	2.41E-	8.79E-	6.12	2.29E	0	4.75	4.20	8.05E-	6.83E-	5.6	-
ems	es,yr	09					12	11			E-17	E-13	E-18	E-19	-21		E-10	E-09	E-12	E-13	3E-	9.8
Resour	USD	0.0003	0	0	0	0.000298	1.37E-	6.19E-	2.10E-05	0	6.00	1.32E-	5.53E-	2.64	6.20E	0	0	0	0	8.23E-	5.9	-
ces	2013	84					05	05			E-10	E-06	E-11	E-12	-14					E-06	1E-	2.1
																					07	1E-
																						05

CCS with SOFC

Damag			CCS	Food	Human	Transpor	Tap	Deioniz	Modified	SOF	MFI	ITM	SOFE	SSA	EMS	CO ₂	CH ₄	NH ₃	N ₂ O	Electrici	Na	S ₂
e categor	Unit	Total	with	Waste	Waste	t, freight,	water	ed	Solar	C			C	S		leak	leak	leak	leak	ty,	O	
y			SOFC			lorry		Water	Electricit	Co-			C							medium	H	
						with			y	GEN										voltage		
Human	DAL	1.70E-	0	0	0	4.14E-09	1.99E-	5.14E-	1.23E-09	9.52	2.77E-	2.16E-	7.31E-	5.41	1.25	0	1.58	1.53	2.73E-	5.27E-10	3.2	-
health	Y	06					09	09		E-16	-14	10	15	E-16	E-18		E-07	E-06	09		4E-	5.0
																					11	11
Ecosyst	speci	4.72E-	0	0	0	9.87E-12	8.81E-	1.55E-	2.94E-12	1.75	3.91E-	2.41E-	8.79E-	6.12	2.29	0	4.75	4.20	8.05E-	6.83E-13	5.6	-
ems	es,yr	09					12	11		E-18	-17	13	18	E-19	E-21		E-10	E-09	E-12		3E-	9.8
Resour	USD	0.0003	0	0	0	0.000298	1.37E-	6.19E-	2.10E-05	1.79	6.00E-	1.32E-	5.53E-	2.64	6.20	0	0	0	0	8.23E-06	5.9	-
ces	2013	84					05	05		E-11	-10	06	11	E-12	E-14						1E-	2.1
																					07	1E-
																						05

CCU without SOFC

Damag			CCU	Food	Human	Transpor	Tap	Deioniz	Modified	MFI	ITM	SOFE	SSA	EMS	CO ₂	CH ₄	NH ₃	N ₂ O	Urea	Compo	Na	S ₂
e categor	Unit	Total	without	Waste	Waste	t, freight,	water	ed	Solar			C	S		leak	leak	leak	leak		st	O	
y			SOFC			lorry		Water	Electricit	Co-											H	
						with			y	GEN												
Human	DAL	1.70E-	0	0	0	4.05E-09	1.99E-	5.14E-	1.23E-09	2.77	2.16	7.31E-	5.41E-	1.25	0	1.58	1.53	2.73	0	0	3.2	-
health	Y	06					09	09		E-14	E-10	15	16	E-18		E-07	E-06	E-09			4E-	5.0
																					11	11
Ecosyst	speci	4.72E-	0	0	0	9.71E-12	8.81E-	1.55E-	2.95E-12	3.91	2.41	8.79E-	6.12E-	2.29	0	4.75	4.20	8.05	0	0	5.6	-
ems	es,yr	09					12	11		E-17	E-13	18	19	E-21		E-10	E-09	E-12			3E-	9.8
Resour	USD	0.0003	0	0	0	0.000295	1.37E-	6.19E-	2.10E-05	6.00	1.32	5.53E-	2.64E-	6.20	0	0	0	0	0	0	5.9	-
ces	2013	72					05	05		E-10	E-06	11	12	E-14							1E-	2.1
																					07	1E-
																						05

