DYNAMIC MODE CONTROLLER DESIGN OF AMMONIA PRODUCTION UNIT

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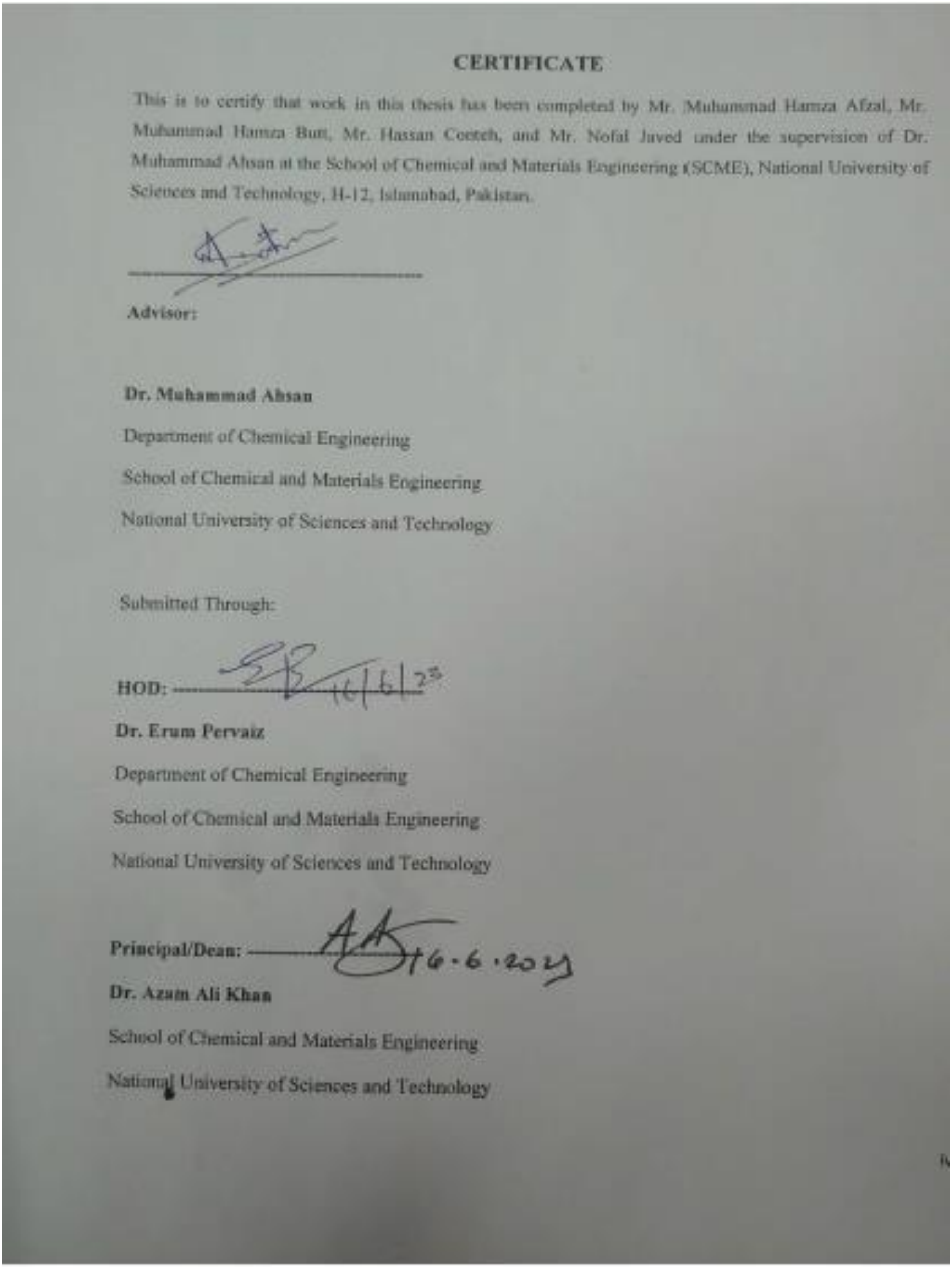

CERTIFICATE

This is to certify that work in this thesis has been completed by Mr. Muhammad Hamza Afzal, Mr. Muhammad Hamza Butt, Mr. Hassan Coeteh, and Mr. Nofal Javed under the supervision of Dr. Muhammad Ahsan at the School of Chemical and Materials Engineering (SCME), National University of Sciences and Technology, H-12, Islamabad, Pakistan.

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DEDICATION

This FYP Thesis is dedicated to, foremost, our parents, who supported us and had our back throughout our life and our friends and teachers here at SCME, who have been so helpful.

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All thanks to Allah, the Generous and Almighty for His countless blessings and rewards, who granted us the strength and ability to complete this thesis.

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We are also thankful to our parents and special thanks to our friends and seniors; without their support and encouragement, it would not have been possible to complete the project successfully.

Sincerely,
Group 22

ABSTRACT

This thesis designs dynamic mode controllers for ammonia unit to increase production, reduce troubleshooting time and automate the plant. The study begins by reviewing literature and selecting the best approach for dynamic calculation. A comprehensive literature review covers process basics, methods for dynamic simulation, comparison of different approaches and choosing the best approach. This literature evaluation lays the groundwork for the planned study and future research. Thesis then presents a process flow diagram and details about process and dynamic procedures. The specifications and design criteria for different equipment such feed tanks, centrifugal pumps, pre-heaters, packed bed reactors, and columns are carefully studied. Equipment undergoes material and energy balances. Thesis also covers critical equipment component design and specifications. The design, function, and design considerations of shell-and-tube heat exchangers are examined. Discussions include packed-bed reactor design and reactions. Aspen Hysys was used for process simulation and for process dynamics and behaviour, providing a complete picture. Component lists, fluid packages, parameters, and reactor and reactor requirements are simulated. Simulations reveal process performance and enable optimization. Operation and process monitoring require instrumentation and control. Ratio and cascade control solutions are described for process stability and production optimization. This thesis assesses primary equipment costs, total investment, direct production expenses, income generation, and payback period for any industrial operation. These financial studies reveal the parallel ammonia plant's economic viability. Hazard and Operability (HAZOP) research identifies process hazards and recommends risk assessment and reduction. Explaining HAZOP and identifying process hazards ensures safety and regulatory compliance. This final-year thesis suggests designing dynamic mode controllers at various points of ammonia plant gives boost production capacity and eliminate bottlenecks. Process overview, material and energy balance calculations, equipment design, simulation, instrumentation and control strategies, cost estimation, and HAZOP studies are examined in detail to inform future research.

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INTRODUCTION

1.1 BACKGROUND

The dynamic mode controller (DMC) has emerged as a powerful control algorithm for optimizing the performance of dynamic systems and processes. In the realm of industrial production, the design and implementation of an effective control strategy play a pivotal role in ensuring operational efficiency, product quality, and resource utilization. Ammonia, a key compound in various industries, serves as a prime example of where the application of a dynamic mode controller can yield significant benefits.

Ammonia, with its wide-ranging applications in agriculture, chemical synthesis, refrigeration, and more, plays a critical role in supporting global food security, sustaining chemical manufacturing, and meeting the demands of a rapidly growing population. As the demand for ammonia continues to rise, the need for efficient and precise control over its production processes becomes increasingly paramount.

1.2 PROBLEM STATEMENT

The ammonia production process plays a critical role in various industries, including agriculture, chemical manufacturing, and refrigeration. However, ensuring efficient and precise control over the production unit presents several challenges. The current control strategies employed in ammonia production units often struggle to optimize key process variables, maintain product quality, and respond effectively to disturbances and variations in feedstock composition.

The problem addressed in this thesis is the design and implementation of a dynamic mode controller (DMC) for an ammonia production unit. The aim is to overcome the limitations of existing control strategies and enhance the efficiency, stability, and overall performance of the production process.

Key Challenges:

- Process Dynamics: The ammonia production unit exhibits complex dynamics due to various factors such as heat transfer, chemical reactions, and interdependent process variables. Capturing and controlling these dynamics effectively is crucial to achieving optimal operation and maximizing the production unit's performance.

- Disturbance Rejection: Ammonia production processes are susceptible to disturbances, including variations in feedstock composition, changes in operating conditions, and external factors. The existing control strategies often struggle to respond quickly and effectively to these disturbances, leading to suboptimal process performance and reduced product quality.
- Energy Efficiency: Ammonia production units consume a significant amount of energy, making energy efficiency a crucial aspect to optimize. Current control strategies may not adequately consider energy optimization objectives, resulting in excessive energy consumption and increased operational costs.
- Product Quality and Yield: Maintaining consistent product quality and maximizing ammonia yield are essential for meeting industry standards and economic viability. The existing control strategies may not adequately address variations in feedstock properties and other process uncertainties, leading to deviations in product quality and yield.
- Adaptability to Changing Operating Conditions: Ammonia production units often encounter variations in feedstock properties, market demands, and process requirements. The control strategies should be able to adapt to these changes and provide robust and flexible control to ensure stable operation and consistent performance.

Research Objective:

The primary objective of this thesis is to design and implement a dynamic mode controller for an ammonia production unit to address the challenges. The goal is to enhance process control, improve energy efficiency, maintain product quality, and enhance the overall performance of the ammonia production process.

By leveraging the predictive capabilities of the dynamic mode controller, this research aims to optimize key process variables, respond effectively to disturbances, and ensure stable and efficient operation of the ammonia production unit. The study will focus on the design, implementation, and evaluation of the dynamic mode controller, considering factors such as control parameter tuning, controller robustness, and adaptability to changing operating conditions.

Through the development and application of an advanced control strategy, this research seeks to contribute to the advancement of ammonia production processes, promote sustainability, and enable more efficient and optimized industrial practices.

1.3 SCOPE OF PROJECT

The scope of this thesis project encompasses the design, implementation, and evaluation of a dynamic mode controller (DMC) for an ammonia production unit. The project will focus on addressing the control challenges specific to the ammonia production process and aims to enhance the overall performance, efficiency, and stability of the production unit.

- Control Strategy Development: The project will involve the development of a dynamic mode controller for the ammonia production unit. The controller will utilize advanced control algorithms, such as model predictive control (MPC) or generalized predictive control (GPC), to optimize key process variables and improve control performance.
- Process Modelling and Identification: A mathematical model of the ammonia production unit will be developed, capturing the system's dynamics and interactions. If necessary, model identification techniques will be employed to estimate model parameters based on available data or experimental measurements. The model will serve as a foundation for the controller design and subsequent evaluation.
- Controller Implementation: The designed dynamic mode controller will be implemented in a simulation environment or a suitable control system platform. The controller will be integrated into the existing control infrastructure of the ammonia production unit, ensuring compatibility with sensors, actuators, and real-time operation.

- Performance Evaluation and Optimization: The performance of the dynamic mode controller will be evaluated through simulation studies and/or experiments on the actual production unit. The controller's ability to meet performance objectives, such as process stability, disturbance rejection, and set point tracking, will be assessed. Sensitivity analysis and tuning techniques will be applied to optimize the controller's performance.
- Comparative Analysis: The effectiveness of the dynamic mode controller will be compared with existing control strategies or conventional control approaches employed in the ammonia production unit. Key performance indicators, including product quality, energy consumption, and process stability, will be analyzed to determine the improvements achieved by the dynamic mode controller.
- Documentation and Reporting: The findings, methodology, and conclusions of the project will be documented in a detailed report or thesis. The report will provide an overview of the project objectives, the methodology followed, the results obtained, and any recommendations for further improvements or future research.

It is important to note that this thesis project will primarily focus on the control aspects of the ammonia production unit and the application of a dynamic mode controller. While process optimization and energy efficiency are essential considerations, the project's scope may not include extensive optimization algorithms or energy management systems unless directly related to the dynamic mode controller design.

Additionally, the project's scope may be influenced by the availability of data, resources, and access to the actual ammonia production unit for experimentation. The project will aim to provide practical insights and recommendations while considering the limitations and constraints of the research context.

1.4 RELEVANCE OF THE PROJECT

The project on the design and implementation of a dynamic mode controller (DMC) for an ammonia production unit holds significant relevance due to several key factors:

- Enhanced Process Control: The ammonia production process is complex and involves various interdependent variables. The application of a dynamic mode controller can significantly improve process control by optimizing key variables such as temperature, pressure, and reactant flow rates. Enhanced control leads to improved process efficiency, stability, and product quality.

- Operational Efficiency and Cost Reduction: By implementing an effective dynamic mode controller, the ammonia production unit can achieve greater operational efficiency. The controller optimizes control inputs, minimizing energy consumption, and reducing waste. This leads to cost savings through improved resource utilization, decreased downtime, and increased production capacity.
- Product Quality Assurance: Ammonia is a critical component in various industries, including agriculture and chemical manufacturing. Consistency in product quality is crucial for meeting industry standards and ensuring customer satisfaction. The dynamic mode controller aids in maintaining stable process conditions, resulting in consistent product quality and reducing the risk of product variations.
- Disturbance Rejection and Robustness: Ammonia production processes are susceptible to disturbances such as variations in feedstock properties, changes in operating conditions, and external factors. The dynamic mode controller's ability to predict and adapt to disturbances enhances the system's robustness, allowing for more effective disturbance rejection and improved process stability.
- Sustainability and Environmental Impact: The implementation of a dynamic mode controller can contribute to sustainable practices in the ammonia production unit. By optimizing energy consumption and reducing waste, the controller helps minimize the environmental impact associated with the production process. This aligns with the growing global focus on sustainability and reducing carbon footprints.
- Advancement of Control Strategies: The project contributes to the advancement of control strategies in the field of ammonia production. By exploring the application of a dynamic mode controller and evaluating its performance, the project provides valuable insights and recommendations for optimizing control systems in similar industrial processes.
- Industrial Relevance and Practical Application: The project's relevance extends beyond academic research, as it directly addresses the control challenges faced in

ammonia production units. The outcomes of the project can be implemented in real-world industrial settings, offering practical benefits to ammonia production facilities, optimizing their operations, and improving their competitiveness.

CHAPTER 2

PROCESS DESCRIPTION

By focusing on the design and implementation of a dynamic mode controller for ammonia production units, this thesis project addresses the industry's need for improved control strategies, enhanced operational efficiency, and consistent product quality. It contributes to the broader goal of optimizing industrial processes, promoting sustainability, and achieving cost-effective production in the ammonia production sector.

2.1 Ammonia Production

Different procedures are followed to produce ammonia worldwide. The main procedure to produce ammonia has been Haber process since its development. Earlier processes like Frank-Caro process, Dry distillation and Birkeland-Eyde process, etc. were used for making ammonia but they have become obsolete due to their inefficiency. Due to significant environmental impacts of the Haber-Bosch process, some novel sustainable processes have been developed and are the main focus of research in ammonia production industry. Major process designs for ammonia production includes ThyssenKrupp, Kellogg’s Process, Haldor Topsøe process and Linde Ammonia Technology. All of these processes have their advantages and disadvantages and all of them use Haber-Bosch process in the Ammonia synthesis reactors. We are also utilising the Kellogg’s process for ammonia production using Natural Gas as feedstock for this study. As hydrogen obtained from natural gas reforming still has the lowest cost. But we have also discussed an alternative process for ammonia production which utilizes electro catalysis of water.

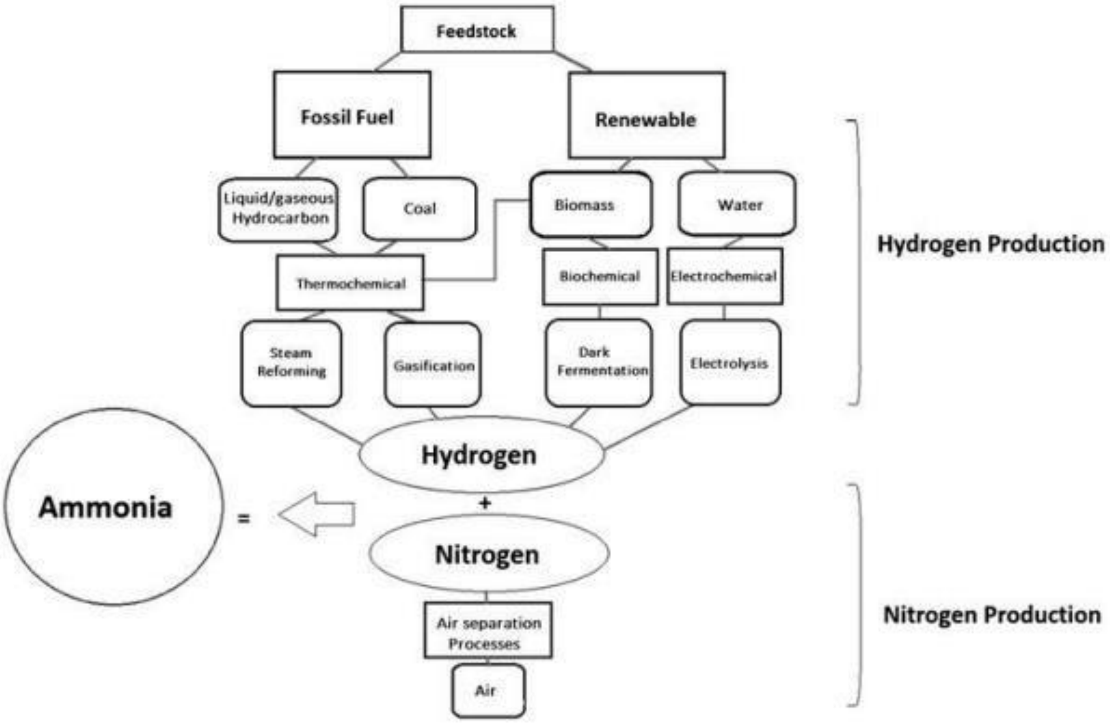


Figure 1: Ammonia Production Routes

2.1.1 Kellogg's Process

This process first desulphurizes natural gas from any sulphur content. Then this natural gas is converted into syngas by Kellogg's steam reforming process in reformers. Steam and natural gas are combined in reformer to produce hydrogen. The carbon dioxide and carbon monoxide produced because of reforming reactions are then removed in water gas shift reactions, carbon dioxide adsorption columns and methanator. Finally, the cleaned syngas is pressurised by a centrifugal compressor and then fed into ammonia synthesis converter. Here nitrogen and hydrogen are combined to form ammonia in the presence of iron catalyst through Haber-Bosch process. Ammonia produced through synthesis reactor is sent to a refrigeration loop where it is liquefied and separated from unreacted reactants. This process utilizes centrifugal compressors as much as possible to consume less energy. Waste heat recovery technology is also used especially after secondary reformer and high temperature shift reactor.

Front End:

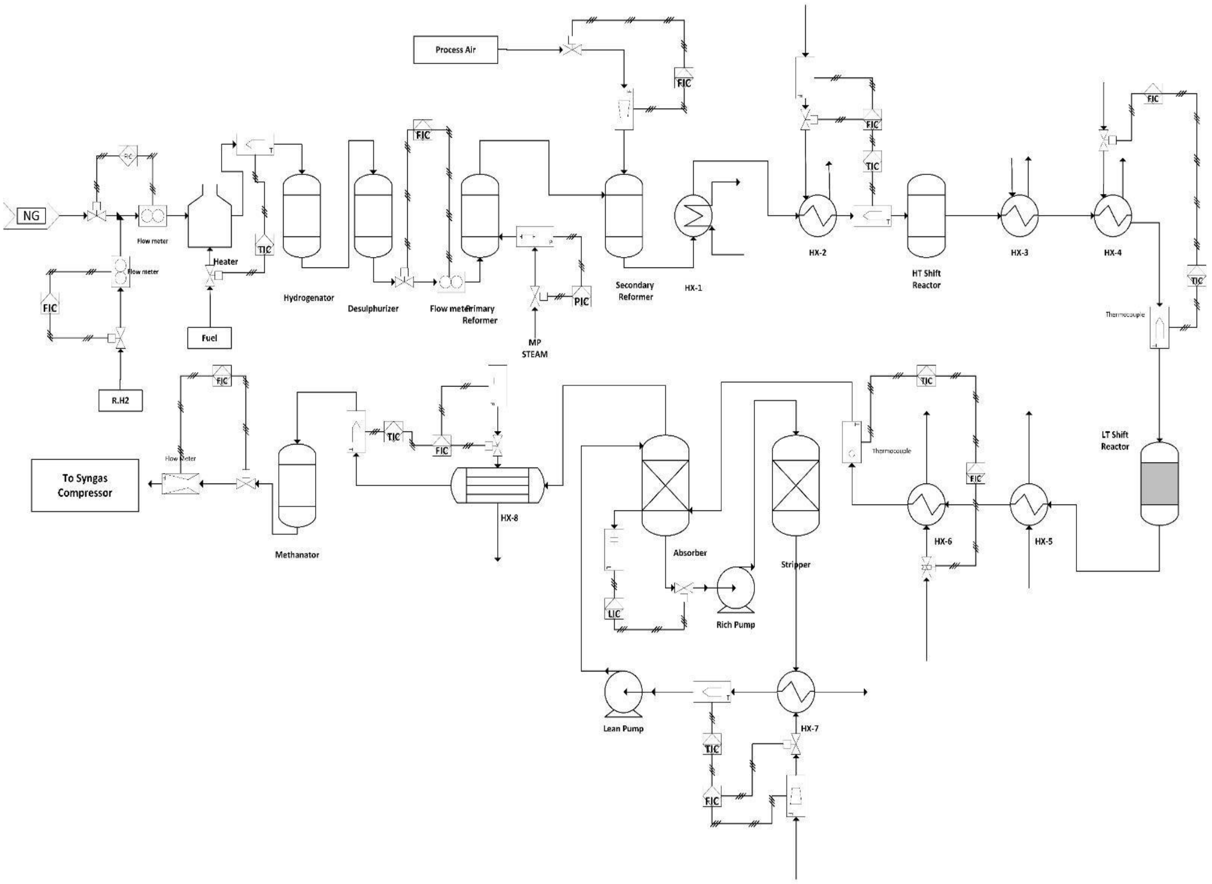


Figure 2: Front end PFD for Kellogg's Process

Backend:

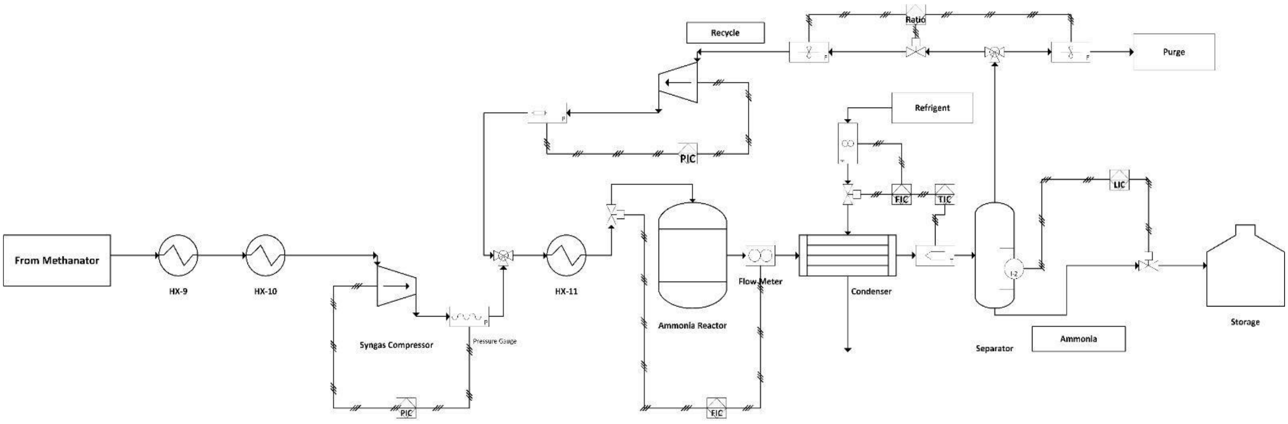


Figure 3: Back end PFD for Kellogg's Process

Following major operations are performed in this process:

2.1.2 Hydrogenator

Feed gas enters at high pressure and contains about 94% methane, 4% nitrogen and 10 ppm of organic sulphur. This sulphur is converted into H_2S by a hydrogen rich stream coming from syngas compressor. Cobalt molybdate or Nickel molybdate are used as catalysts for this reaction. It converts all of the organic sulphur into hydrogen sulphide.