CCU with SOFC

Damag			CCU	Food	Human	Transpor	Tap	Deioniz	Modified	SOF	MFI	ITM	SOFE	SSA	EMS	CO ₂	CH ₄	NH ₃	N ₂ O	Urea	Na	S ₂
e categor	Unit	Total	with	Waste	Waste	t, freight,	water	ed	Solar	C			C	S		leak	leak	leak	leak		O	
y			SOFC			lorry		Water	Electricit	Co-											H	
						with			y	GEN												
Human	DAL	1.70E-	0	0	0	4.14E-09	1.99E-	5.14E-	1.23E-09	9.52	2.77	2.16E-	7.31E-	5.41	1.25E	0	1.58	1.53	2.73E-	0	3.2	-
health	Y	06					09	09		E-16	E-14	10	15	E-16	-18		E-07	E-06	09		4E-	5.0
																					11	11
Ecosyst	speci	4.72E-	0	0	0	9.87E-12	8.81E-	1.55E-	2.95E-12	1.75	3.91	2.41E-	8.79E-	6.12	2.29E	0	4.75	4.20	8.05E-	0	5.6	-
ems	es,yr	09					12	11		E-18	E-17	13	18	E-19	-21		E-10	E-09	E-12		3E-	9.8
Resour	USD	0.0003	0	0	0	0.000298	1.37E-	6.19E-	2.10E-05	1.79	6.00	1.32E-	5.53E-	2.64	6.20E	0	0	0	0	0	5.91	-
ces	2013	76					05	05		E-11	E-10	06	11	E-12	-14						E-07	1E-
																					07	1E-
																						05

Integrated CO₂-to-Urea process (mass allocation)

Damag			Integrate	Food	Human	Transpor	Tap	Deioniz	Modified	SOF	MFI	ITM	SOFE	SSA	EMS	CO ₂	CH ₄	NH ₃	N ₂ O	Urea	Na	S ₂
e categor	Unit	Total	d CO ₂ -	Waste	Waste	t, freight,	water	ed	Solar	C			C	S		leak	leak	leak	leak		O	
y			to-Urea			lorry		Water	Electricit	Co-											H	
			process			with			y	GEN												
Human	DAL	1.06E-	0	0	0	2.33E-09	5.68E-	2.89E-	9.61E-09	0	1.56	1.21E-	4.11E-	3.04	7.04E	0	8.86	4.76	1.53E-	0	1.82E	-
health	Y	07					11	09			E-14	10	15	E-16	-19		E-08	E-10	09		11	11
Ecosyst	speci	3.10E-	0	0	0	5.55E-12	2.51E-	8.71E-	2.30E-11	0	2.19	1.36E-	4.94E-	3.44	1.28E	0	2.67	1.31	4.52E-	0	3.16E	-
ems	es,yr	10					13	12			E-17	13	18	E-19	-21		E-10	E-12	12		14	14
Resour	USD	0.0003	0	0	0	0.000168	3.91E-	3.48E-	0.000164	0	3.37	7.41E-	3.10E-	1.48	3.48E	0	0	0	0	0	3.32E	-
ces	2013	56					07	05			E-10	07	11	E-12	-14						07	1E-
																						05

Integrated CO₂-to-Urea and SOFC process (mass allocation)

Damag			Integrate	Food	Human	Transpor	Tap	Deioniz	Modified	SOF	MFI	ITM	SOFE	SSA	EMS	CO ₂	CH ₄	NH ₃	N ₂ O	Urea	Na	S ₂
e categor	Unit	Total	d CO ₂ -	Waste	Waste	t, freight,	water	ed	Solar	C			C	S		leak	leak	leak	leak		O	
y			to-Urea			lorry		Water	Electricit	Co-											H	
			and			with			y	GEN												
Human	DAL	1.06E-	0	0	0	2.33E-09	5.68E-	2.89E-	9.61E-09	5.35	1.56	1.21E-	4.11E-	3.04	7.04E	0	8.86	4.33	1.53E-	0	1.82	-
health	Y	07					11	09		E-16	E-14	10	15	E-16	-19		E-08	E-10	09		11	2.8

Damag e category	Unit	Total	Integrate d CO ₂ -to-Urea process (per tonne of waste)	Food Waste	Human Waste	Transport, freight, lorry with reefer, cooling	Tap water	Deionized Water	Modified Solar Electricity	SOF C Co-GEN	MFI	ITM	SOFE C	SSA S	EMS	CO ₂ leak	CH ₄ leak	NH ₃ leak	N ₂ O leak	Urea	NaOH	S ₂
Human health	DAL Y	0.000338	0	0	0	7.45E-06	1.82E-07	9.26E-06	3.08E-05	0	4.99E-11	3.89E-07	1.32E-11	9.73E-13	2.25E-15	0	0.000284	1.53E-06	4.91E-06	0	5.84E-08	-9.14E-08
Ecosystems	speci es.yr	9.94E-07	0	0	0	1.78E-08	8.05E-10	2.79E-08	7.36E-08	0	7.03E-14	4.34E-10	1.58E-14	1.10E-15	4.12E-18	0	8.55E-07	4.20E-09	1.45E-08	0	1.01E-10	-1.77E-10
Resources	USD 2013	1.139669	0	0	0	0.536567	0.001252	0.111437	0.52494	0	1.08E-06	0.002373	9.94E-08	4.74E-09	1.12E-10	0	0	0	0	0	0.001064	-0.03796

Integrated CO₂-to-Urea and SOFC process (avoided product)

Damag e category	Unit	Total	Integrate d CO ₂ -to-Urea and SOFC process (per tonne of waste)	Food Waste	Human Waste	Transport, freight, lorry with reefer, cooling	Tap water	Deionized Water	Modified Solar Electricity	SOF C Co-GEN	MFI	ITM	SOFE C	SSA S	EMS	CO ₂ leak	CH ₄ leak	NH ₃ leak	N ₂ O leak	Urea	NaOH	S ₂
Human health	DAL Y	0.000372	0	0	0	8.19E-06	2.00E-07	1.02E-05	3.39E-05	1.88E-12	5.49E-11	4.28E-07	1.45E-11	1.07E-12	2.48E-15	0	0.000312	1.53E-06	5.40E-06	0	6.42E-08	-1.01E-07
Ecosystems	speci es.yr	1.09E-06	0	0	0	1.95E-08	8.85E-10	3.07E-08	8.10E-08	3.47E-15	7.73E-14	4.78E-10	1.74E-14	1.21E-15	4.53E-18	0	9.40E-07	4.20E-09	1.59E-08	0	1.12E-10	-1.94E-10
Resources	USD 2013	1.25362	0	0	0	0.590217	0.001377	0.122579	0.577426	3.55E-08	1.19E-06	0.00261	1.09E-07	5.22E-09	1.23E-10	0	0	0	0	0	0.01417	-0.04176

Integrated CO₂-to-Urea and SOFC process with Grid (avoided product)

Damag e category	Unit	Total	Integrate d CO ₂ -to-Urea and SOFC process with Grid (per tonne of waste)	Food Waste	Human Waste	Transport, freight, lorry with reefer, cooling	Tap water	Deionized Water	Electricity, medium voltage	SOF C Co-GEN	MFI	ITM	SOFE C	SSA S	EMS	CO ₂ leak	CH ₄ leak	NH ₃ leak	N ₂ O leak	Urea	NaOH	S ₂
Human health	DAL Y	0.000911	0	0	0	8.19E-06	2.00E-07	1.02E-05	0.000573	1.88E-12	5.49E-11	4.28E-07	1.45E-11	1.07E-12	2.48E-15	0	0.000312	1.53E-06	5.40E-06	0	6.42E-08	-1.01E-07
Ecosystems	speci es.yr	1.75E-06	0	0	0	1.95E-08	8.85E-10	3.07E-08	7.41E-07	3.47E-15	7.73E-14	4.78E-10	1.74E-14	1.21E-15	4.53E-18	0	9.40E-07	4.20E-09	1.59E-08	0	1.12E-10	-1.94E-10
Resources	USD 2013	9.672019	0	0	0	0.590217	0.001377	0.122579	8.995826	3.55E-08	1.19E-06	0.00261	1.09E-07	5.22E-09	1.23E-10	0	0	0	0	0	0.01117	-0.04176