2.1.3 Desulphurizer

It consists of a vessel containing ZnO beds. The hydrogen sulphide present in the natural gas is absorbed on these beds and the gas leaves the desulphurizer at 0.25 ppm of sulphur.

2.1.4 Primary Reformer

In primary reformer most of the hydrocarbons present in the natural gas are converted into hydrogen, carbon dioxide and carbon monoxide by steam methane reformation reaction.

$$CH_4 + H_2O \rightleftharpoons CO + 3H_2$$

Steam and heated natural gas are passed through metallic nickel catalyst and are converted to water and oxides of carbon. Temperature of primary reformer is about 820 °C. 9-10% methane content remains at the outlet of the primary reformer. Reforming is an endothermic reaction.

2.1.5 Secondary Reformer

It is a refractory lined vessel. Feed coming from primary reformer enters secondary reformer and combines with process air coming from compressor.

$$CH_4 + H_2O \rightleftharpoons CO + 3H_2$$

The compressed air burns at a burner gun at the inlet of the secondary reformer. This burning increases the temperature as well as separates nitrogen from oxygen. Again, steam methane reforming takes place in the presence of metallic nickel catalyst. Leaving gas is at 1000 °C and contains 0.3-0.4%of methane.

2.1.6 High Temperature Shift Reactor

The outlet gas of secondary reformer contains about 7.5% carbon dioxide and 12.5% carbon monoxide.

$$CO + H_2O \rightarrow CO_2 + H_2$$

In high temperature shift reactor, this carbon monoxide reacts with steam already mixed with the gas to form carbon dioxide through water gas shift reaction. It is an exothermic reaction, and the gas leaves the reactor at 430 °C and contains 3.1% carbon monoxide. Reduced iron is used as a catalyst in the high temperature shift reactor.

2.1.7 Low Temperature Shift Reactor

The syngas is passed through heat exchangers to reduce its temperature and recover the waste heat.

$$CO + H_2O \rightarrow CO_2 + H_2$$

The gas enters the low temperature shift reactor at 242°C and leaves at 255 °C because of exothermic reaction. Here the same water gas shift reaction takes place but with different copper catalyst and at a lower temperature. The carbon monoxide content is reduced to 0.5%.

2.1.8 CO_2 Absorber

The carbon dioxide content of the syngas has increased to 17.5% after shift reactors and is reduced to 0.1% in an absorption column utilising catacarb solution. The catacarb solution consists of 25% potassium carbonate with additives to inhibit corrosion and foaming. The syngas enters from the bottom of absorber, comes into intimate contact with lean catacarb solution flowing downwards throgh the packed beds of absorption column. CO_2 is absorbed by the catacarb solution during this counter current contact and the rich catacarb solution leaves through the bottom of the absorber.

2.1.9 Stripper

In the stripping section, the CO_2 absorbed in the rich catacarb solution is stripped by flashing under low pressure and by heating the solution. The lean catacarb solution is regenerated and cooled before being sent to absorber. While the CO_2 maybe vented or sent to another process of the plant.

2.1.10 Methanator

In methanator, the leftover carbon dioxide and carbon monoxide in the syngas are converted to methane and water by methanation reaction. It is the opposite of reforming reaction. Nickel is used to catalyse this reaction. The outlet gas of methanator contains less than 10 ppm of the oxides of carbon. These reactions are highly exothermic.

$$CO + 3H_2 \rightarrow CH_4 + H_2O$$

$$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$$

2.1.11 Syngas Compressor

Two case barrel type compressor is used to compress the syngas to bring it to its reaction pressure. Ammonia synthesis reaction being reversible requires high pressure of about 200-300 atms. It is driven by two turbines in tandem. Centrifugal compressor is used here to minimise the energy consumption and make the process more efficient.

2.1.12 Ammonia Synthesis Reactor

It is the main part of ammonia plant. Here Haber-Bosch process is used to form ammonia. Compressed syngas is fed into the ammonia reactor and forms ammonia under high pressure and temperature.

$$N_2 + 3H_2 \rightleftharpoons 2NH_3$$

It is a reversible reaction which gives only 12-15% conversion. A recycle stream is therefore used to increase the overall conversion of ammonia to reactor to 98%. A purge stream is introduced to purge the recycle of inert components and prevent the build-up of inert components in the recycle loop. Reduced iron catalyst modified with aluminium, magnesium and potassium oxides is used to catalyse this reaction. It is a highly exothermic reaction and requires an internal heat exchanger or some sort of quenching.

2.1.13 Ammonia Refrigeration

Ammonia produced above is liquefied and separated from reactants in a refrigeration loop. The refrigeration loop utilises cold ammonia as a refrigerant. The liquid ammonia is then stored in insulated storage tanks.

2.2 Alternate Ammonia Process

As the world is moving to more sustainable processes, it is essential that ammonia production industry keeps pace with the rising tide of sustainability and efficiency. Reforming of natural gas generates significant amounts of carbon dioxide which is the top contributor to global warming. To produce cleaner hydrogen and thus cleaner and environment friendly ammonia, we propose the combination of Kellogg's process with electrolysis of water.

2.2.1 Electrolysis of water

In this process alkaline water can be electrolysed into hydrogen and oxygen in an electrochemical cell with the help of electric current.

$$2H_2O(l) \rightarrow 2H_2(g) + O_2(g)$$

The electricity coverts water into hydrogen and oxygen while coagulating any impurities. These impurities are then removed though gravity separators and clean hydrogen is produced without any harmful by-products. This hydrogen is then sent to ammonia synthesis reactor which combines hydrogen with nitrogen to form ammonia through Haber-Bosch process. This process becomes further clean if renewable sources of electricity production are used.

2.2.2 Non-Thermal Plasma Synthesis

This alternative has the advantage of operating at temperatures around 50ºC and atmospheric pressure conditions. This solves some of the problems posed by HB since the reduction of these conditions has a direct impact on the cost of energy and fossil fuels. However, it comprises two challenges yet to be developed (A review on the non-thermal plasma-assisted ammonia synthesis, 2018).

- Nitrogen gas fixation
- Reverse reactions

In addition, the state of conversion and efficiency still needs to be advanced, so it is in the small and medium scale development phase.

2.2.3 Functional catalyst with nitrogenase motivated peptide

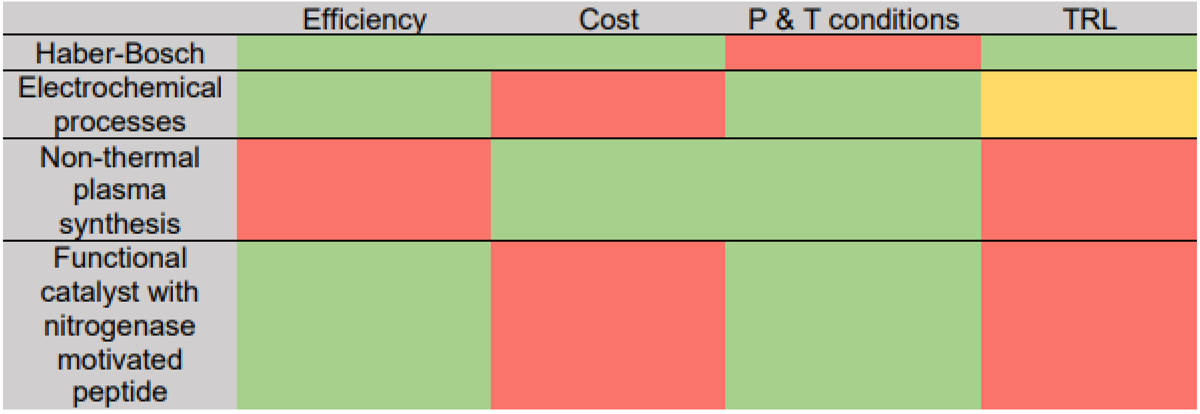
Ammonia is produced in nature by nitrogenase enzymes with an efficiency of about 75%. Since this percentage is very high, it is intended to use these enzymes for the industrial production of NH3. This type of ammonia synthesis is very promising but its low temperatures and working pressures present an efficiency of less than 1%, which requires catalysts to improve this efficiency (Renner, et al., 2020). On the other hand, peptide functional catalyst has been developed and tested in anion exchange-based systems. The materials used for such a catalyst show promising results compared to conventional catalysts.

2.4 Discussion of the selected technology

In accordance with the previous description, different alternatives exist to carry out a complete and reliable process of ammonia synthesis being necessary to select the best one in order to suit the proposed project.

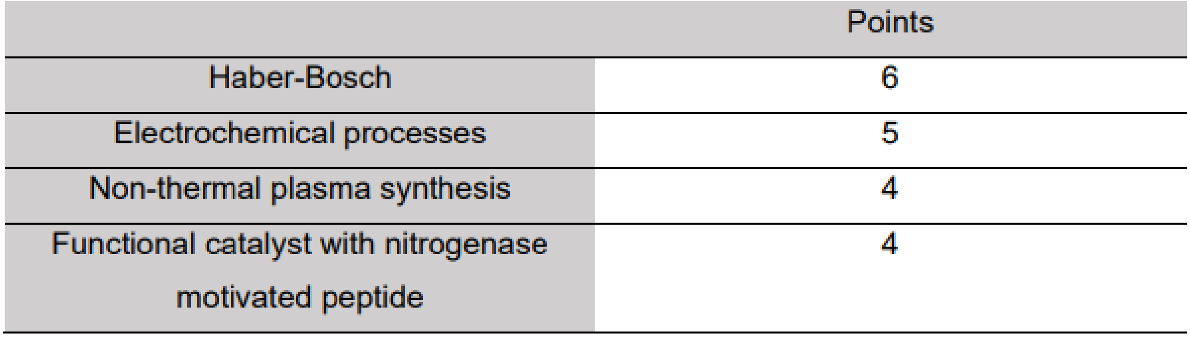
The process to be carried out is then selected under qualitative and subjective comparing different factors that influence production. Based on different articles, research and reports, using the same weighting technique as in Table 1 and Table 2: (green=good (2 points), yellow=acceptable (1 point), red=bad (0 points)) results are obtained in Table 1 and 2:

Table 1: Ammonia production comparison



	Efficiency	Cost	P & T conditions	TRL
Haber-Bosch	🟩	🟩	🟥	🟩
Electrochemical processes	🟩	🟥	🟩	🟨
Non-thermal plasma synthesis	🟥	🟩	🟩	🟥
Functional catalyst with nitrogenase motivated peptide	🟩	🟥	🟩	🟥

Table 2: Production technologies ranking



	Points
Haber-Bosch	6
Electrochemical processes	5
Non-thermal plasma synthesis	4
Functional catalyst with nitrogenase motivated peptide	4

Despite using Haber-Bosch process due to more practicality to implement the dynamic mode controller in Pakistan’s current ammonia industry landscape, a sustainable alternative for future means can be suggested.

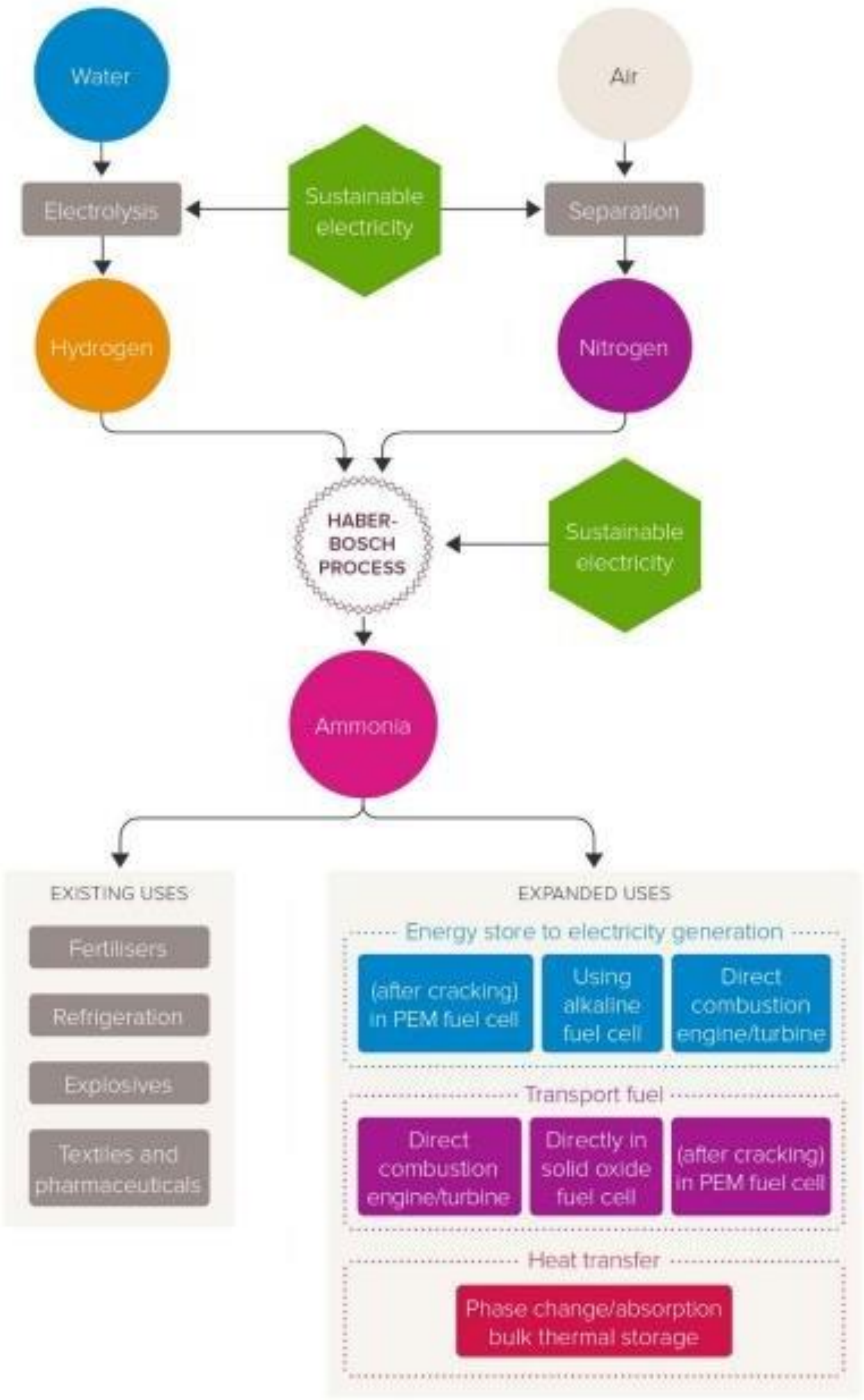


Figure 4: Ammonia production alternative for Pakistan's future needs

CHAPTER 3

MATERIAL AND ENERGY BALANCE

3.1 Material Balance:

Basis

1 hour of steady state operation in an open system.

Formulas

$$Mass\ Out = Mass\ In + Generation - Consumption - Accumulation$$

$$X_A = \frac{(N_{A_0} - N_A)}{N_{A_0}} \qquad \xi = \frac{(n_i - n_{io})}{\gamma}$$

3.1.1 Hydrogenator

Reactions

$$CH_3 - SH + H_2 \rightarrow CH_4 + H_2S$$

Table 3 Hydrogenator Mass Balance

Streams	NG		H2	OUTLET	
Species	Molar Flow	Mass Flow	Molar Flow	Molar Flow	Mass Flow
Nitrogen	17.4	487.6	7.7	25.1	702.3
Hydrogen	0.0	0.0	322.0	321.9	643.7
Argon	1.4	55.3	0.0	1.4	55.3
CO	0.0	0.0	0.0	0.0	0.0
CO2	146.4	6439.6	0.0	146.4	6439.6
H2S	0.0	0.0	0.0	0.1	4.7
Methane	1191.4	19062.8	0.0	1191.6	19065.0

Ethane	19.8	592.9	0.0	19.8	592.9
Propane	2.8	121.9	0.0	2.8	121.9
n-Butane	1.4	80.3	0.0	1.4	80.3
n-Pentane	1.4	99.7	0.0	1.4	99.7
M-Mercaptan	0.1	6.6	0.0	0.0	0.0
TOTAL	1382.0	26946.6	329.7	1711.7	27805.4

3.1.2 Desulphurizer

Reactions

$$ZnO + H_2S \rightarrow ZnS + H_2O$$

Table 4 Desulphurizer Mass Balance

Streams	Inlet		Outlet	
Species	Molar Flow	Mass Flow	Molar Flow	Mass Flow
Nitrogen	25.1	702.3	25.1	702.3
Hydrogen	321.9	643.7	321.9	643.7
Argon	1.4	55.3	1.4	55.3
CO	0.0	0.0	0.0	0.0
CO2	146.4	6439.6	146.4	6439.6
H2S	0.1	4.7	0.0	0.1
Methane	1191.6	19065.0	1191.6	19065.0

Ethane	19.8	592.9	19.8	592.9
Propane	2.8	121.9	2.8	121.9
n-Butane	1.4	80.3	1.4	80.3
n-Pentane	1.4	99.7	1.4	99.7
H2O	0.0	0.0	0.1	2.4
TOTAL	1711.7	27805.4	1711.7	27803.2

3.1.3 Primary Reformer

Reactions

$$CH_4 + H_2O \rightarrow CO + 3H_2$$

$$C_2H_6 + 2H_2O \rightarrow 2CO + 5H_2$$

$$C_3H_8 + 3H_2O \rightarrow 3CO + 7H_2$$

$$C_4H_{10} + 4H_2O \rightarrow 4CO + 9H_2$$

$$C_5H_{12} + 5H_2O \rightarrow 5CO + 11H_2$$

$$CO + H_2O \rightarrow CO_2 + H_2$$

Table 5 Primary Reformer Mass Balance

Streams	Inlet		Steam		Outlet	
Species	Molar Flow	Mass Flow	Molar Flow	Mass Flow	Molar Flow	Mass Flow
Nitrogen	25.1	702.3	0	0	25.1	702.3
Hydrogen	321.9	643.7	0	0	3038.8	6077.6

Argon	1.4	55.3	0	0	1.38	55.3
CO	0.0	0.0	0	0	348.8	9767.41
CO2	146.4	6439.6	0	0	572.7	25199
H2S	0.1	0.1	0	0	0.1	0.1
Methane	1191.6	19065.0	0	0	476.6	7626
Ethane	19.8	592.9	0	0	0	0
Propane	2.8	121.9	0	0	0	0
n-Butane	1.4	80.3	0	0	0	0
n-Pentane	1.4	99.7	0	0	0	0
H2O	0.1	2.4	1887.9	33982.1	686.5	12356.7
TOTAL	1711.7	27805.4	1887.9	33982.1	5149.9	61784.7

3.1.4 Secondary Reformer

Reactions

$$CH_4 + H_2O \rightarrow CO + 3H_2$$

$$CH_4 + O_2 \rightarrow CO_2 + 2H_2$$

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

Table 6 Secondary Reformer Mass Balance

STREAMS	Feed Inlet		Air		Outlet	
Species	Molar Flow	Mass Flow	Molar Flow	Mass Flow	Molar Flow	Mass Flow
Nitrogen	25.1	702.3	1171.2	32793.6	1196.3	33495.9
Hydrogen	3038.8	6077.7	0.0	0.0	3900.8	7801.6
Argon	1.4	55.3	14.1	564.0	15.5	619.3

CO	348.8	9767.4	0.0	0.0	754.0	21111.1
CO2	572.7	25199.2	0.0	0.0	641.7	28235.2
H2S	0.0	0.1	0.0	0.0	0.0	0.1
Methane	476.6	7626.0	0.0	0.0	2.5	39.9
H2O	686.5	12356.7	0.0	0.0	772.8	13909.6
O2	0.0	0.0	314.7	10070.4	0.0	0.0
TOTAL	5149.9	61784.7	1500.0	43428.0	7283.5	105212.7

3.1.5 High Temperature Shift Reactor

Reactions

$$CO + H_2O \rightarrow CO_2 + H_2$$

Table 7 HTS Mass Balance

STREAMS	FEED INLET		OUTLET	
Species	Molar Flow	Mass Flow	Molar Flow	Mass Flow
Nitrogen	1196.3	33495.9	1196.3	33495.9
Hydrogen	3900.8	7801.6	4466.3	8932.6
Argon	15.5	619.3	15.5	619.3
CO	754.0	21111.1	188.5	5277.8
CO2	641.7	28235.2	1207.2	53116.1
H2S	0.0	0.1	0.0	0.1
Methane	2.5	39.9	2.5	39.9
H2O	772.8	13909.6	207.3	3731.0
TOTAL	7283.5	105212.7	7283.5	105212.7

3.1.6 Low Temperature Shift Reactor

Reactions

$$CO + H_2O \rightarrow CO_2 + H_2$$

Table 8 LTS Mass Balance

STREAMS	FEED INLET		OUTLET	
Species	Molar Flow	Mass Flow	Molar Flow	Mass Flow
Nitrogen	1196.2	33495.9	1196.3	33495.9
Hydrogen	4466.2	8932.6	4635.9	9271.9
Argon	15.5	619.3	15.4	619.2
CO	188.5	5277.8	18.8	527.7
CO2	1207.2	53116.1	1376.8	60580.3
H2S	0	0.1	0.	0.1
Methane	2.5	39.9	2.5	39.9
H2O	207.3	3731.0	37.6	677.5
TOTAL	7283.5	105212.7	7283.5	105212.7

3.1.7 Absorber

Reactions

$$K_2CO_3 + CO_2 + H_2O \rightarrow 2KHCO_3$$

Table 9 Absorber Mass Balance

STREAMS	FEED INLET		OUTLET	
Species	Molar Flow	Mass Flow	Molar Flow	Mass Flow
Nitrogen	1196.3	33495.9	1196.3	33495.9
Hydrogen	4635.9	9271.9	4635.9	9271.9
Argon	15.5	619.3	15.5	619.3
CO	18.8	527.8	18.8	527.8

CO2	1376.8	60580.4	27.5	1211.6
H2S	0.0	0.1	0.0	0.1
Methane	2.5	39.9	2.5	39.9
H2O	37.6	677.5	37.6	677.5
K2CO3	0.0	0.0	0.0	0.0
KHCO3	0.0	0.0	0.0	0.0
TOTAL	7283.5	105212.7	5934.2	45843.9

Table 10 Absorber Mass Balance 2

STREAMS	LEAN Catacarb Solution INLET		RICH Catacarb Solution OUT	
Species	Molar Flow	Mass Flow	Molar Flow	Mass Flow
Nitrogen	0.0	0.0	0.0	0.0
Hydrogen	0.0	0.0	0.0	0.0
Argon	0.0	0.0	0.0	0.0
CO	0.0	0.0	0.0	0.0
CO2	0.0	0.0	0.0	0.0
H2S	0.0	0.0	0.0	0.0
Methane	0.0	0.0	0.0	0.0
H2O	1349.3	24287.2	0.0	0.0
K2CO3	1349.3	186478.6	0.0	0.0
KHCO3	0.0	0.0	2698.6	270168.4
TOTAL	2698.6	210765.9	2698.6	270168.4

3.1.8 Stripper

Reactions

$$2KHCO_3 \rightarrow K_2CO_3 + CO_2 + H_2O$$

Table 11 Stripper Mass Balance

STREAMS	RICH Catacarb Solution IN		LEAN Catacarb Solution OUT		CO2 OUT	
Species	Molar Flow	Mass Flow	Molar Flow	Mass Flow	Molar Flow	Mass Flow
KHCO3	2698.5	270168.3	0	0	0	0
K2CO3	0	0	1349.3	186478.6	0	0
H2O	0	0	1349.3	24287.2	0	0
CO2	0	0	0	0	1349.3	59368.8
TOTAL	2698.5	270168.3	2698.6	210765.8	1349.3	59368.8

3.1.9 Methanator

Reactions

$$CO + 3H_2 \rightarrow CH_4 + H_2O$$

$$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$$

Table 12 Mehanator Mass Balance

STREAMS	FEED INLET		OUTLET	
Species	Molar Flow	Mass Flow	Molar Flow	Mass Flow
Nitrogen	1196.3	33495.9	1196.2	33495.9
Hydrogen	4635.93	9271.8	4469.2	8938.5
Argon	15.5	619.2	15.5	619.2
CO	18.8	527.7	0	0
CO2	27.5	1211.6	0	0
H2S	0.0	0.1	0.0	0.1

Methane	2.5	39.9	48.9	782.1
H2O	37.6	677.4	111.6	2008.1
TOTAL	5934.2	45843.9	5841.4	45843.9

3.1.10 Ammonia Synthesis Reactor

Reactions

$$N_2 + 3H_2 \rightarrow 2NH_3$$

Table 13 Ammonia Reactor Material Balance

STREAMS	FEED INLET		MIX		RECYCLE		REACTOR OUTLET	
Species	Molar Flow	Mass Flow	Molar Flow	Mass Flow	Molar Flow	Mass Flow	Molar Flow	Mass Flow
Nitrogen	1196.3	33496	3279.9	91838.5	2214.0	61991.0	2460.0	68879
Hydrogen	4469.2	8939	11511.8	23023.5	8146.6	16293.2	9051.8	18104
Argon	15.5	619.3	50.1	2002.2	45.1	1802.0	50.1	2002.2
Methane	48.9	782.1	104.8	256.0	94.3	230.4	104.8	256.0
NH3	0.0	0.0	0.0	0.0	0.0	0.0	1640.0	27880
H2S	0.0	0.1	0.0	0.3	0.0	0.1	0.0	0.1
TOTAL	5729.9	43836	14946.6	117121	10500	80316.8	13307	117120

STREAMS	PURGE		TO SPLITTER		TO STORAGE	
Species	Molar Flow	Mass Flow	Molar Flow	Mass Flow	Molar Flow	Mass Flow
Nitrogen	246.0	6887.9	2460.0	68878.9	0.0	0.0

Hydrogen	905.2	1810.4	9051.8	18103.6	0.0	0.0
Argon	5.0	200.2	50.1	2002.2	0.0	0.0
Methane	10.5	25.6	104.8	256.0	0.0	0.0
NH3	0.0	0.0	0.0	0.0	1640.0	27879.5
H2S	0.0	0.0	0.0	0.1	0.0	0.0
TOTAL	1166.7	8924.1	11666.6	89240.9	1640.0	27879.5

3.2 Energy Balance:

Energy balance is applied on each equipment using the standard formulae for calculation of work and heat duty. Energy balance is applied on reactor by using standard heat of reactions.

First law of thermodynamics was used:

$\Delta E = \Delta KE + \Delta PE + \Delta U = Q - W$

Overall energy balance equation was used to calculate heat duty:

$\Delta\dot{H}=\xi\,\Delta\dot{H}^{\circ}_{r}+\sum\dot{n}_{out}\cdot H_{out}-\sum\dot{n}_{in}\cdot H_{in}$

3.2.1 Hydrogenator:

Table 14 Hydrogenator Energy Balance

		Inlet T 399 °c	Ref T 25 °c	Out T 401 °c
Hydrogenator	INLET		OUTLET	
Components	Mole Percent	Molar FLOW kgmol	Mole Percent	Molar FLOW kgmol
Nitrogen	1.02	17.41	1.46	25.08
Hydrogen	18.89	322	18.80	321.86
Argon	0.08	1.38	0.08	1.38
CO	0	0	0	0
CO2	8.58	146.35	8.55	146.35
H2S	0	0	0.008	0.13
Methane	69.91	1191.42	69.61	1191.5
Ethane	1.15	19.76	1.15	19.76

Propane	0.16	2.76	0.16	2.76
n-Butane	0.08	1.38	0.08	1.38
n-Pentane	0.08	1.38	0.08	1.38
M-Mercaptan	0.008	0.13	0	0
TOTAL	100	1704	100	1711.6
Cp of NG	51.62	kj/kgmol	Cp out	51.62 KJ/Kgmol
Hin	32897220	Kj/hr	Hout	33054131 KJ/hr

$CH_3\text{-}SH+H_2 \rightarrow CH_4+H_2S$

Heat of reaction	-72000	kj/kgmol				
ΔH_{298}	-99504	KJ/hr	Heat Duty	$\Delta H^{\cdot}$	57407.74	kj/hr

3.2.2 Primary Reformer:

Table 15 Primary Reformer Energy Balance

PRIMARY REFORMER		In T	716 °c		Out T	1044 °c		Ref 25 °c
Component	Mol Frac	Kg mol/hr	Cp kj/kgmol °c	Hi (KJ/hr)	Mol Frac	Kg mol/hr	Cp (kJ/kgmol °c	Hout (kj/hr)
Nitrogen	0.006	25.08	33.35	349670	0.004	25.08	34.33	642440.7
Hydrogen	0.08	321.8	30.58	4E+06	0.59	3038.8	32.50	73684462
Argon	0.0003	1.38	20.93	12091	0.0003	1.38	20.93	21578.24
CO	0	0	33.71	0	0.06	348.83	37.10	9656663
CO2	0.04	146.3	51.62	3E+06	0.11	572.70	48.83	20864770
H2S	7.6E-07	0.002	46.13	53.297	5E-07	0.002	52.94	109.1667
Methane	0.33	1191.6	80.34	4E+07	0.09	476.62	100.4	35697184
Ethane	0.005	19.76	119.2	984858	0	0	0	0
Propane	0.0007	2.76	188.3	217605	0	0	0	0
n-Butane	0.00038	1.38	212.6	122821	0	0	0	0
n-Pentane	0.00038	1.38	196.6	113552	0	0	0	0

H_2O	0.52	1887.1	47.7	4E+07	0.13	686.48	55.71	28560507
TOTAL	1	3598.7	1098	9E+07	1	5149.94		1.69E+08
				86736 MJ/hr				169127.7

1	$CH_4+H_2O \rightarrow CO + 3H_2$	Conv 60 %	Reac 1	210	MJ/kg	Reac 4	650	MJ/kg
2	$C_2H_6+2H_2O \rightarrow 2CO + 5H_2$	100 %	ΔH298	150137	MJ/hr	$\Delta H298$	3593.2	MJ/hr
3	$C_3H_8+3H_2O \rightarrow 3CO + 7H_2$	100 %	Reac 2	350	MJ/kg	Reac 5	800	MJ/Kg
4	$C_4H_{10}+4H_2O \rightarrow 4CO + 9H_2$	100 %	$\Delta H298$	13834	MJ/hr	$\Delta H298$	5528	MJ/hr
5	$C_5H_{12}+5H_2O \rightarrow 5CO + 11H_2$	100 %	Reac 3	500	MJ/Kg	Reac 6	-41	MJ/kg
6	$CO+H_2O \rightarrow CO_2 + H_2$	55%	$\Delta H298$	4146	MJ/hr	$\Delta H298$	-17480.6	Mj/hr
		$\Delta \dot{H}=\xi\Delta \dot{H}^{\circ}_{r}+\sum \dot{n}_{out}\cdot \hat{H}_{out}-\sum \dot{n}_{in}\cdot \hat{H}_{in}$						

	Heat Duty	$\Delta H^{\cdot}$	242149	MJ/hr				

3.2.3 Secondary Reformer:

Table 16 Secondary Reformer Energy Balance

	SECONDARY REFORMER			Ref T	25 °c				
	STREAMS	FEED INLET	In T	1096 °c		Out T	918.4 °c		
Sr.No.	Components	Mole Percent	Kgmol/hr	Cp kJ/kgmol °c	Hi Kj/hr	Mole Perc	Kgmol/hr	Cp	Hout (kJ/hr)
1	Nitrogen	17.98	1196.28	34.68	44433450.5	16.42	1196.28	34.56	36944222.36
2	Hydrogen	45.69	3038.82	35.10	114258565.4	53.55	3900.81	33.59	117078547
3	Argon	0.23	15.48	20.93	347044.97	0.21	15.48	20.93	289495.78
4	CO	5.24	348.83	41.22	15402220.79	10.35	753.96	38.87	26187833.34
5	CO2	8.61	572.70	39.95	24505870.75	8.81	641.70	45.57	26127410.4

6	H_2S		4.15E-05	0.002	60.33	178.60	3.7E-05	0.002	56.20	138.79
7	Methane		7.16	476.62	121.04	61787596.83	0.03	2.49	109.63	244253.83
8	H_2O		10.32	686.48	57.12	82915.55	10.60	772.75	52.44	36203588.4
9	O_2		4.73	314.7	32.56	10977282.02	0	0	33.51	0
10	TOTAL		100	6649.94		271795125.5		7283.50		243075489.9
						271795.12	MJ/hr			243075.48
	Reac 1	210 MJ/kgmol			$CH_4+H_2O \rightarrow CO+3H_2$ 85% conv					MJ/hr
	ΔH298	85077.4	MJ/hr		$CH_4+O_2 \rightarrow CO_2+2H_2$					
	Reac 2	-320	MJ/kgmol		$2H_2+O_2 \rightarrow 2H_2O$					
	ΔH298	-22080	MJ/hr	$\Delta \dot{H}=\xi\Delta \dot{H}^{\circ}_r+\sum \dot{n}_{out}\cdot\hat{H}_{out}-\sum \dot{n}_{in}\cdot\hat{H}_{in}$						
	Reac 3	-480	MJ/kgmol							
	ΔH298	4146	MJ/hr		Heat Duty	$\Delta \dot{H}$	38423	MJ/hr		

3.2.4 Hight Temp shift Reactor:

Table 17 HTS Energy Balance

High Temp Shift Reactor		IN T	339 °c			Out T	397°c	
Components	Mole %	Kgmol/hr	Cp (kJ/kgmol°c)	Hi (kJ/hr)	Mole %	Kgmol/hr	Cp kJ/kgmol°c	Hout (kJ/hr)
Nitrogen	16.42	1196.28	31.43	11808665	16.42	1196.28	31.78	14145183
Hydrogen	53.55	3900.81	29.243	35819465	61.32	4466.29	29.38	48827998
Argon	0.21	15.48	20.93	101748	0.21	15.48	20.93	120542
CO	10.35	753.96	30.75	7280169	2.58	188.49	31.14	2183563
CO2	8.81	641.70	47.14	9498975	16.57	1207.18	48.36	21719318
H2S	3.7E-05	0.002	39.10	33	3.7E-05	0.002	40.12	41
Methane	0.03	2.49	58.27	4562	0.03	2.49	61.59	57140

H2O	10.60	772.75	4E+01	9.83E+06	2.84	207.27	41.48	3198664
TOTAL	100	7283.51		7438630	100	7283.51		90252452
				74386	MJ/hr			90252
								MJ/hr
			Reac	CO+H2O→ CO2 +H2		Conv	65%	
					-410	MJ/kg mol		
				ΔH298	-200932.12	MJ/hr		
			ΔH˙=ξΔH˙∘r+∑n˙out·H^out−∑n˙in·H^in					
		Heat Duty	ΔH˙	-185065.97	MJ/hr			

3.2.5 Low Temp Shift Reactor:

Table 18 LTS Energy Balance

			In T	227 °c		OUT T	236 °c	
Components	Mole percent	Kgmol /hr	Cp (kJ/kgmol°c)	Hi kJ/hr	Mole Percent	**Kgmol /hr**	Cp (kJ/kgmol°c)	Hout (kJ/hr)
Nitrogen	16.42	1196.28	30.70	742024	16.42	1196.28	3.08E+01	7.77E+06
Hydrogen	61.32	4466.29	29.02	26187719	63.64	4635.93	2.90E+01	2.84E+07
Argon	0.21	15.48	20.93	65455.72	0.21	15.48	20.93	68372.0
CO	2.58	188.49	30.06	1144764.69	0.25	18.84	3.01E+01	1.20E+05
CO2	16.57	1207.18	44.23	10785847	18.90	1376.82	4.45E+01	1.29E+07
H2S	3.7E-05	0.002	37.17	20.75	3.7E-05	0.002	3.73E+01	2.18E+01
Methane	0.03	2.49	51.9	26149.34	0.03	2.49	5.24E+01	2.76E+04
H2O	2.84	207.27	39.16	1639971.77	0.51	37.63	38.93	309170.25

TOTAL		100	7283.51		47270170.1	100	7283.51		4.96E+07
		Ref T c	25		47270.1701	MJ/hr			4.96E+04
									MJ/hr
			Reac	$CO+H_2O \rightarrow CO_2 + H_2$			65	% conv	
					-410	MJ/kg mol			
				ΔH298	-200932.12	MJ/hr			
				$\Delta\dot{H}=\xi\Delta\dot{H}^{\circ}_{r}+\sum\dot{n}_{out}\cdot\hat{H}_{out}-\sum\dot{n}_{in}\cdot\hat{H}_{in}$					
Heat Duty				$\Delta\dot{H}$	-1.99E+05	MJ/hr			

3.2.6 Methanator:

Table 19 Methanator Energy Balance

INLET				In T	325 °c		Out T	342 °c	
Sr. No.	Components	Mole %	Kgmol/hr	Cp (kJ/kgmol°c)	Hin (kJ/hr)	Mole %	Kgmol/hr	Cp (kJ/kgmol	Hout (kJ/hr)
1	Nitrogen	20.15	1196.28	31.34	11250866	20.47	1196.28	31.45	11928516.55
2	Hydrogen	78.12	4635.93	29.21	40627707	76.50	4469.24	29.25	41440981.27
3	Argon	0.26	15.48	20.93	97211	0.26	15.48	20.93	102720.12
4	CO	0.31	18.84	30.66	173377	0	0	30.77	0
5	CO2	0.46	27.53	46.81	386760.4	0	0	47.21	0
6	H2S	4.6E-05	0.002	38.85	32.21	4.73E-05	0.002	39.15	34.30
7	Methane	0.04	2.49	57.47	42993.28	0.83	48.87	58.44	905546.78
8	H2O	0.63	37.63	40.29	454951	1.90	111.55	40.56	1434623.61

	TOTAL	100	5934.21		53033899	100	5841.44		55812422.66
					53033.9	MJ/hr			55812.42 MJ/hr
		REACTIONS		CONVERSION		ζ			
	Reac 1	$CO+3H_2 \rightarrow CH_4+H_2O$		100		18.8			
		-210	MJ/kgml						
		ΔH_{298}	-3958.32						
	Reac 2	$CO_2+4H_2 \rightarrow CH_4+2H_2O$			100	27.5			
		-160	MJ/Kgml						
				Heat Duty	$\Delta H^{\cdot}$	-1.7E+04			

3.2.7 Ammonia Reactor:

Table 20 Ammonia Reactor Energy Balance

			INLET	In T 380 °c	OUT T 423 °c	
Sr. No.	Components		Mole %	kgmol	Mole %	kgmol
1	Nitrogen		21.94	3279.94	18.48	2459.96
2	Hydrogen		77.01	11511.76	68.02	9051.8
3	Argon		0.33	50.05	0.37	50.05
4	Methane		0.70	104.79	0.78	104.79
5	NH_3		0	0	12.32	1639.97
6	H_2S		5.5E-05	0.008	6.24E-05	0.008
7	TOTAL		100	14946.57	100	13306.59
			Cp kJ/kgmol°c	33.27	Cp kJ/kgmol°c	34.25
			Hin (kJ/hr)	1.77E+08	Hout (kj/hr)	1.81E+08
				Heat of Reac		
Reac	$N_2+3H_2 \rightarrow 2NH_3$		25% conv	-819.98 Kj/kgmol		
	ΔH298	-91000	kJ/kgmol			
			Heat Duty	ΔH˙	4776052	KJ/hr

3.2.8 Heater for primary reformer feed:

Table 21 Heater for Reformer Feed Energy Balance

	INLET	In T 382 °c	OUTLET	Out T 444 °c
Component	Mol Frac	Kg mol	Mol Frac	Kg mol
Nitrogen	0.006	25.08	0.006	25.08
Hydrogen	0.08	321.86	0.08	321.86
Argon	0.0003	1.38	0.0003	1.38
CO	0	0	0	0
CO2	0.04	146.35	0.04	146.35
H2S	7.6E-07	0.002	7.6E-07	0.002
Methane	0.33	1191.56	0.33	1191.56
Ethane	0.005	19.76	0.005	19.76
Propane	0.0007	2.76	0.0007	2.76
n-Butane	0.00038	1.38	0.00038	1.38
n-Pentane	0.00038	1.38	0.00038	1.38
H2O	0.52	1887.13	0.52	1887.13
TOTAL	1	3598.67	1	3598.67
	Cp	42.12	Cp	42.77
	Hin	54112625	Hout	64490433.56 kj/hr
	$\Delta H^{\cdot}$	10377808.56	Kj/hr	

3.2.9 Compressor:

$$\text{Isentropic Power} = ZRT_1 \frac{\gamma}{\gamma - 1}\left(\frac{T2 - T1}{MW}\right) * Q_m$$

$$\text{Isentropic Efficiency} = 75\%$$

$$\text{Actual power required} = \frac{\text{Isentropic power}}{\text{Efficency}}$$

Table 22 Compressor Energy Balance

Multistage Compressor Power		IN	OUT
	Compressor 1		
Qm 43513 kg/hr	Pressure [bar]	26.11	44.21
	Power [kW]	3086.02	
	Actual Power	**3615.87**	**KW**
	Compressor 2		
Qm 43513 kg/hr	Pressure [bar]	44.21	74.17
	Total Rotor [kW]	3724.34	
	Actual Power	**4587.90**	**kW**
	Compressor 3		
Qm 43513 kg/hr	Pressure [bar]	74.17	126.26
	Total Rotor [kW]	4711.95	

	Actual Power	**6037.09**	**kW**

CHAPTER 4

EQUIPMENT DESIGN

4.1 Shell-and-Tube Heat Exchanger:

1. Tube Layout and Size: The tube layout and size must be meticulously chosen to provide sufficient heat transfer area and to accommodate the desired fluid flow rates. Tube diameter, length, and pitch have an effect on heat transfer performance and pressure decrease.
2. Baffles and passes: Baffles are used to improve heat transfer by directing fluid flow and generating turbulence. Overall heat transfer coefficient and pressure drop are affected by the number and design of baffles, as well as the configuration of multiple tube passes.
3. Shell side: The design should take into account the fluid properties, flow rates, and pressure decrease on the shell side. Heat transfer efficacy is affected by the selection of shell-side baffles, inlet and outlet configurations, and flow arrangements (such as parallel or counter-flow).
4. Material Selection: Appropriate material selection is necessary to assure compatibility with the process fluids, temperature, and pressure conditions, and to prevent corrosion, erosion, and fouling.

4.1.1 Design Criteria and Specifications

Design criteria and specifications are crucial for achieving optimal performance and efficient operation in various industrial processes.

4.1.2 Heat Exchanger:

1. Heat Transfer Rate: The heat exchanger should be designed to provide the requisite heat transfer rate based on the heat load and temperature requirements of the process.

2. Fluid Compatibility: The selection of materials must take into account the heat exchanger's compatibility with the process fluids, including factors such as corrosion resistance and thermal expansion.

3. Pressure Drop: The design must guarantee an acceptable pressure drop across the heat exchanger in order to maintain fluid flow efficiency and reduce pumping costs.

4. Proper design should address potential fouling issues, such as scaling or deposition, by implementing features such as adequate cleaning mechanisms or fouling-resistant materials.

4.1.3 Heat Exchanger Design:

Shell and tube heat exchanger design using Kern's method follows a systematic approach to determine the required heat transfer area and size the heat exchanger appropriately. The method involves several steps:

1) Determine the Overall Heat Transfer Coefficient (U):
    - Calculate the individual heat transfer coefficients for the hot and cold fluids inside the shell and tubes based on their properties, flow conditions, and heat transfer mechanisms (convection, conduction).
    - Consider fouling factors to account for any surface fouling that may reduce the heat transfer coefficients.
    - Calculate the overall heat transfer coefficient (U) using the appropriate equation, such as the Kern method equation for shell and tube heat exchangers.
2) Determine the Logarithmic Mean Temperature Difference (LMTD):
    - Identify the temperature profiles of the hot and cold fluids at the inlet and outlet of the heat exchanger.
    - Calculate the temperature differences between the fluids at each end and determine the logarithmic mean temperature difference (LMTD) using the appropriate equation based on the flow arrangement (parallel, counter-flow, or crossflow) and the number of shell and tube passes.
3) Determine the Required Heat Transfer Area:
    - Calculate the required heat transfer area (A) using the equation: $Q = U \times A \times LMTD$

      where Q is the heat duty or the desired heat transfer rate.
    - Rearrange the equation to solve for the required heat transfer area (A):

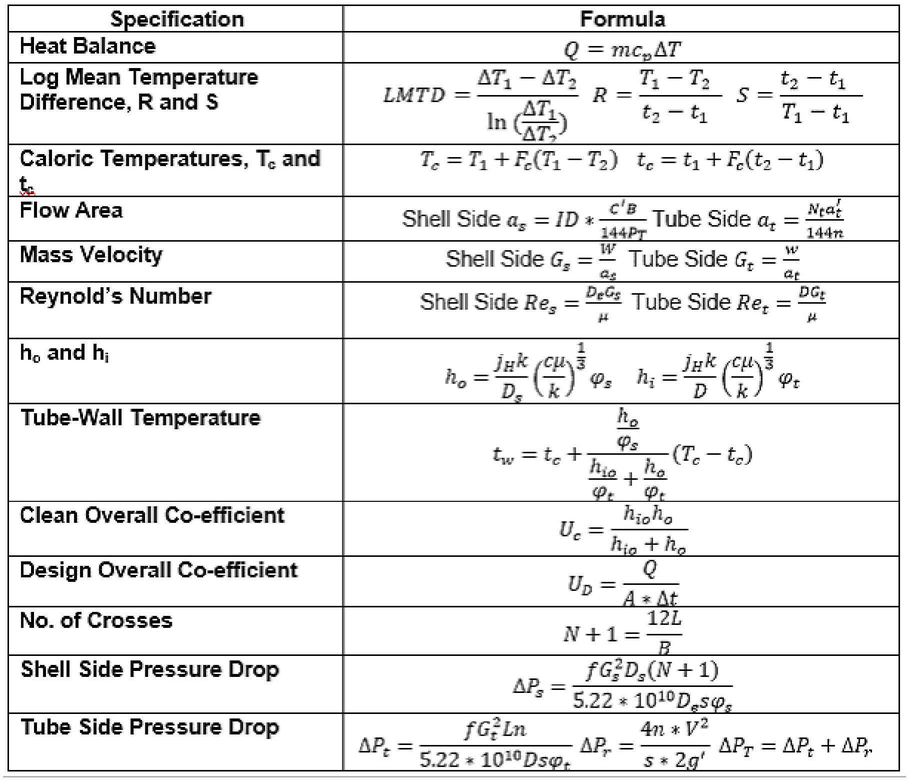
      $A = Q \div (U \times LMTD)$

4) Perform Iterative Sizing Calculations:

- Estimate the initial heat exchanger dimensions and configuration based on the required heat transfer area.
- Calculate dimensions, taking into account tube diameter, tube length, number of tubes, and overall dimensions.
- Identifying and calculating the baffle type and spacing.
- Calculate and verify that the pressure decrease across the heat exchanger meets the design specifications.

If necessary, iterate the sizing calculations to obtain an optimal design.

Table 23 Heat Exchanger Formulae



Specification	Formula
Heat Balance	$Q = mc_p\Delta T$
Log Mean Temperature Difference, R and S	$LMTD = \frac{\Delta T_1 - \Delta T_2}{\ln\left(\frac{\Delta T_1}{\Delta T_2}\right)}$ $R = \frac{T_1 - T_2}{t_2 - t_1}$ $S = \frac{t_2 - t_1}{T_1 - t_1}$
Caloric Temperatures, T_c and t_c	$T_c = T_1 + F_c(T_1 - T_2)$ $t_c = t_1 + F_c(t_2 - t_1)$
Flow Area	Shell Side $a_s = ID * \frac{c'B}{144P_T}$ Tube Side $a_t = \frac{N_t a_t'}{144n}$
Mass Velocity	Shell Side $G_s = \frac{W}{a_s}$ Tube Side $G_t = \frac{w}{a_t}$
Reynold's Number	Shell Side $Re_s = \frac{D_e G_s}{\mu}$ Tube Side $Re_t = \frac{DG_t}{\mu}$
h_o and h_i	$h_o = \frac{j_H k}{D_s}\left(\frac{c\mu}{k}\right)^{\frac{1}{3}}\varphi_s$ $h_i = \frac{j_H k}{D}\left(\frac{c\mu}{k}\right)^{\frac{1}{3}}\varphi_t$
Tube-Wall Temperature	$t_w = t_c + \frac{\frac{h_o}{\varphi_s}}{\frac{h_{io}}{\varphi_t} + \frac{h_o}{\varphi_t}}(T_c - t_c)$
Clean Overall Co-efficient	$U_c = \frac{h_{io}h_o}{h_{io} + h_o}$
Design Overall Co-efficient	$U_D = \frac{Q}{A * \Delta t}$
No. of Crosses	$N + 1 = \frac{12L}{B}$
Shell Side Pressure Drop	$\Delta P_s = \frac{fG_s^2 D_s(N+1)}{5.22 * 10^{10} D_e s\varphi_s}$
Tube Side Pressure Drop	$\Delta P_t = \frac{fG_t^2 Ln}{5.22 * 10^{10} Ds\varphi_t}$ $\Delta P_r = \frac{4n * V^2}{s * 2g'}$ $\Delta P_T = \Delta P_t + \Delta P_r$

- The tube side fluid is the process stream to be cooled.
- The shell side fluid is the steam to be heated.

Table 24 HE Data

Hot **Fluid – Tube Side**	
Parameters	Value
Inlet Temperature (°C)	397
Outlet T (°C)	332
Mass flowrate (kg/hr)	180615
Avg. Cp (kJ/kg.K)	2.239
Avg. density (kg/m^3)	7.89
Avg. viscosity (Cp)	0.0198
Thermal conductivity (W/mK)	0.1109

Table 25: HE Data

Cold Fluid - Shell Side	
Parameters	Value
Inlet T (°C)	310
Outlet T (°C)	312
Mass Flowrate (kg/hr)	253530
Cp (kJ/kg.K) vapor	7.91
Density (kg/m^3) vapor	702
Viscosity (Cp) vapor	0.021
Thermal Conductivity (W/mK)	0.0598

4.1.4 Calculated Parameters:

Table 26 Calculated Parameters

Parameters	Tube Side	Shell Side
Duty (kW)	7158	
LMTD (°C)	34.8	
Reynold number	110490	109000
Prandtl number	1.345	-
h (film coefficient)	5217	31364
U_c (W/m^2K)	3520	
U_d (W/m^2K)	1969	
R_d (m^2K/W)	0.0001	
Area (m^2)	34.1	
Pressure Drop (kPa)	2.47	1.88

- The exchanger geometry was chosen based on Aspen Exchanger Design and Rating (EDR) recommendation.
- The design was modified considering operation warnings provided by EDR.

Table 27 HE Geometry Tube Side

Tube Side	
Number	374
Length (m)	1.7
OD (mm)	19.1
ID (mm)	14.83
Pitch	Rotated Sq. Pitch
Passes	2
Material	Stainless Steel

Table 28: HE Geometry Shell Side

Shell Side	
OD (mm)	690
ID (mm)	620
Baffle spacing (mm)	150
Passes	1
Material	Stainless Steel

4.2 Reactor Design (Packed Bed Reactor)

4.2.1 Secondary Reformer:

Assumptions

- Adiabatic and steady state meaning no accumulation.
- Plug flow with no axial mixing.
- LHHW kinetic model

$$-r_{CH_4} = r_1 + r_2$$

For reaction kinetics, Langmuir-Hinshelwood-Hogan-Watson Mechanism is followed:

$$r_1 = \left(\frac{k_1}{P_{H_2}{}^{2.5}}\right)\left(P_{CH_4}\ P_{H_2O} - \frac{P_{H_2}{}^{3}\,P_{CO}}{K_1}\right)\left(\frac{1}{\Omega}\right)^2$$

$$r_2 = \left(\frac{k_2}{P_{H_2}{}^{3.5}}\right)\left(P_{CH_4}\ P_{H_2O}{}^{2} - \frac{P_{H_2}{}^{4}\,P_{CO_2}}{K_2}\right)\left(\frac{1}{\Omega}\right)^2$$

$$\text{where } \Omega = 1 + K_{CO}P_{CO} + K_{H_2}P_{H_2} + K_{CH_4}P_{CH_4} + \left(\frac{K_{H_2O}\,P_{H_2O}}{P_{H_2}}\right)$$

$$k_1 = 4.225*10^{16}\exp\left(\frac{240.1}{RT}\right) \qquad \frac{kmol.kPa^{0.5}}{kg.hr}$$

$$K_1 = 4.70*10^{16}\exp\left(\frac{224}{RT}\right) \qquad kPa^2$$

$$k_2 = 1.02*10^{16}\exp\left(\frac{243.9}{RT}\right) \qquad \frac{kmol.kPa^{0.5}}{kg.hr}$$

$$K_2 = 5.37*10^{14}\exp\left(\frac{186.7}{RT}\right) \qquad kPa^2$$

$$K_{H_2} = 6.12*10^{-11}\exp\left(\frac{-82.9}{RT}\right) \qquad kPa^{-1}$$

$$K_{CO} = 8.23*10^{-7}\exp\left(\frac{-70.65}{RT}\right) \qquad kPa^{-1}$$

$$K_{CH_4} = 6.64*10^{-6}\exp\left(\frac{-38.28}{RT}\right) \qquad kPa^{-1}$$

$$K_{H_2O} = 1.77*10^{5}\exp\left(\frac{88.68}{RT}\right)$$

Where T is in Kelvin and E is in kJ/mol.

Finding the Inlet Partial P

H2	435.18

CO	69.91
CO2	1298.83
CH4	190.81
H2o	2049.27

Putting the Partial Pressures in terms of CH4:

$PCH4 = PCH4*(1-X)$

$PH2O = 10.7395*(1-X)$

$PCO=0.3664*(1-X)$

$PH2 = 2.281*(1-X)$

Ratio is calculated by dividing the partial pressure of component with the partial pressure of CH4.

Now, the temperature relation with the conversion is:

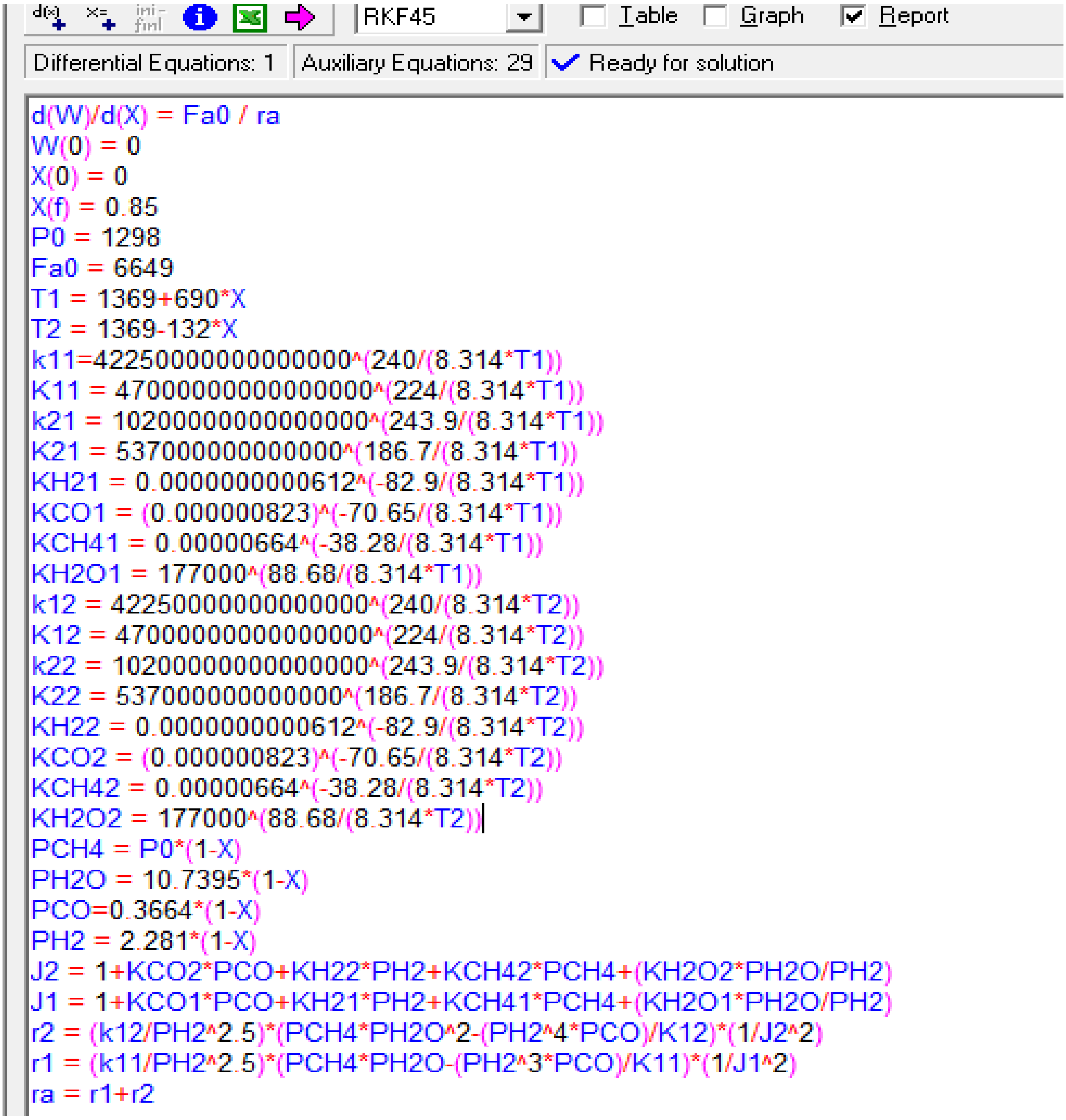
$T/To = 1 + (del\ Hrxn / Cp0) * X$

From the material and energy balances:

$T1 = 1369+690*X$

$T2 = 1369-132*X$

Plugging into the ODE Solver:



RKF45 ☐ Table ☐ Graph ☑ Report

Differential Equations: 1 | Auxiliary Equations: 29 | ✓ Ready for solution

```
d(W)/d(X) = Fa0 / ra
W(0) = 0
X(0) = 0
X(f) = 0.85
P0 = 1298
Fa0 = 6649
T1 = 1369+690*X
T2 = 1369-132*X
k11=42250000000000000^(240/(8.314*T1))
K11 = 47000000000000000^(224/(8.314*T1))
k21 = 10200000000000000^(243.9/(8.314*T1))
K21 = 537000000000000^(186.7/(8.314*T1))
KH21 = 0.0000000000612^(-82.9/(8.314*T1))
KCO1 = (0.000000823)^(-70.65/(8.314*T1))
KCH41 = 0.00000664^(-38.28/(8.314*T1))
KH2O1 = 177000^(88.68/(8.314*T1))
k12 = 42250000000000000^(240/(8.314*T2))
K12 = 47000000000000000^(224/(8.314*T2))
k22 = 10200000000000000^(243.9/(8.314*T2))
K22 = 537000000000000^(186.7/(8.314*T2))
KH22 = 0.0000000000612^(-82.9/(8.314*T2))
KCO2 = (0.000000823)^(-70.65/(8.314*T2))
KCH42 = 0.00000664^(-38.28/(8.314*T2))
KH2O2 = 177000^(88.68/(8.314*T2))
PCH4 = P0*(1-X)
PH2O = 10.7395*(1-X)
PCO=0.3664*(1-X)
PH2 = 2.281*(1-X)
J2 = 1+KCO2*PCO+KH22*PH2+KCH42*PCH4+(KH2O2*PH2O/PH2)
J1 = 1+KCO1*PCO+KH21*PH2+KCH41*PCH4+(KH2O1*PH2O/PH2)
r2 = (k12/PH2^2.5)*(PCH4*PH2O^2-(PH2^4*PCO)/K12)*(1/J2^2)
r1 = (k11/PH2^2.5)*(PCH4*PH2O-(PH2^3*PCO)/K11)*(1/J1^2)
ra = r1+r2
```

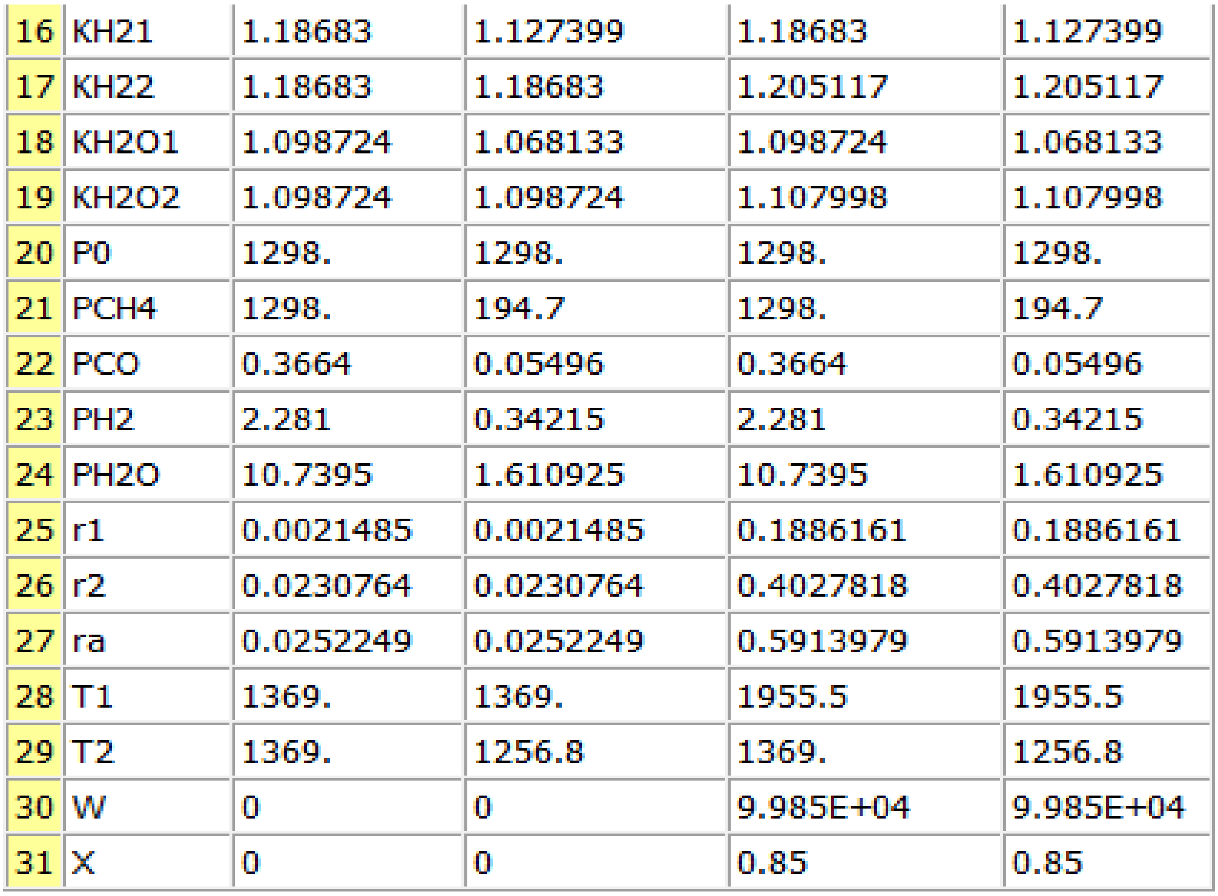
Figure 5 Polymath Code

The result from polymath is:

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	Fa0	6649.	6649.	6649.	6649.
2	J1	1360.385	206.7162	1360.385	206.7162
3	J2	1360.385	210.082	1360.385	210.082
4	k11	2.241687	1.759663	2.241687	1.759663
5	K11	2.128698	1.69709	2.128698	1.69709
6	k12	2.241687	2.241687	2.409198	2.409198
7	K12	2.128698	2.128698	2.277226	2.277226
8	k21	2.203157	1.738434	2.203157	1.738434
9	K21	1.744295	1.476225	1.744295	1.476225
10	k22	2.203157	2.203157	2.364126	2.364126
11	K22	1.744295	1.744295	1.833118	1.833118
12	KCH41	1.040913	1.028469	1.040913	1.028469
13	KCH42	1.040913	1.040913	1.044646	1.044646
14	KCO1	1.090859	1.062774	1.090859	1.062774
15	KCO2	1.090859	1.090859	1.099361	1.099361

Figure 6 Polymath results



16	KH21	1.18683	1.127399	1.18683	1.127399
17	KH22	1.18683	1.18683	1.205117	1.205117
18	KH2O1	1.098724	1.068133	1.098724	1.068133
19	KH2O2	1.098724	1.098724	1.107998	1.107998
20	P0	1298.	1298.	1298.	1298.
21	PCH4	1298.	194.7	1298.	194.7
22	PCO	0.3664	0.05496	0.3664	0.05496
23	PH2	2.281	0.34215	2.281	0.34215
24	PH2O	10.7395	1.610925	10.7395	1.610925
25	r1	0.0021485	0.0021485	0.1886161	0.1886161
26	r2	0.0230764	0.0230764	0.4027818	0.4027818
27	ra	0.0252249	0.0252249	0.5913979	0.5913979
28	T1	1369.	1369.	1955.5	1955.5
29	T2	1369.	1256.8	1369.	1256.8
30	W	0	0	9.985E+04	9.985E+04
31	X	0	0	0.85	0.85

Figure 7 Polymath Results 2

4.2.2 Volume of reactor:

Volume of catalyst (m^3) = Weight of catalyst/ bulk density of catalyst

= 9985 kg;/1028kg/m3 = 97.1 m3

The average bed porosity is 0.45, therefore the overall volume of packed bed reactor is calculated to be:

= 97.1/0.55 = 178 m3

Assuming length to be 15 m, as suggested by literature:

$$V = \pi \times D^2 \times \frac{H}{4}$$

$$178 = 3.142 \times D^2 \times 15/4$$

Diameter = 3.92 m

4.2.3 Pressure Drop:

Using the general form of Ergun Equation:

$$-\frac{\Delta P}{L} = \frac{150*Visc*Vo*(1-E)^\wedge 2}{(Dp^\wedge 2*E^\wedge 3)} + \frac{1.75*\boldsymbol{\rho}*Vo^\wedge\ 2*(1\ \boldsymbol{\varepsilon})}{(Dp*\boldsymbol{\varepsilon}^\wedge 3)}$$

Cross-sectional Area	11.93	m2
Volumetric flow rate	10.22	m3/s
Vo	0.85	m/s
Visc	0.0000244	kg/ms
ε	0.45	
Φs	1	
Dp	0.0012	m
L	15	m

$$del\,P/15 = 150 * \frac{0.00002 * 0.85}{0.0012^2} \left(\frac{(1-4.5)^2}{0.45^3}\right) + 1.75 \left(\frac{4.12 * 0.85^2}{0.0012}\right) \frac{1-0.45}{0.45^3}$$

Del P= 90 kpa

4.3 Reactor Design (Packed Bed Reactor)

4.3.1 Low-Temperature Shift Converter

4.3.2 Theoretical Background

The process gas exiting reforming section contains 10% to 15% of CO (On dry basis). Water gas shift reactions take place in shift converters namely High Temperature Shift Converter and Low Temperature Shift Converter. In water-Gas shift reaction, CO gets converted into CO_2 and H_2 after reacting with steam in presence of a catalyst (Which is CuO. ZnO. Al_2O_3 in case of LTSC). Percentage conversion of CO into CO_2 in shift converters because of water-Gas shift reaction will dictate overall performance of Hydrogen synthesis plant, otherwise H_2 may get converted into CH_4 leading towards reduced feedstock efficiency. Usually, Water-Gas shift reaction is conducted in two (2) steps with heat being removed between HTSC and LTSC to shift equilibrium in forward direction. First, the process stream passes through catalytic bed of iron oxide/chromium oxide at around 350oC to 380oC (HTSC) and followed by process stream being passed through catalytic bed of CuO. ZnO. Al_2O_3 at around 200oC to 230oC (LTSC). Process gas having residual CO content of 0.2% to 0.4% (On dry basis) at outlet of LTSC is obtained. Modern technological advancements are focused on an isothermal shift conversion which goes to completion in only one step. Process gas obtained at outlet is sent to CO_2 removal section after cooling it to such an extent that most of steam is condensed and removed.

The reaction in LTSC is carried out as:

$$CO + H_2O \longrightarrow CO_2 + H_2 \text{ (exothermic)}$$

4.3.3 Equipment Selection

To find suitable type of reactor, we must consider:

- Reaction Conditions i.e., Temperature, Pressure, Conversion, and Capacity.
- Whether desired reaction is exothermic or endothermic in nature or is there any need to remove or supply heat for stable operation of reactor.
- Process type i.e., Batch process or Continuous process.

In our case, as we need to design LTSC for a continuous process we only need to consider reactors which are suitable for continuous heterogeneous processes as there will be more than one phase involved in our case. Reactor types available for desired operation:

- Fixed and Fluidized bed reactors
- Trickle bed reactors

Comparison between Fixed Bed and Partially Fluidized Bed Reactors.

Table 29 Comparison of Fixed Bed and Partially Fluidized Bed Reactors

Parameters	Partially Fluidized Bed	Fixed Bed
Pressure Changes	Either Low or Medium	High
Catalyst Activity	High	Low (But thermally stable)
Catalyst Consumption	Chance of entrainment	No chance of entrainment
Catalyst Handling	Technical difficulties	No technical difficulties
Maximum Capacity	50 m^3	300 m^3
Process Nature	Can be Batch or Continuous	Continuous
Capital Cost	High	Low
Residence Time	High	Low
Operating Cost	High	Low

Selected: Packed Bed Reactor

- Primarily used for gas phase solid catalyzed reactions.
- Due to their low operating cost.
- Suitable for continuous operation.
- They have high conversion per unit mass of catalyst.
- Economically superior in terms of capital cost and operating cost.
- Suitable for handling large capacities.

4.3.4 Reaction Kinetics

For reaction kinetics, Langmuir-Hinshelwood model is followed.

Following assumptions are made:

- Adiabatic and steady state meaning no accumulation.
- Plug flow with no axial mixing.

Estimating the Weight of Catalyst:

$$\frac{W}{Fao} = \int_{xo}^{xf} \frac{dXa}{-rco}$$

Weight of catalyst is determined by using polymath with making units consistent.

$$r = \frac{kK_{CO}K_{H_2O}\left[P_{CO}P_{H_2O} - \frac{P_{CO_2}P_{H_2}}{K_{eq}}\right]}{\left(1 + K_{CO}P_{CO} + K_{H_2O}P_{H_2O} + K_{CO_2}P_{CO_2}\right)^2} \times \frac{\rho_{cat}}{60}$$

Equilibrium Constant $K_{eq} = \exp\left(\frac{4577.8}{T} - 4.33\right)$

Rate Constant $k = \exp\left(-\frac{29364}{1.987 \times T} + \frac{40.32}{1.987}\right)$ mol/g cat. Min

$K_{CO} = \exp\left(\frac{3064}{1.987 \times T} - \frac{6.74}{1.987}\right)$, $K_{H_2O} = \exp\left(-\frac{6216}{1.987 \times T} + \frac{12.77}{1.987}\right)$

$K_{CO_2} = \exp\left(\frac{12542}{1.987 \times T} - \frac{18.45}{1.987}\right)$

r is rate of reaction (mol/cm^{3}s), Pi is partial pressure of species (Pa), ρ_{cat} is density of catalyst(g cat/cm^3), T is temperature(K)

Finding the Inlet Partial Pressures in kPa from simulation

Hydrogen	**1136.1**
CO	38.94
CO2	341.66
H2O	912.79

Putting the Partial Pressures in terms of CH4:

PCO=PCO*(1-X)

PH2=29.2*(1-X)

PH2O=23.4*(1-X)

PCO2=8.77*(1-X)

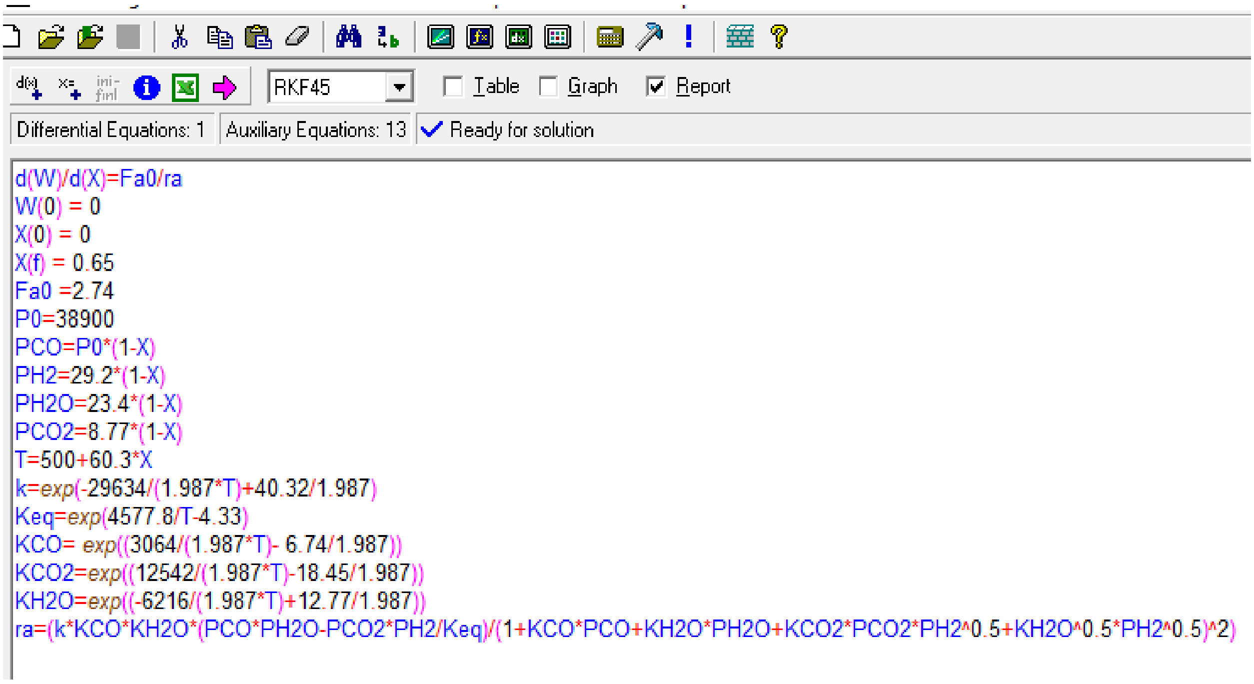
Now, the temperature relation with the conversion is:

*T/To = 1 + (del Hrxn / Cp0) * X*

From the material and energy balances:

T=500+60.3*X

Plugging into the ODE Solver:

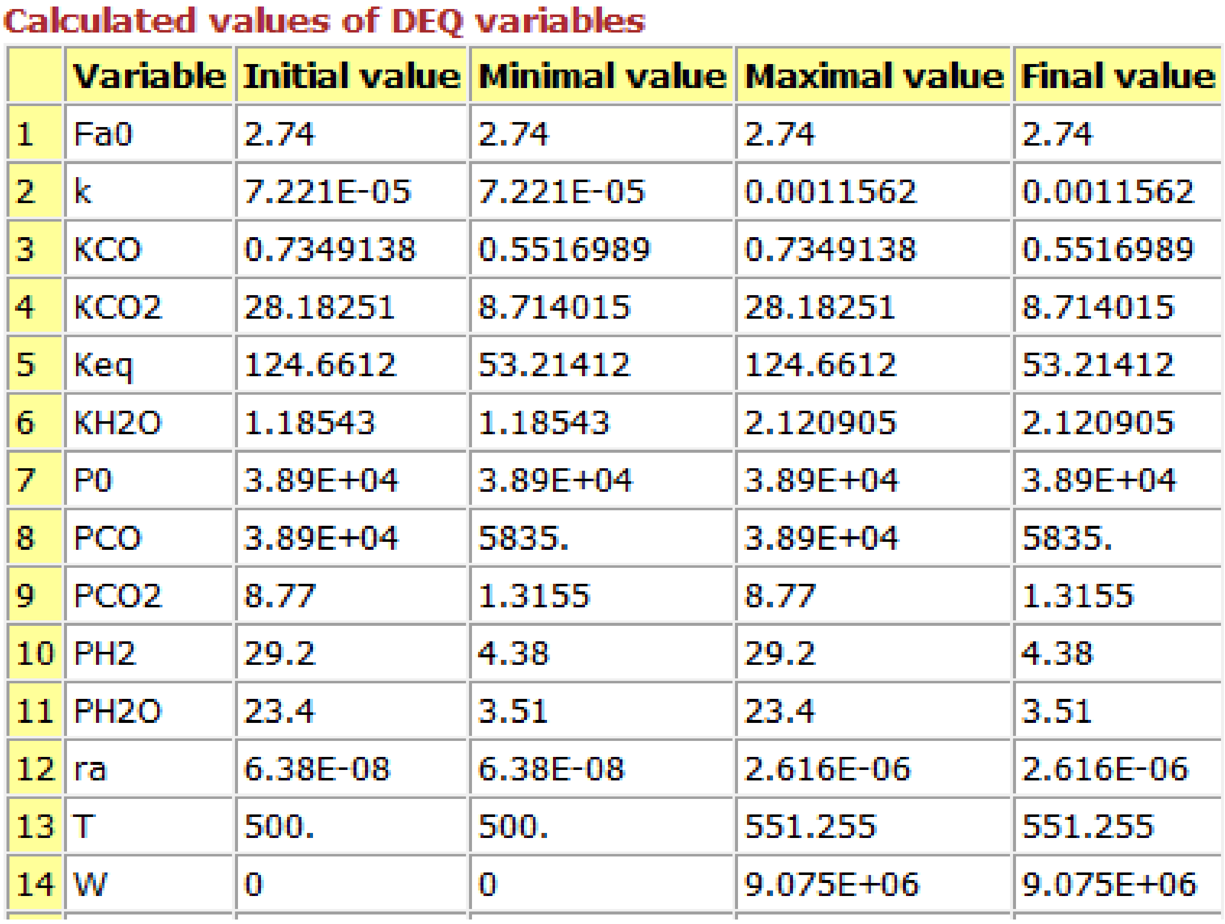


Differential Equations: 1 | Auxiliary Equations: 13 | ✓ Ready for solution

```
d(W)/d(X)=Fa0/ra
W(0) = 0
X(0) = 0
X(f) = 0.65
Fa0 =2.74
P0=38900
PCO=P0*(1-X)
PH2=29.2*(1-X)
PH2O=23.4*(1-X)
PCO2=8.77*(1-X)
T=500+60.3*X
k=exp(-29634/(1.987*T)+40.32/1.987)
Keq=exp(4577.8/T-4.33)
KCO= exp((3064/(1.987*T)- 6.74/1.987))
KCO2=exp((12542/(1.987*T)-18.45/1.987))
KH2O=exp((-6216/(1.987*T)+12.77/1.987))
ra=(k*KCO*KH2O*(PCO*PH2O-PCO2*PH2/Keq)/(1+KCO*PCO+KH2O*PH2O+KCO2*PCO2*PH2^0.5+KH2O^0.5*PH2^0.5)^2)
```

Figure 8 Polymath code for second Reactor

The results:



Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	Fa0	2.74	2.74	2.74	2.74
2	k	7.221E-05	7.221E-05	0.0011562	0.0011562
3	KCO	0.7349138	0.5516989	0.7349138	0.5516989
4	KCO2	28.18251	8.714015	28.18251	8.714015
5	Keq	124.6612	53.21412	124.6612	53.21412
6	KH2O	1.18543	1.18543	2.120905	2.120905
7	P0	3.89E+04	3.89E+04	3.89E+04	3.89E+04
8	PCO	3.89E+04	5835.	3.89E+04	5835.
9	PCO2	8.77	1.3155	8.77	1.3155
10	PH2	29.2	4.38	29.2	4.38
11	PH2O	23.4	3.51	23.4	3.51
12	ra	6.38E-08	6.38E-08	2.616E-06	2.616E-06
13	T	500.	500.	551.255	551.255
14	W	0	0	9.075E+06	9.075E+06

Figure 9 Polymath result for second Reactor

4.3.5 Volume of Reactor

Volume of catalyst (m^3) = Weight of catalyst/ bulk density of catalyst

= 9075 kg;/600kg/m3 = 15.12 m3

The average bed porosity is 0.45, therefore the overall volume of packed bed reactor is calculated to be:

= 15.12/0.55 = 27 m3

Consider L/D=1.5

Diameter = 2.85 m

Length = 4.28 m

4.3.6 Pressure Drop:

Using Ergun Equation:

$$\frac{\Delta P}{L} = \frac{150 * \text{Visc} * \text{Vo} * (1 - \text{E})\text{^}2}{(\text{Dp}\text{^}2 * \text{E}\text{^}3)} + \frac{1.75 * \rho * \text{Vo}\text{^}\ 2 * (1\ \varepsilon)}{(\text{Dp} * \varepsilon\text{^}3)}$$

Vo = 4.08 m/s

ε = 0.45

Φs = 0.874

Dp = 0.006 m

Lb= 2.89 m

$$del\ P/4.28 = 150 * \frac{0.00001419 * 4.085}{0.006^2} \left(\frac{(1 - 4.5)^2}{0.45^3}\right) + 1.75 \left(\frac{4.1 * 0.85^2}{0.006}\right) \frac{1 - 0.45}{0.45^3}$$

Del P= 80.3 kpa

CHAPTER 5

ECONOMIC ANALYSIS

5.1 Background

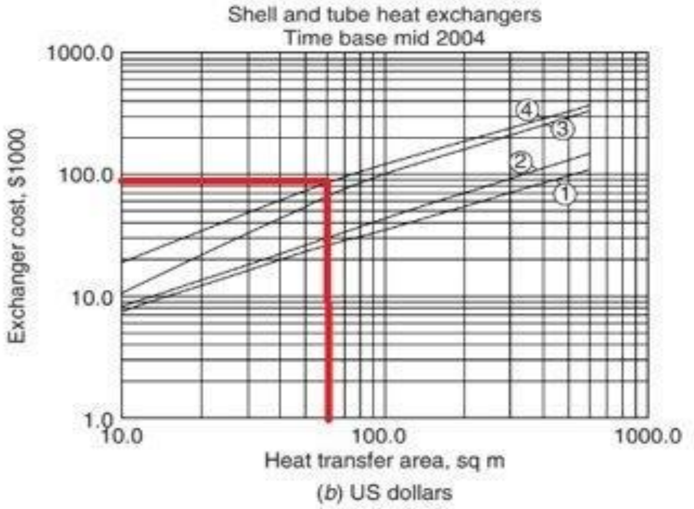
Economic analysis and costing of the whole process was done with the help of Aspen HYSYS Economic Analyzer. We provided the prices of our raw material that is natural gas, and the sale price of our product ammonia. As economic analyzer cannot provide accurate costs for reactors, we calculated the cost of reactors with the help of graphs provided in Coulson's and Richardson Chemical Engineering Design book. All the values were updated to the current year using indexing.

Table 30 Summary of Costing

Summary	
Total Capital Cost [USD]	415005503
Total Operating Cost [USD/Year]	82139300
Total Raw Materials Cost [USD/Year]	11834100
Total Product Sales [USD/Year]	429384000
Total Utilities Cost [USD/Year]	100695470.1
Desired Rate of Return [Percent/'Year]	20
P.O.Period [Year]	4
Equipment Cost [USD]	98217502.54
Total Installed Cost [USD]	222558000

5.1.1 Costing of Heat Exchanger

Heat Exchanger Area = 60.32 m^2



Materials	
Shell	Tubes
① Carbon steel	Carbon steel
② C.S.	Brass
③ C.S.	Stainless steel
④ S.S.	S.S.

Pressure factors	
1–10 bar	× 1.0
10–20	× 1.1
20–30	× 1.25
30–50	× 1.3
50–70	× 1.5

Type factors	
Floating head	× 1.0
Fixed tube sheet	× 0.8
U tube	× 0.85
Kettle	× 1.3

Cost from Graph (2004) = 90000 USD

Type Factor = 1

Pressure Factor = 1

Index Factor = 1.75

Cost in 2023 = 90000*1.75

Cost in 2023 = 157500 USD

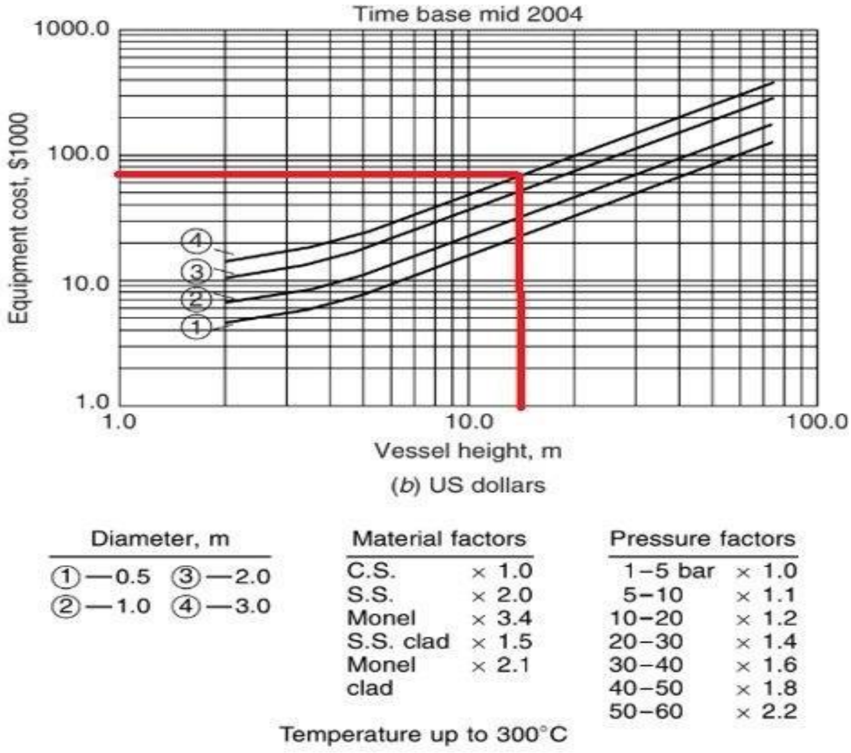
Costing of Secondary Reformer

Diameter= 3965 mm

Height = 15490 mm

Pressure Factor= 1.8

Material Factor= 2



Cost (2004) = Ce = 252000 USD

Index Factor = 1.75

Cost (2023) = 442703 USD

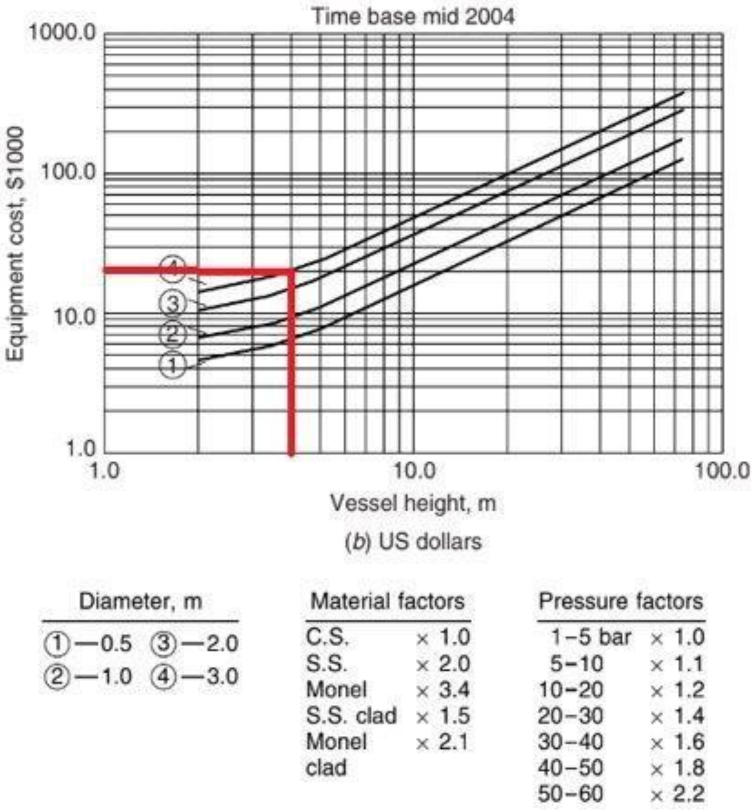
5.1.2 Costing of High Temperature Shift Reactor

Diameter= 3966 mm

Height = 4310 mm

Pressure Factor= 1.8

Material Factor= 2



(b) US dollars

Diameter, m

①—0.5 ③—2.0
②—1.0 ④—3.0

Material factors	
C.S.	× 1.0
S.S.	× 2.0
Monel	× 3.4
S.S. clad	× 1.5
Monel clad	× 2.1

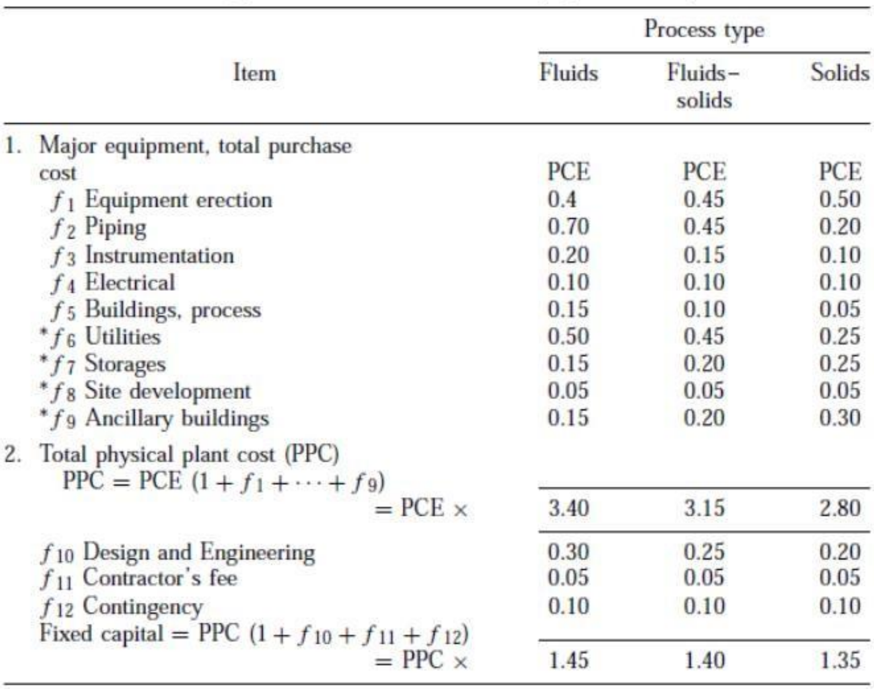
Pressure factors	
1–5 bar	× 1.0
5–10	× 1.1
10–20	× 1.2
20–30	× 1.4
30–40	× 1.6
40–50	× 1.8
50–60	× 2.2

Cost (2004) =Ce= 39600 USD

Index Factor = 1.75

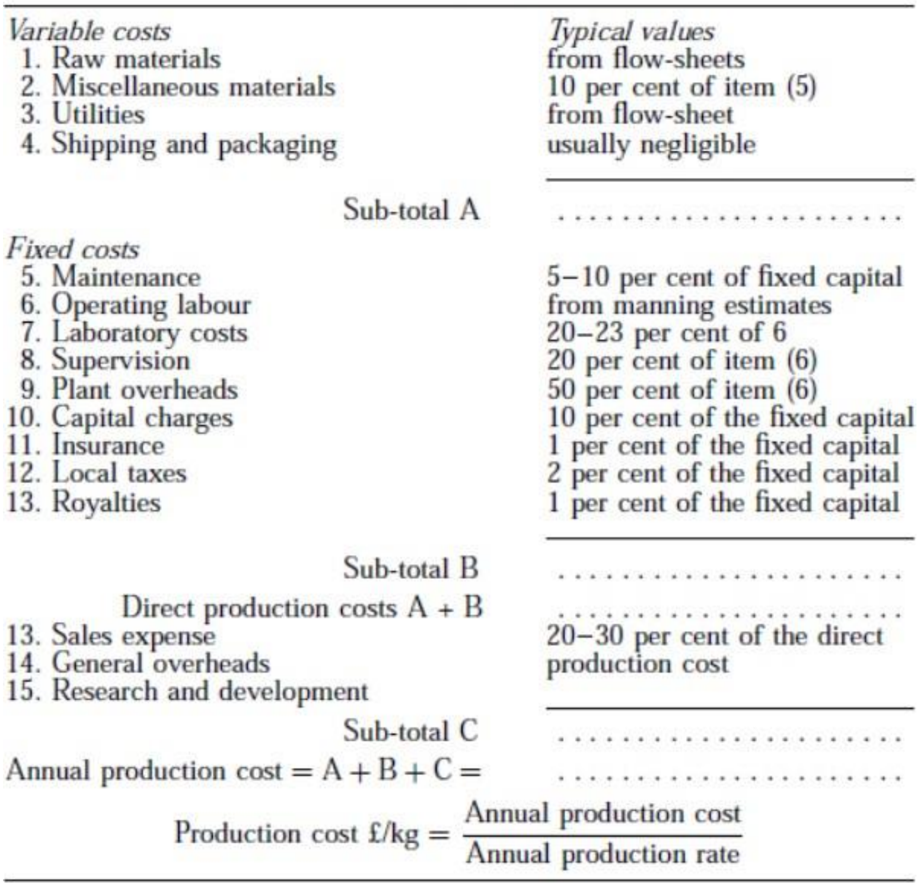
Cost (2023) = 69568 USD

Table 6.1. Typical factors for estimation of project fixed capital cost



Item	Process type		
	Fluids	Fluids–solids	Solids
1. Major equipment, total purchase cost	PCE	PCE	PCE
f_1 Equipment erection	0.4	0.45	0.50
f_2 Piping	0.70	0.45	0.20
f_3 Instrumentation	0.20	0.15	0.10
f_4 Electrical	0.10	0.10	0.10
f_5 Buildings, process	0.15	0.10	0.05
*f_6 Utilities	0.50	0.45	0.25
*f_7 Storages	0.15	0.20	0.25
*f_8 Site development	0.05	0.05	0.05
*f_9 Ancillary buildings	0.15	0.20	0.30
2. Total physical plant cost (PPC)			
$\text{PPC} = \text{PCE}\ (1 + f_1 + \cdots + f_9)$			
$= \text{PCE} \times$	3.40	3.15	2.80
f_{10} Design and Engineering	0.30	0.25	0.20
f_{11} Contractor's fee	0.05	0.05	0.05
f_{12} Contingency	0.10	0.10	0.10
$\text{Fixed capital} = \text{PPC}\ (1 + f_{10} + f_{11} + f_{12})$			
$= \text{PPC} \times$	1.45	1.40	1.35

Table 6.6. Summary of production costs



Variable costs	*Typical values*
1. Raw materials	from flow-sheets
2. Miscellaneous materials	10 per cent of item (5)
3. Utilities	from flow-sheet
4. Shipping and packaging	usually negligible
Sub-total A	. . . .
Fixed costs	
5. Maintenance	5–10 per cent of fixed capital
6. Operating labour	from manning estimates
7. Laboratory costs	20–23 per cent of 6
8. Supervision	20 per cent of item (6)
9. Plant overheads	50 per cent of item (6)
10. Capital charges	10 per cent of the fixed capital
11. Insurance	1 per cent of the fixed capital
12. Local taxes	2 per cent of the fixed capital
13. Royalties	1 per cent of the fixed capital
Sub-total B	. . . .
Direct production costs A + B	. . . .
13. Sales expense	20–30 per cent of the direct production cost
14. General overheads	
15. Research and development	
Sub-total C	. . . .
Annual production cost = A + B + C =	. . . .

$$\text{Production cost £/kg} = \frac{\text{Annual production cost}}{\text{Annual production rate}}$$

Table 31: FCC

Project Fixed Capital Cost (USD)		
Purchase Cost of Equipment	PCE	98217502.54
Equipment Erection	f_1	39287001.02
Piping	f_2	68752251.78
Instrumentation	f_3	19643500.51
Electrical	f_4	9821750.254
Building, process	f_5	14732625.38
Utilities	f_6	49108751.27
Storages	f_7	14732625.38
Site Development	f_8	4910875.127
Ancillary buildings	f_9	14732625.38
Total physical plant cost	PPC	333939508.65
Design and Engineering	f_{10}	100181852.6
Contractors Fee	f_{11}	16696975.43
Contingency	f_{12}	33393950.87
Fixed Capital	FC	484212287.55

Table 32: Variable Costs

Variable Costs (USD)	
Raw materials (USD)	11834100
Miscellaneous materials (USD)	4842122.875
Utilities (USD)	100695470.1
Shipping and packaging (USD)	Negligible
Total	117371693

Table 33: Fixed Costs

Fixed Costs (USD)	
Maintenance	48421228.75
Operating labor	41069650
Laboratory costs	8213930
Supervision	8213930
Plant overheads	20534825
Capital charges	48421228.75
Total	174874792

Direct Production Cost = Total Fixed Cost + Total Variable Cost

Direct Production Cost = 174874792 + 117371693

Direct Production Cost = 292246485 USD/year

Annual Production Cost = Direct Production Cost + Sales Expense + General Overheads

Annual Production Cost = 292246485 + 73061621

Annual Production Cost = 365308107 USD/year

Production Rate = 307200000 kg/year

Production Cost= 1.2 USD/kg

CHAPTER 6

PROCESS SIMULATION

This chapter entails everything that is related to modelling and simulation of ammonia production unit (both in steady and dynamic state). Despite studying alternatives production methods for the environmentally cleaner ammonia in the previous literature review, we believed it to be the best to use Kellogg's process to maximize the productivity of this simulation tool for the industry. The flowsheet simulation was integrated on Aspen HYSYS V11 -- a powerful software tool that allowed us to model a digital twin of the ammonia plant with a high level of detail and analysis in our further instrumentation analysis.

6.1.1 Units Used:

When starting the simulation, it is necessary to specify the units you are going to work with. In this case the following units were chosen due to the ease of adapting the information obtained from literature and research

Pressure: kg/cm^2

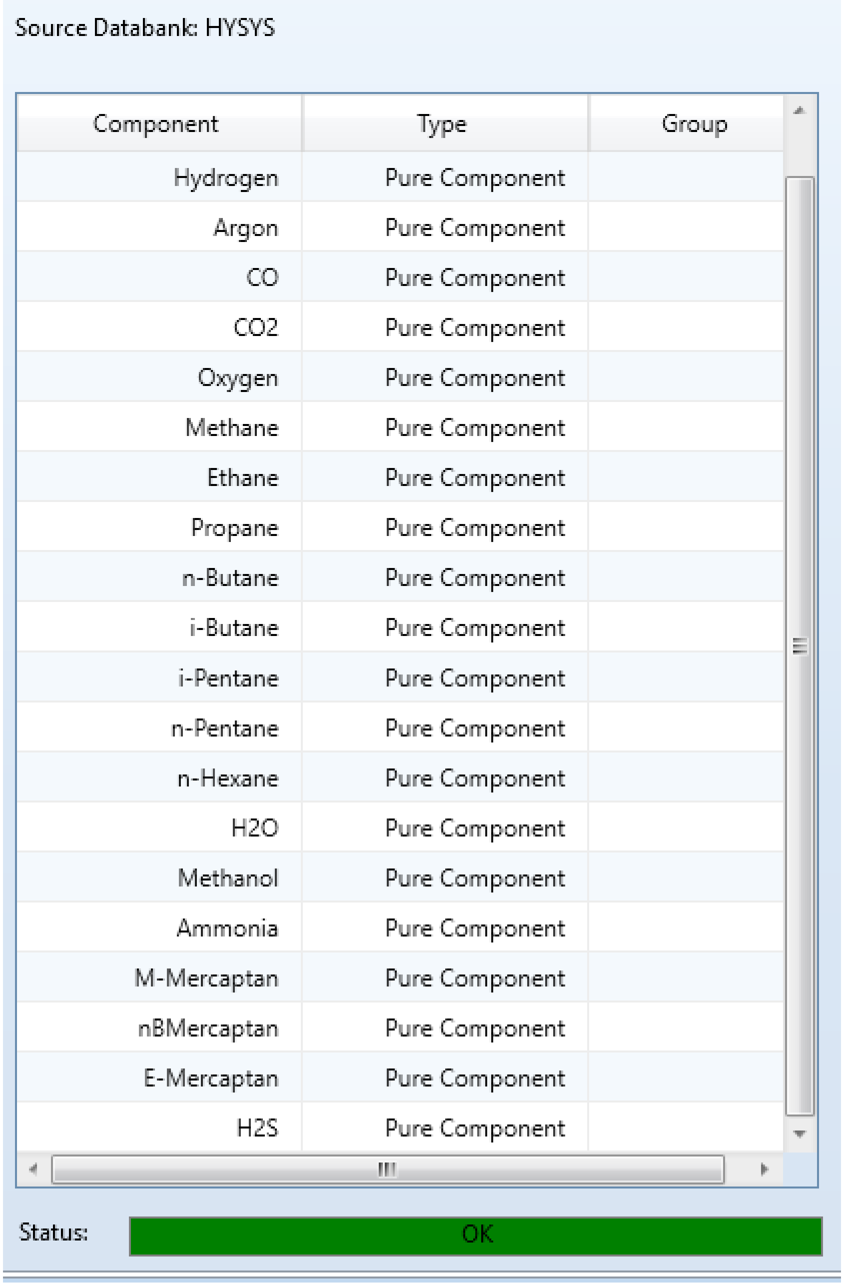
Temperature: ^{o}C

Molar flow: kgmole/hr

Mass Flow: kg/hr

6.1.2 Component Lists:

Subsequently, all the components involved in the process are selected from the Aspen HYSYS databank. The following elements were selected for this process, which are the ones that interact in the plant:



Source Databank: HYSYS

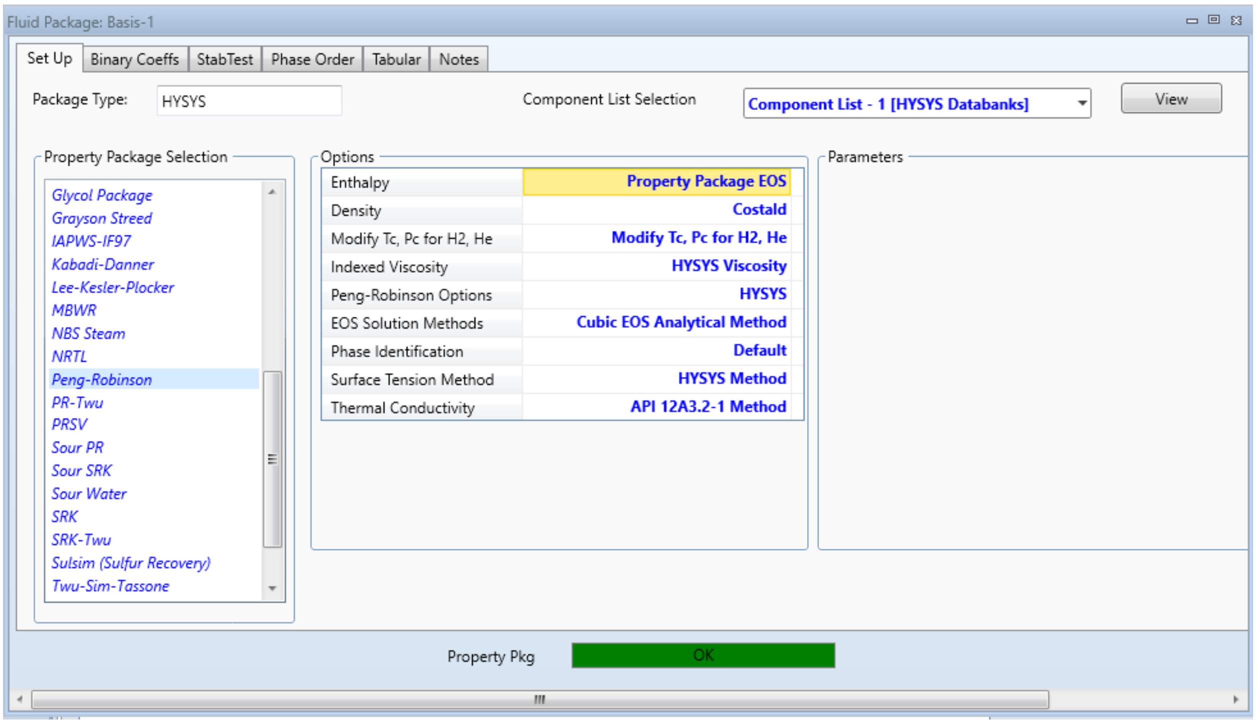
Component	Type	Group
Hydrogen	Pure Component	
Argon	Pure Component	
CO	Pure Component	
CO2	Pure Component	
Oxygen	Pure Component	
Methane	Pure Component	
Ethane	Pure Component	
Propane	Pure Component	
n-Butane	Pure Component	
i-Butane	Pure Component	
i-Pentane	Pure Component	
n-Pentane	Pure Component	
n-Hexane	Pure Component	
H2O	Pure Component	
Methanol	Pure Component	
Ammonia	Pure Component	
M-Mercaptan	Pure Component	
nBMercaptan	Pure Component	
E-Mercaptan	Pure Component	
H2S	Pure Component	

Status: OK

Figure 10 Component list

6.1.3 Property Package:

For the specified model, Peng-Robinson was used to give accurate results.



Package Type: HYSYS

Component List Selection: Component List - 1 [HYSYS Databanks]

Enthalpy	Property Package EOS
Density	Costald
Modify Tc, Pc for H2, He	Modify Tc, Pc for H2, He
Indexed Viscosity	HYSYS Viscosity
Peng-Robinson Options	HYSYS
EOS Solution Methods	Cubic EOS Analytical Method
Phase Identification	Default
Surface Tension Method	HYSYS Method
Thermal Conductivity	API 12A3.2-1 Method

Property Pkg: OK

Figure 11 Fluid Package

Why use Peng-Robinson:

The Peng Robinson (PR) equation of state is widely used in process simulation software like Aspen HYSYS due to its ability to accurately predict the thermodynamic properties of complex mixtures, such as those encountered in ammonia production units.

- Wide Applicability: The PR equation of state is applicable to a wide range of substances, including hydrocarbons, non-hydrocarbons, and mixtures of both. It can handle the complex mixture of gases involved in the ammonia production process, which includes methane (from natural gas), nitrogen (from air), and hydrogen.

- Mixture Behavior: The PR equation of state accounts for the interactions between different components in a mixture, including non-ideal behavior, phase equilibria, and vapor-liquid equilibrium. These interactions are crucial in accurately predicting the behavior of the natural gas and air mixture throughout the different stages of the ammonia production process.

- Phase Equilibria: Ammonia production involves multiple phases, such as gas-phase reactions, liquid-phase reactions, and vapor-liquid separation. The PR equation of state can accurately predict phase equilibria, ensuring that the simulation adequately captures the behavior of the gas and liquid phases at various process conditions.

- Reliable Property Calculations: The PR equation of state provides reliable predictions of key thermodynamic properties, such as enthalpy, entropy, density, and heat capacity. These properties are essential for process design, optimization, and equipment sizing in the ammonia production unit.

- Established Model: The PR equation of state has been extensively validated and used in the industry for several decades. Its reliability and accuracy have been demonstrated in various applications, including the simulation of chemical processes, making it a trusted choice for ammonia production simulations.

6.1.5 Reaction Sets

Primarily ammonia production involves the reaction of Nitrogen and Hydrogen. However, on industrial scale this reaction is preceded by a number of separation and purification reactions:

.

- **Hydrogenator:**
  $RSH + H2 \rightleftharpoons H2S + RH$

This section primarily focusses on removing the mercaptans from the feed stream.

- **Desulphurizer:**

  $H_2S + ZnO \rightarrow ZnS + H_2O$

  This section removes the sulphur from the feed that would have caused catalytic poisoning in the later stages.

- **Primary Reforming:**

  $CH_4 + H_2O \rightleftharpoons CO + 3H_2$ C_3H_8

  $+ H_2O \rightleftharpoons 3CO + 4H_2$ $C_4H_{10} +$

  $H_2O \rightleftharpoons 4CO + 5H_2$ $C_5H_{12} +$

  $H_2O \rightleftharpoons 5CO + 6H_2$ $C_6H_{14} +$

  $H_2O \rightleftharpoons 6CO + 7H_2$

  This reaction involves the reforming of methane (CH4) with steam (H2O) to produce carbon monoxide (CO) and hydrogen gas (H2) and reforming of reactions of other hydrocarbons present in the NG feed.

- **Secondary Reforming:**

  $CH_4 + 2O_2 \rightarrow CO_2 + H_2O$

  $2CH_4 + 3O_2 \rightarrow 2\,CO + 4H_2O$

  $2H_2 + O_2 \rightarrow 2H_2O$

  $CH_4 + H_2O \rightleftharpoons CO/CO_2 + H_2$

  Secondary reformer reaction converts remaining methane at high temperature meanwhile O2 of air is combusted leaving behind Nitrogen sufficient for ammonia synthesis.

- **Shift Conversion:**

  $CO + H_2O \rightleftharpoons CO_2 + H_2$

This reaction, also known as the water-gas shift reaction, converts additional carbon monoxide (CO) to carbon dioxide (CO2) and hydrogen gas (H2) using steam (H2O).

- **Methanation:**

  $CO + 3H_2 \rightleftharpoons CH_4 + H_2O$

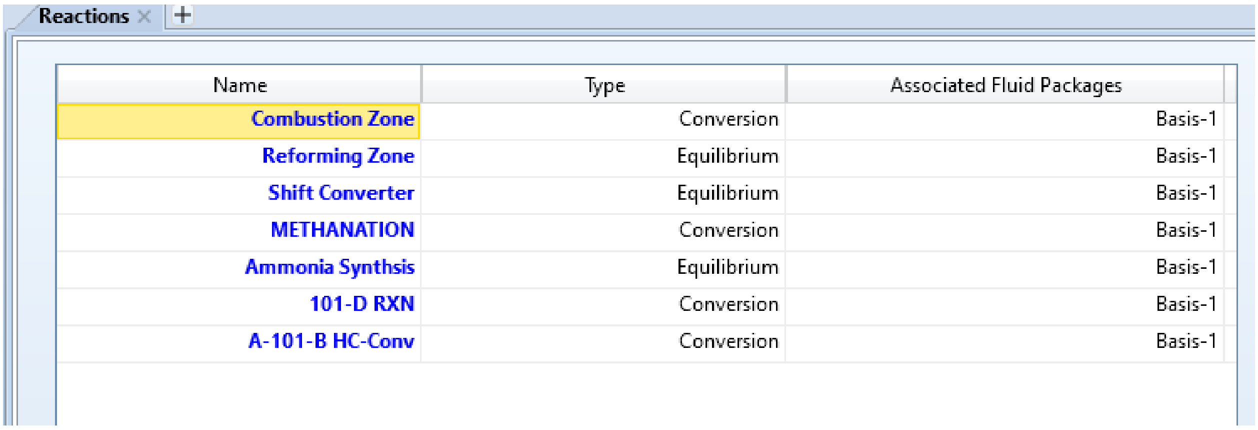
  In this reaction, carbon monoxide (CO) and hydrogen gas (H2) are reacted to form methane (CH4) and steam (H2O).

- **Ammonia Synthesis:**

  $N_2 + 3H_2 \rightleftharpoons 2NH_3$

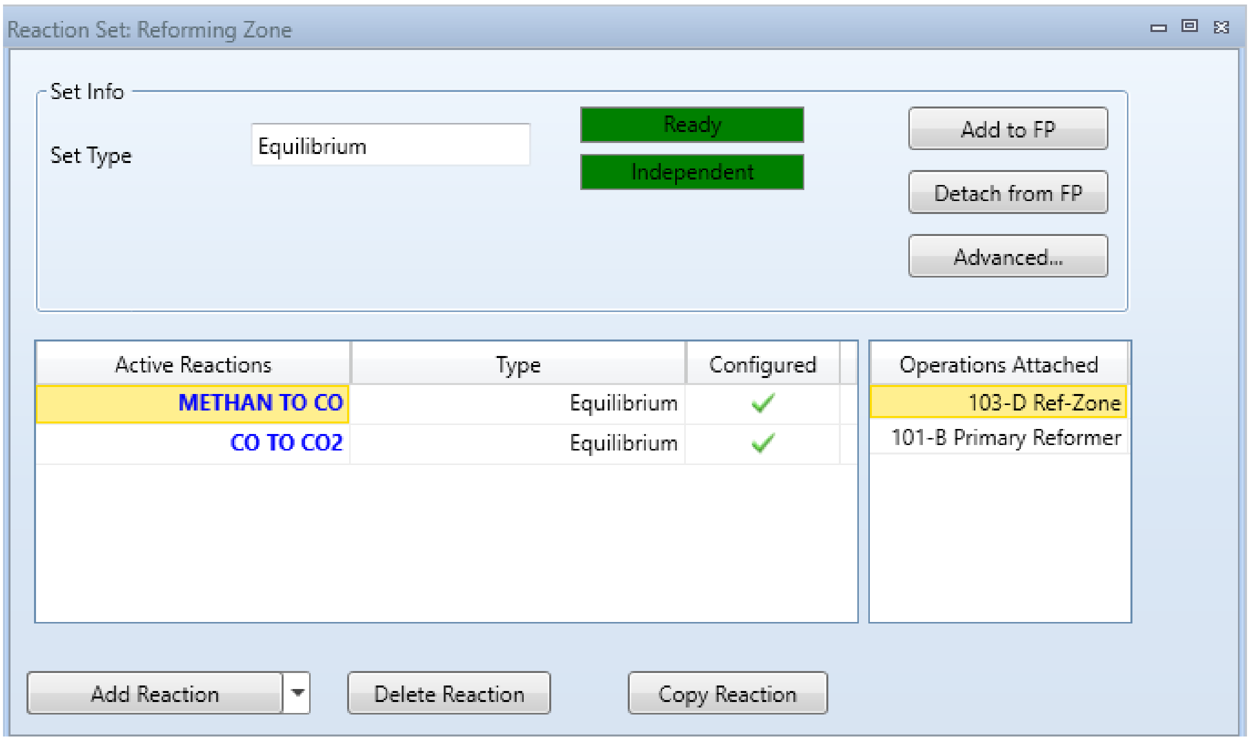
  This is the final reaction where nitrogen gas (N2) and hydrogen gas (H2) combine to produce ammonia (NH3).

Following reaction sets were associated with the main flowsheet with each having its own sub-set of reactions:



Name	Type	Associated Fluid Packages
Combustion Zone	Conversion	Basis-1
Reforming Zone	Equilibrium	Basis-1
Shift Converter	Equilibrium	Basis-1
METHANATION	Conversion	Basis-1
Ammonia Synthsis	Equilibrium	Basis-1
101-D RXN	Conversion	Basis-1
A-101-B HC-Conv	Conversion	Basis-1

Figure 12 Reactions

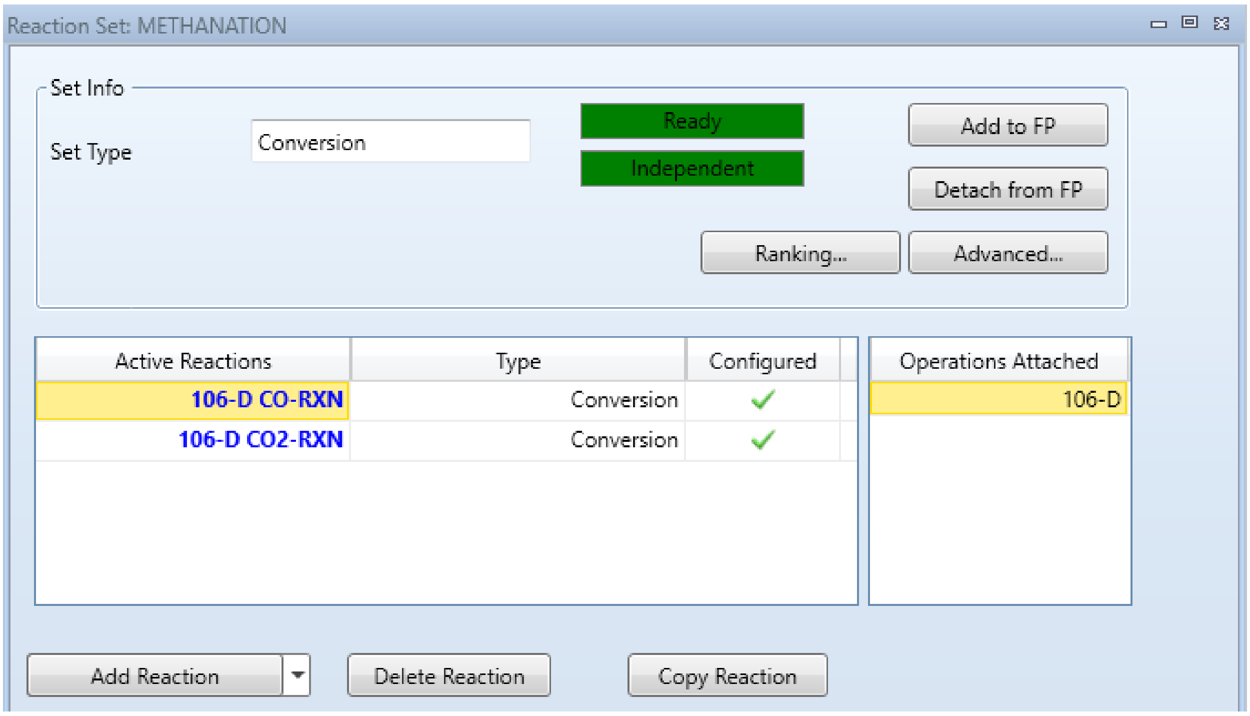


Set Type: Equilibrium

Active Reactions	Type	Configured
METHAN TO CO	Equilibrium	✓
CO TO CO2	Equilibrium	✓

Operations Attached
103-D Ref-Zone
101-B Primary Reformer

Figure 13 Reaction Set 1

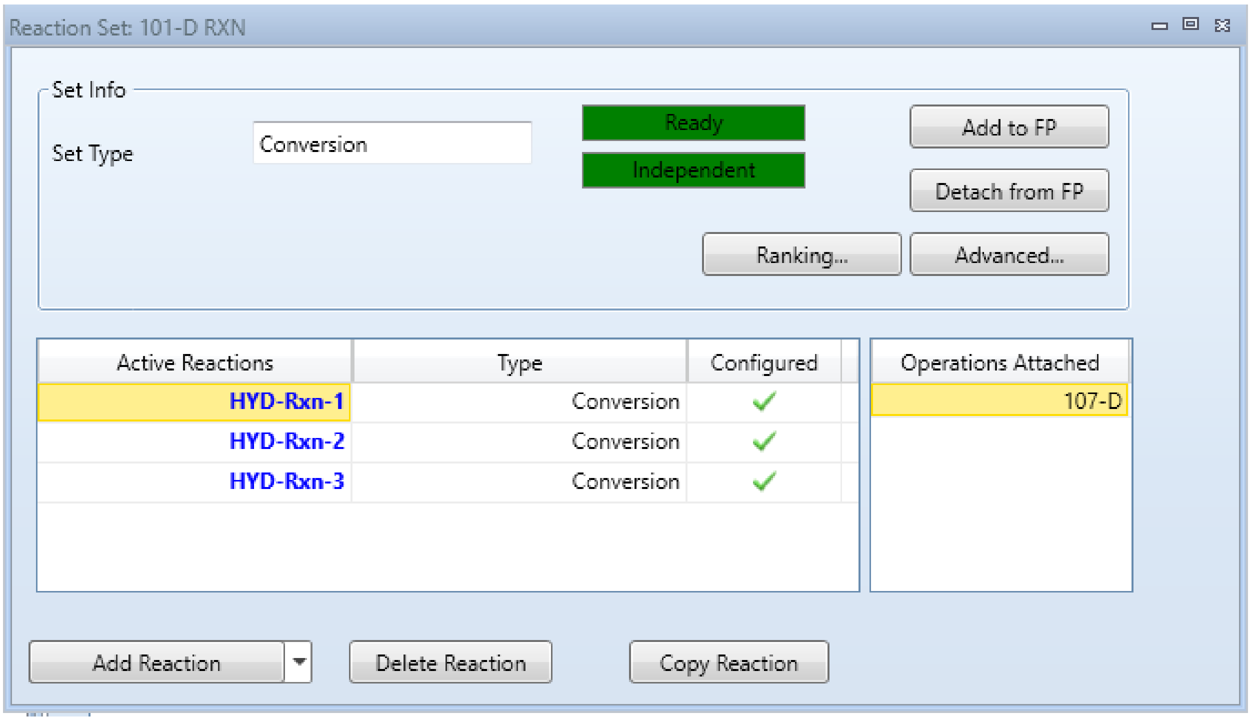


Set Type: Conversion

Active Reactions	Type	Configured
106-D CO-RXN	Conversion	✓
106-D CO2-RXN	Conversion	✓

Operations Attached
106-D

Figure 14 Reaction Set 2

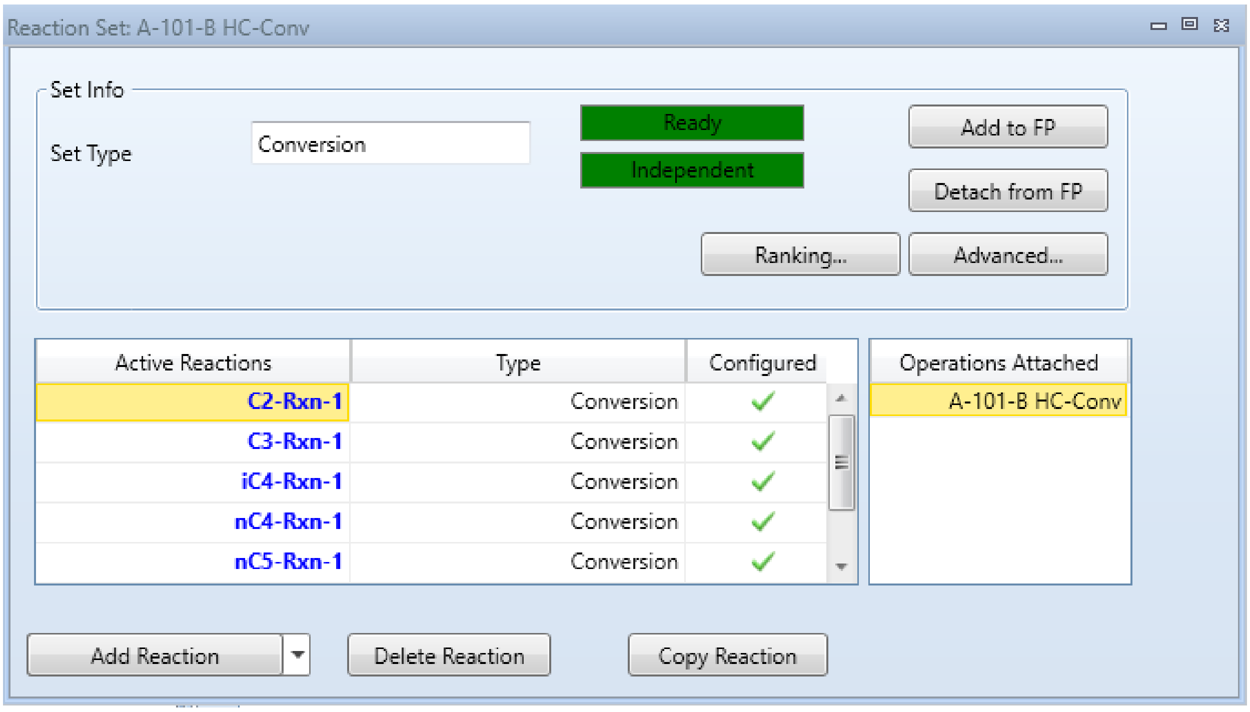


Set Type: Conversion

Active Reactions	Type	Configured
HYD-Rxn-1	Conversion	✓
HYD-Rxn-2	Conversion	✓
HYD-Rxn-3	Conversion	✓

Operations Attached
107-D

Figure 15 Reaction Set 3

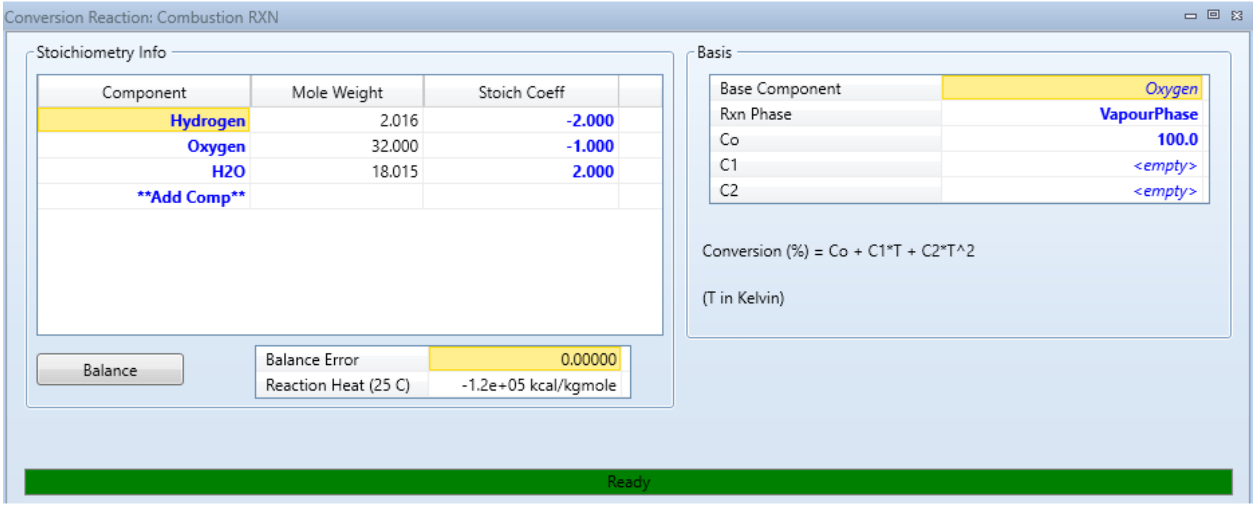


Set Type: Conversion

Active Reactions	Type	Configured
C2-Rxn-1	Conversion	✓
C3-Rxn-1	Conversion	✓
iC4-Rxn-1	Conversion	✓
nC4-Rxn-1	Conversion	✓
nC5-Rxn-1	Conversion	✓

Operations Attached
A-101-B HC-Conv

Figure 16 Reaction Set 4



Conversion Reaction: Combustion RXN

Stoichiometry Info

Component	Mole Weight	Stoich Coeff
Hydrogen	2.016	-2.000
Oxygen	32.000	-1.000
H2O	18.015	2.000
Add Comp		

Balance Error	0.00000
Reaction Heat (25 C)	-1.2e+05 kcal/kgmole

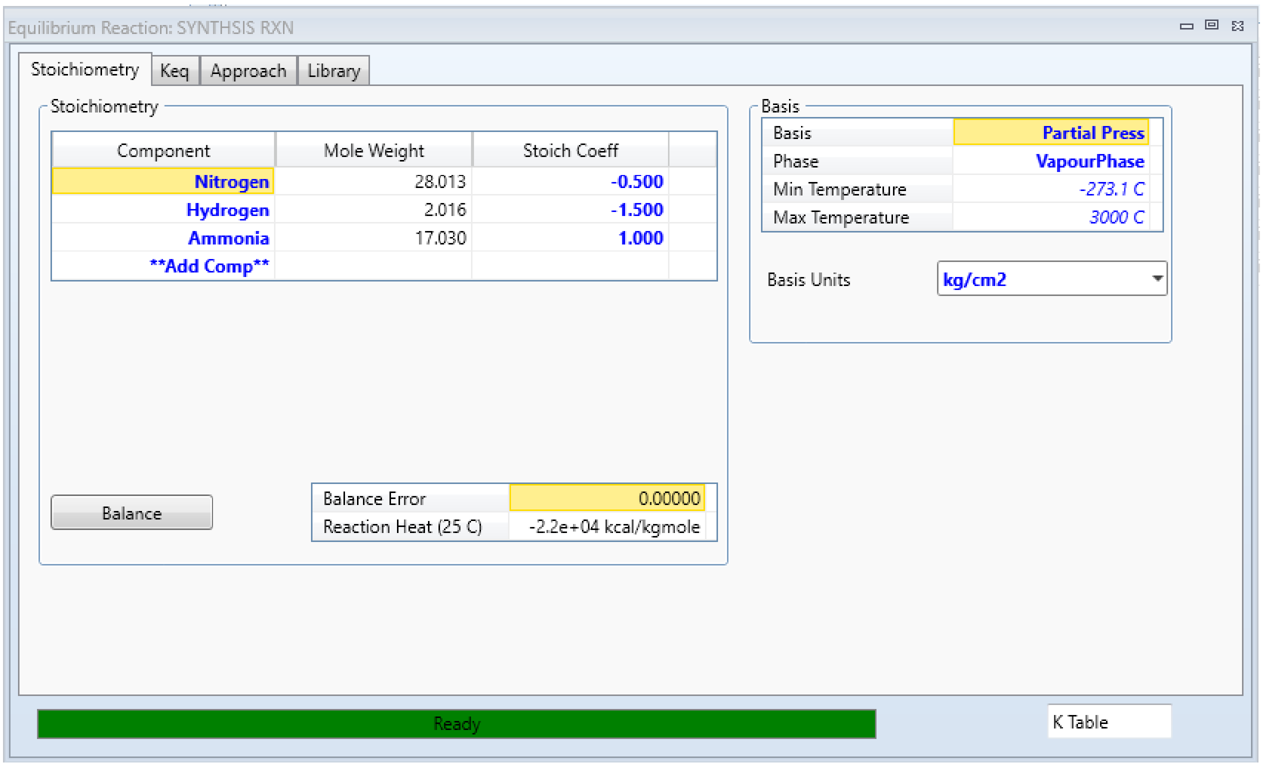
Basis

Base Component	Oxygen
Rxn Phase	VapourPhase
Co	100.0
C1	<empty>
C2	<empty>

Conversion (%) = Co + C1*T + C2*T^2

(T in Kelvin)

Figure 17 Reaction Set 5



Equilibrium Reaction: SYNTHSIS RXN

Stoichiometry

Component	Mole Weight	Stoich Coeff
Nitrogen	28.013	-0.500
Hydrogen	2.016	-1.500
Ammonia	17.030	1.000
Add Comp		

Balance Error	0.00000
Reaction Heat (25 C)	-2.2e+04 kcal/kgmole

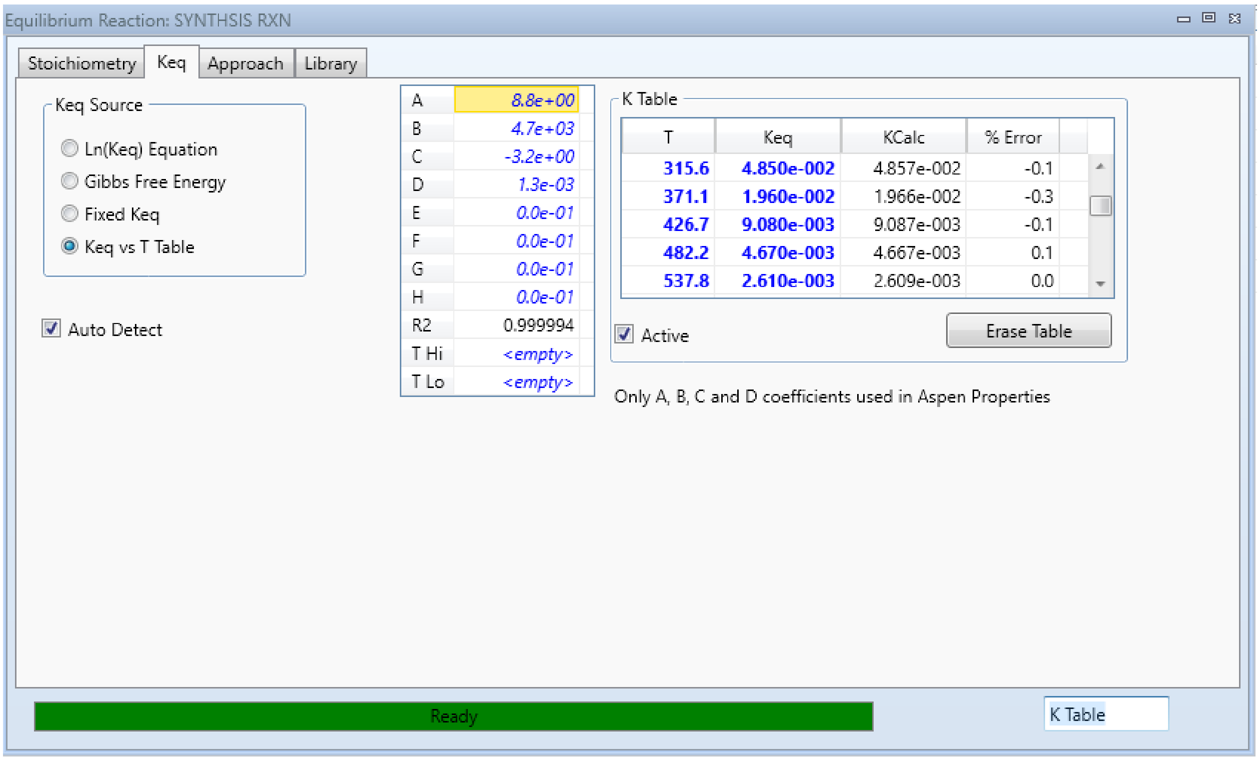
Basis

Basis	Partial Press
Phase	VapourPhase
Min Temperature	-273.1 C
Max Temperature	3000 C

Basis Units: kg/cm2

Figure 18 Reaction Set 6

For all equilibrium reaction sets K_{eq} vs Temperature data was obtained from literature and industry:



Keq Source

○ Ln(Keq) Equation
○ Gibbs Free Energy
○ Fixed Keq
● Keq vs T Table

☑ Auto Detect

A	8.8e+00
B	4.7e+03
C	-3.2e+00
D	1.3e-03
E	0.0e-01
F	0.0e-01
G	0.0e-01
H	0.0e-01
R2	0.999994
T Hi	<empty>
T Lo	<empty>

K Table

T	Keq	KCalc	% Error
315.6	**4.850e-002**	4.857e-002	-0.1
371.1	**1.960e-002**	1.966e-002	-0.3
426.7	**9.080e-003**	9.087e-003	-0.1
482.2	**4.670e-003**	4.667e-003	0.1
537.8	**2.610e-003**	2.609e-003	0.0

☑ Active

Only A, B, C and D coefficients used in Aspen Properties

Ready

Figure 19 Reaction Set 7

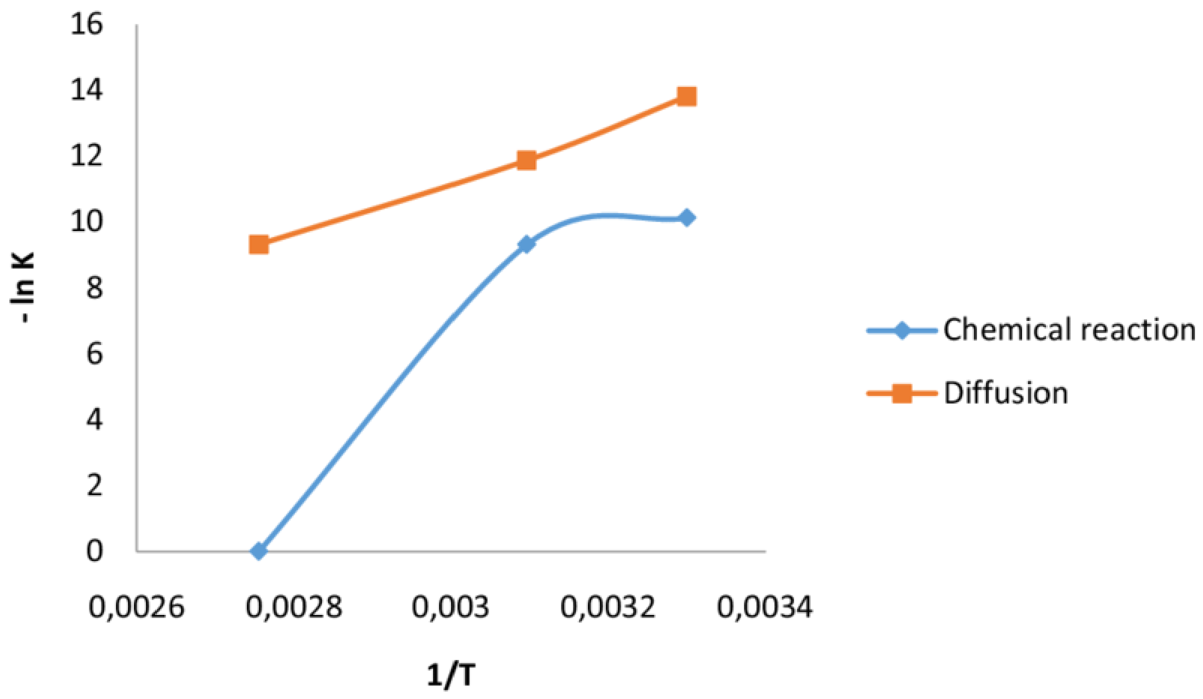


Figure 20 Keq vs T Graph for ammonia from literature

6.2.1 PFD developed on HYSYS:

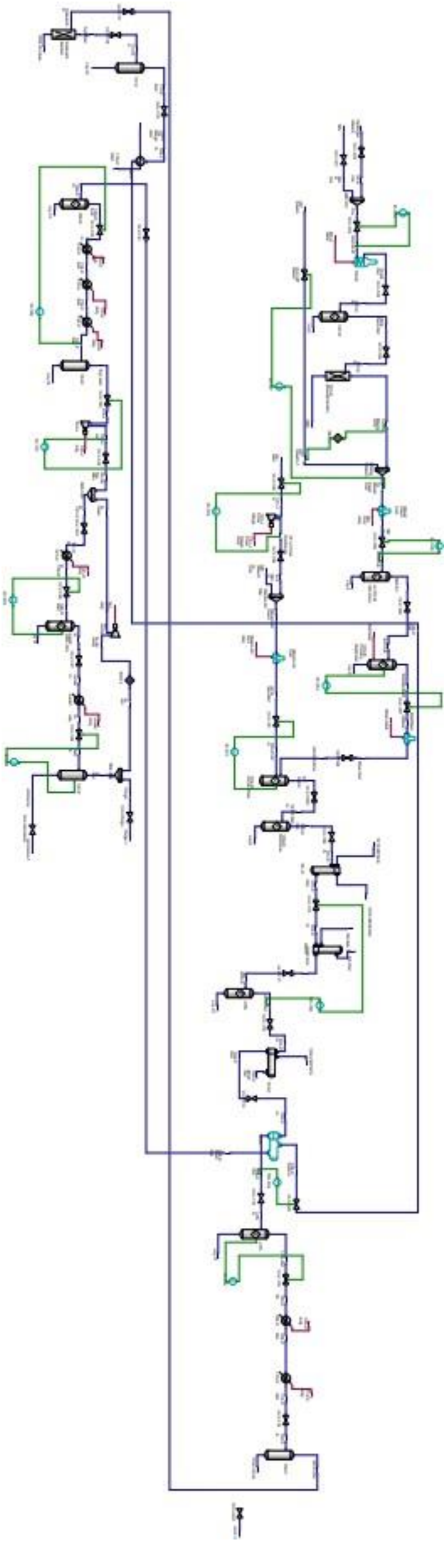


Figure 21 Main flowsheet on HYSYS

6.2.2 Feed and Product Specifications:

Subsequently, following data was inputted into the simulation and proceeded with the results.

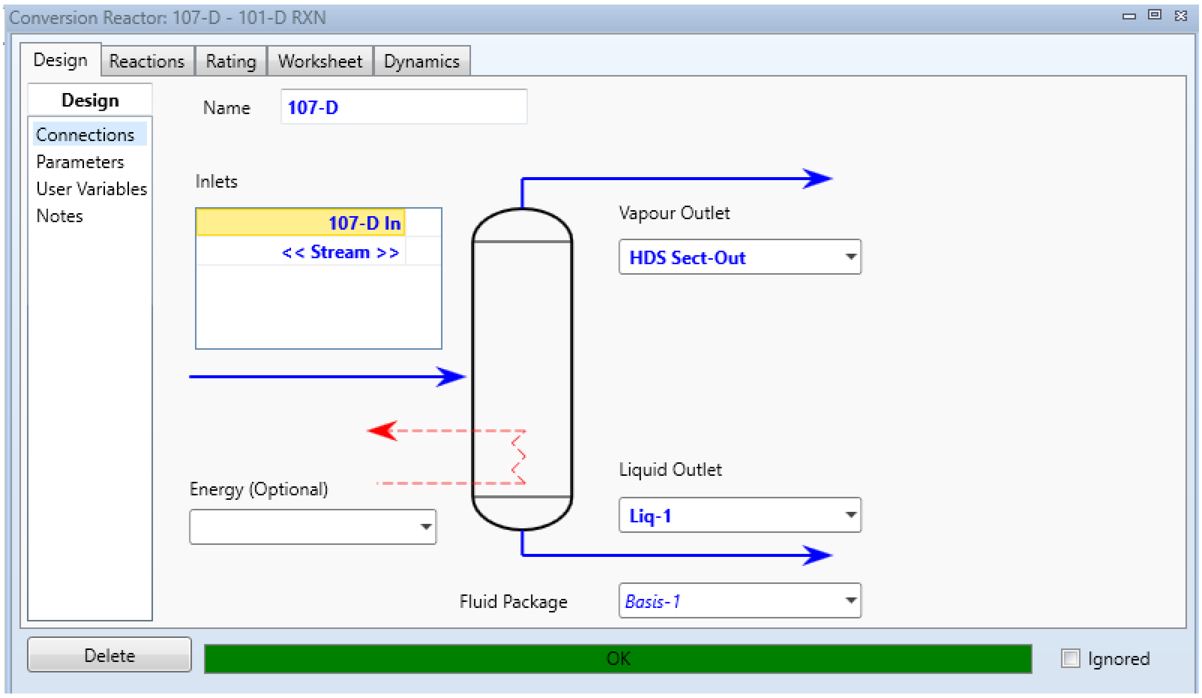
Table 34 Feed and Product Specifications

	Natural Gas	Air	Ammonia
T (°C)	40	40	26.8
Pressure (kg/cm^2)	35	2.039	96
Mass flow (kg/h)	2.7 x 10^4	4.3 x 10^4	4.01 x 10^4
Molar composition			
Nitrogen	0.0126	0.78	0.0006
Hydrogen	0.00	0.00	0.0106
Argon	0.0010	0.01	0.0001
CO	0.00	0.00	0.00
CO2	0.1059	0.00	0.00
Oxygen	0.00	0.21	0.00
Methane	0.8621	0.00	0.0033
Ethane	0.0142	0.00	0.00
Propane	0.002	0.00	0.00
n-Butane	0.001	0.00	0.00
i-Butane	0.001	0.00	0.00
i-Pentane	0.001	0.00	0.00
n-Pentane	0.001	0.00	0.00
n-Hexane	0.001	0.00	0.00
H2O	0.00	0.00	0.0047
Methanol	0.00	0.00	0.00

Ammonia	0.00	0.00	0.9807
M-Mercaptan	0.0001	0.00	0.00
nB-Mercaptan	0.00	0.00	0.00
E-Mercaptan	0.00	0.00	0.00
H2S	0.00	0.00	0.00

The ammonia synthesis process only has one product stream apart from the final product, this stream is SEP5-1, and it is one of the most important steps of the process as it is the purge necessary to ensure that the percentage of inert components entering the reactor is lower than 12%.

6.2.3 Hydrogenator Specification:



Conversion Reactor: 107-D - 101-D RXN

Name: 107-D

Inlets: 107-D In

Vapour Outlet: HDS Sect-Out

Liquid Outlet: Liq-1

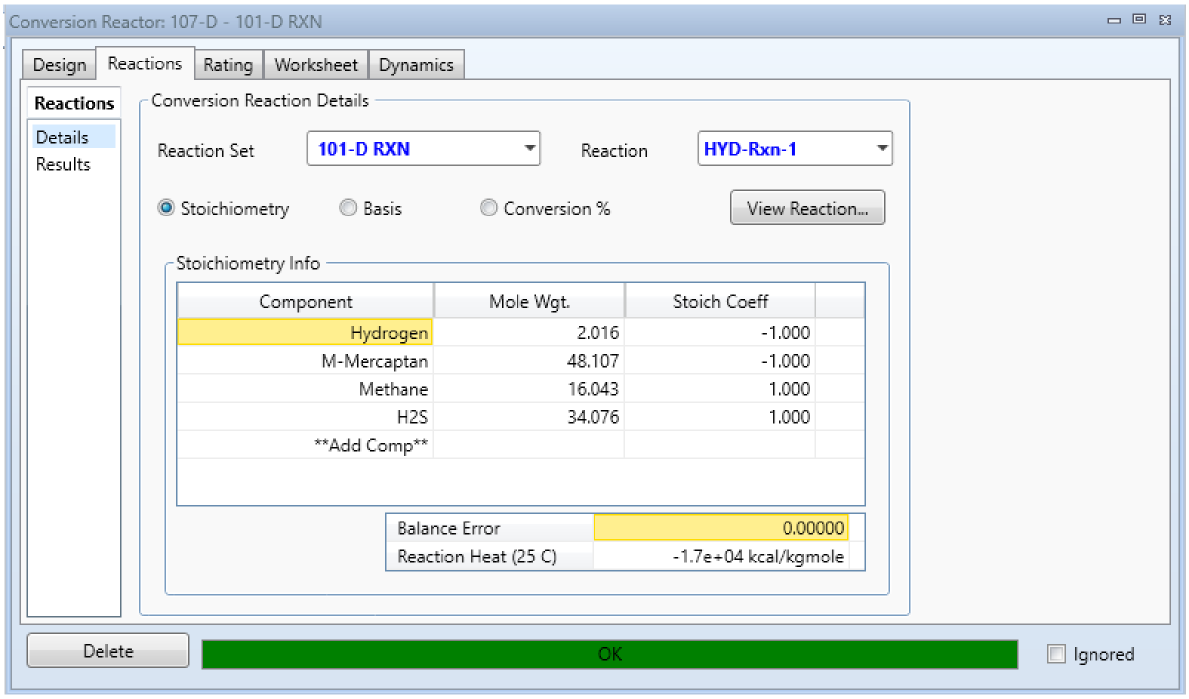
Energy (Optional):

Fluid Package: Basis-1

OK

☐ Ignored

Figure 22 Hydrogenator



Reaction Set: 101-D RXN

Reaction: HYD-Rxn-1

● Stoichiometry ○ Basis ○ Conversion %

Component	Mole Wgt.	Stoich Coeff
Hydrogen	2.016	-1.000
M-Mercaptan	48.107	-1.000
Methane	16.043	1.000
H2S	34.076	1.000
Add Comp		

Balance Error	0.00000
Reaction Heat (25 C)	-1.7e+04 kcal/kgmole

Figure 23 Hydrogenator Specification 2

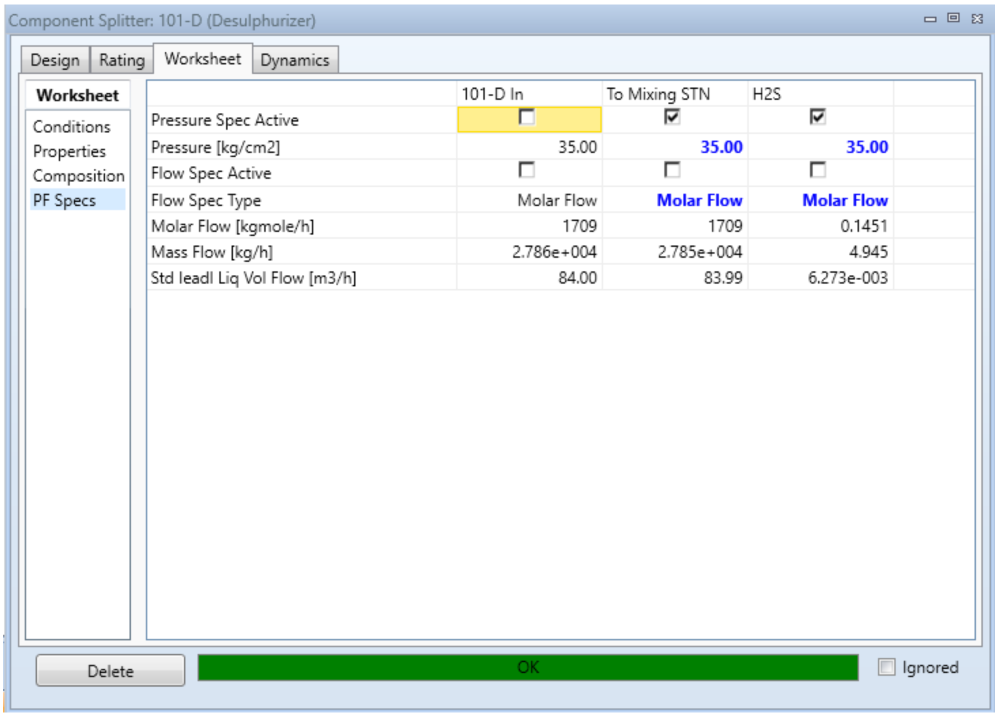
6.2.4 Dynamic Data and Specification

Dynamic Tab Data for Hydrogenator:

Height	Diameter	Volume
6.84 m	1.79 m	17.21 m^3

Desulphurizer Specifications:

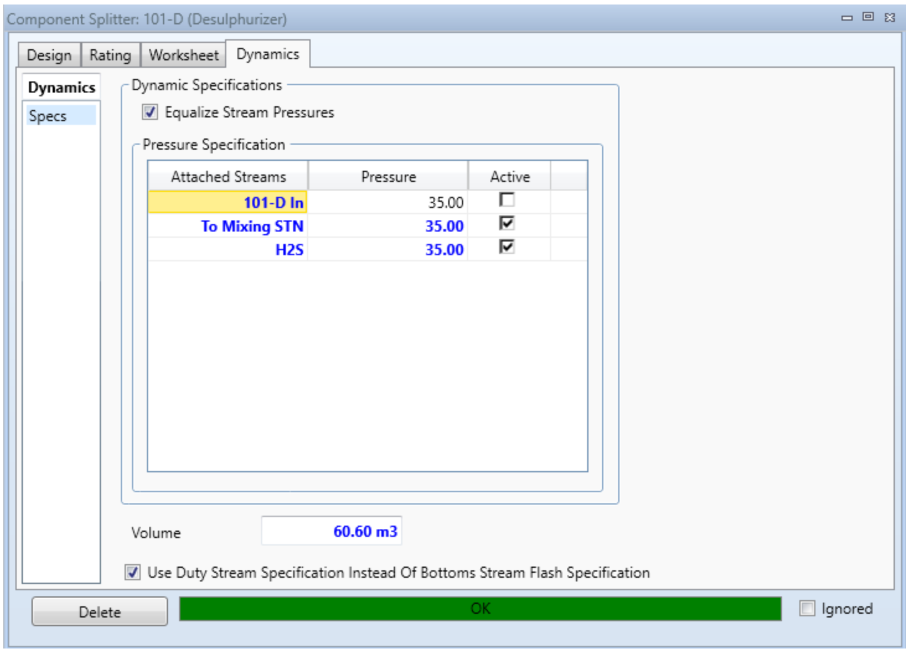
Due to constraint of using solid ZnO in the reaction, this section was simulated using Aspen HYSYS component splitter block to remove the H2S achieving same results.



	101-D In	To Mixing STN	H2S
Pressure Spec Active	☐	☑	☑
Pressure [kg/cm2]	35.00	35.00	35.00
Flow Spec Active	☐	☐	☐
Flow Spec Type	Molar Flow	Molar Flow	Molar Flow
Molar Flow [kgmole/h]	1709	1709	0.1451
Mass Flow [kg/h]	2.786e+004	2.785e+004	4.945
Std Ideal Liq Vol Flow [m3/h]	84.00	83.99	6.273e-003

Figure 24 Desulphurizer Specifications

Dynamics Tab Data for Desulphurizer:



Dynamic Specifications

☑ Equalize Stream Pressures

Pressure Specification

Attached Streams	Pressure	Active
101-D In	35.00	☐
To Mixing STN	35.00	☑
H2S	35.00	☑

Volume 60.60 m3

☑ Use Duty Stream Specification Instead Of Bottoms Stream Flash Specification

Figure 25 Dynamic Tab for Desulphurizer 2

Primary Reformer Specifications:

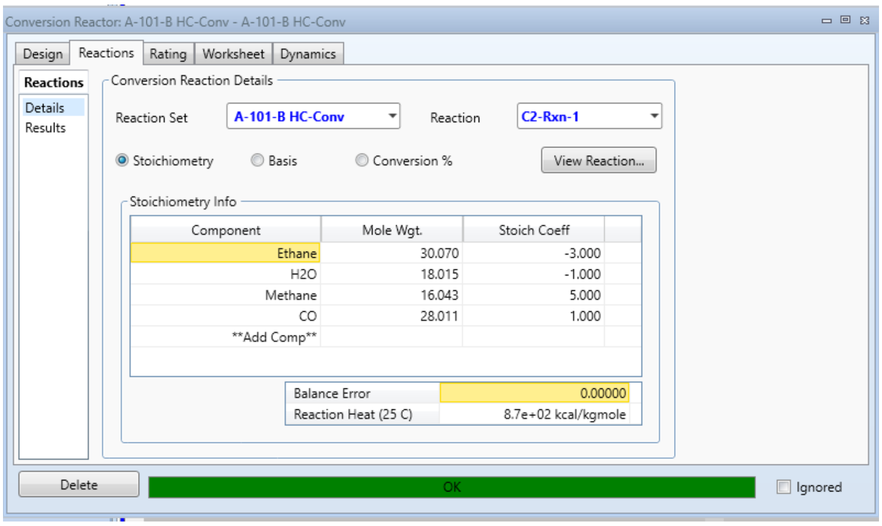
Following Reactions were simulated in the first section of the primary reformer 103-D:

$C3H8 + H2O \rightleftharpoons 3CO + 4H2\ C4H10$

$+ H2O \rightleftharpoons 4CO + 5H2\ C5H12 + H2O$

$\rightleftharpoons 5CO + 6H2\ C6H14 + H2O \rightleftharpoons 6CO$

$+ 7H2$



Conversion Reactor: A-101-B HC-Conv - A-101-B HC-Conv

Conversion Reaction Details

Reaction Set: A-101-B HC-Conv

Reaction: C2-Rxn-1

● Stoichiometry ○ Basis ○ Conversion %

Stoichiometry Info

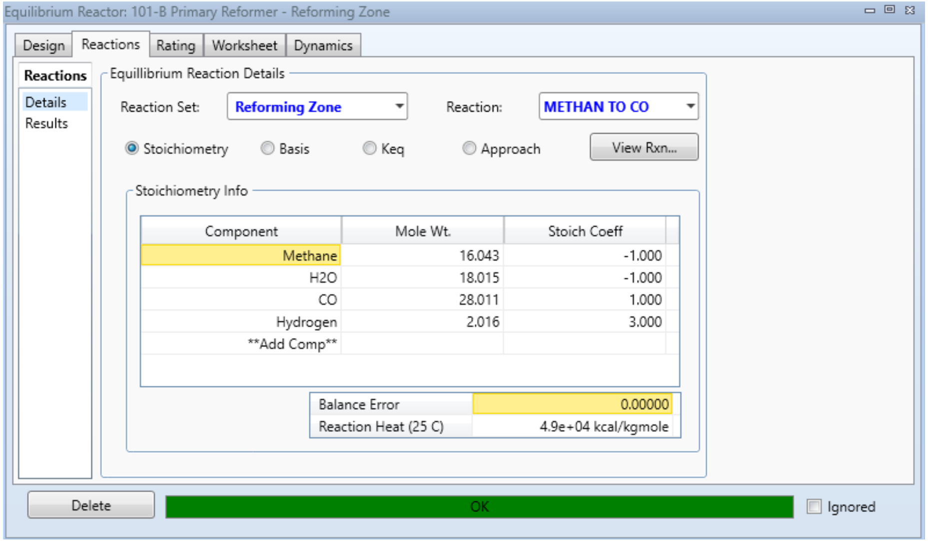
Component	Mole Wgt.	Stoich Coeff
Ethane	30.070	-3.000
H2O	18.015	-1.000
Methane	16.043	5.000
CO	28.011	1.000
Add Comp		

Balance Error	0.00000
Reaction Heat (25 C)	8.7e+02 kcal/kgmole

Figure 26 Primary Reformer Specifications

It is then proceeded for the main primary reformer reaction:

$CH4 + H2O \rightleftharpoons CO + 3H2$



Equilibrium Reactor: 101-B Primary Reformer - Reforming Zone

Equillibrium Reaction Details

Reaction Set: Reforming Zone

Reaction: METHAN TO CO

● Stoichiometry ○ Basis ○ Keq ○ Approach

Stoichiometry Info

Component	Mole Wt.	Stoich Coeff
Methane	16.043	-1.000
H2O	18.015	-1.000
CO	28.011	1.000
Hydrogen	2.016	3.000
Add Comp		

Balance Error	0.00000
Reaction Heat (25 C)	4.9e+04 kcal/kgmole

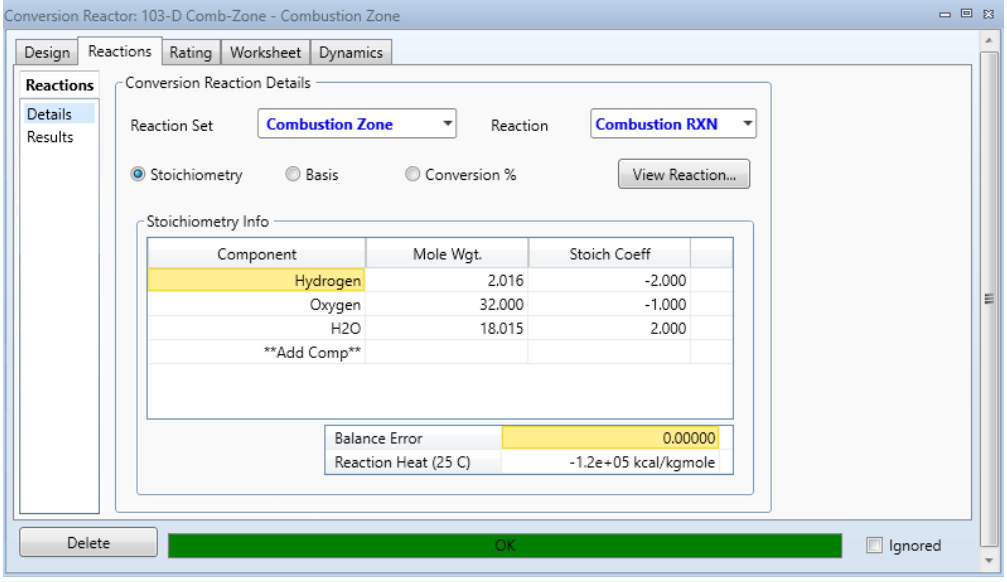
Figure 27 Primary Reformer Specifications 2

Dynamic Tab Data for Primary Reformer:

Height	Diameter	Volume
21.4	3.9	348 m^3

Secondary Reformer Specifications

In the first zone, combustion reaction takes place.



Conversion Reactor: 103-D Comb-Zone - Combustion Zone

Conversion Reaction Details

Reaction Set: Combustion Zone

Reaction: Combustion RXN

● Stoichiometry ○ Basis ○ Conversion %

Stoichiometry Info

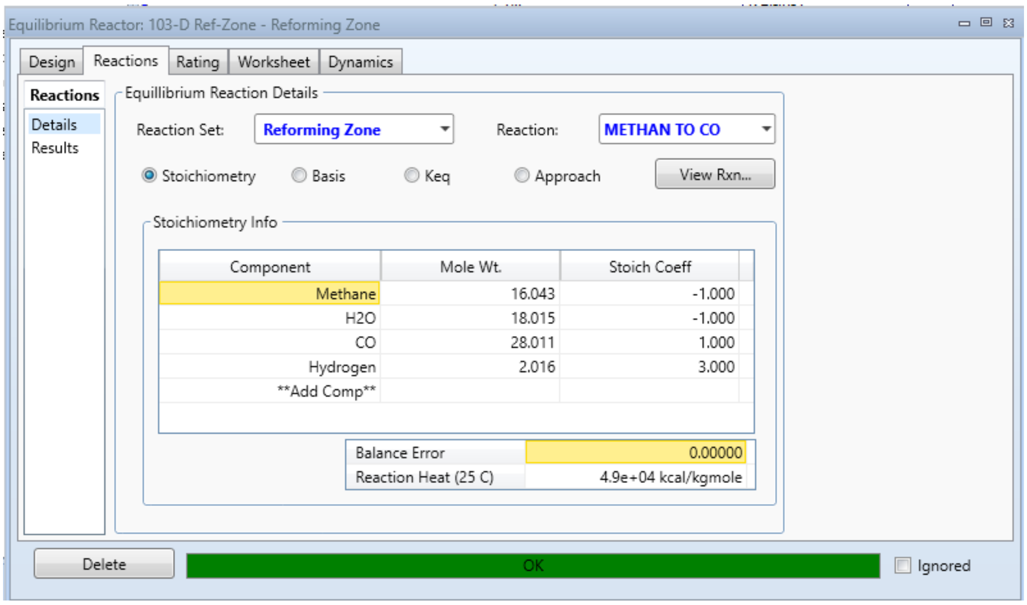
Component	Mole Wgt.	Stoich Coeff
Hydrogen	2.016	-2.000
Oxygen	32.000	-1.000
H2O	18.015	2.000
Add Comp		

Balance Error	0.00000
Reaction Heat (25 C)	-1.2e+05 kcal/kgmole

☐ Ignored

Figure 28 Secondary Reformer Specifications 1

Second zone, for reforming reaction:



Equilibrium Reactor: 103-D Ref-Zone - Reforming Zone

Equillibrium Reaction Details

Reaction Set: Reforming Zone

Reaction: METHAN TO CO

● Stoichiometry ○ Basis ○ Keq ○ Approach

Stoichiometry Info

Component	Mole Wt.	Stoich Coeff
Methane	16.043	-1.000
H2O	18.015	-1.000
CO	28.011	1.000
Hydrogen	2.016	3.000
Add Comp		

Balance Error	0.00000
Reaction Heat (25 C)	4.9e+04 kcal/kgmole

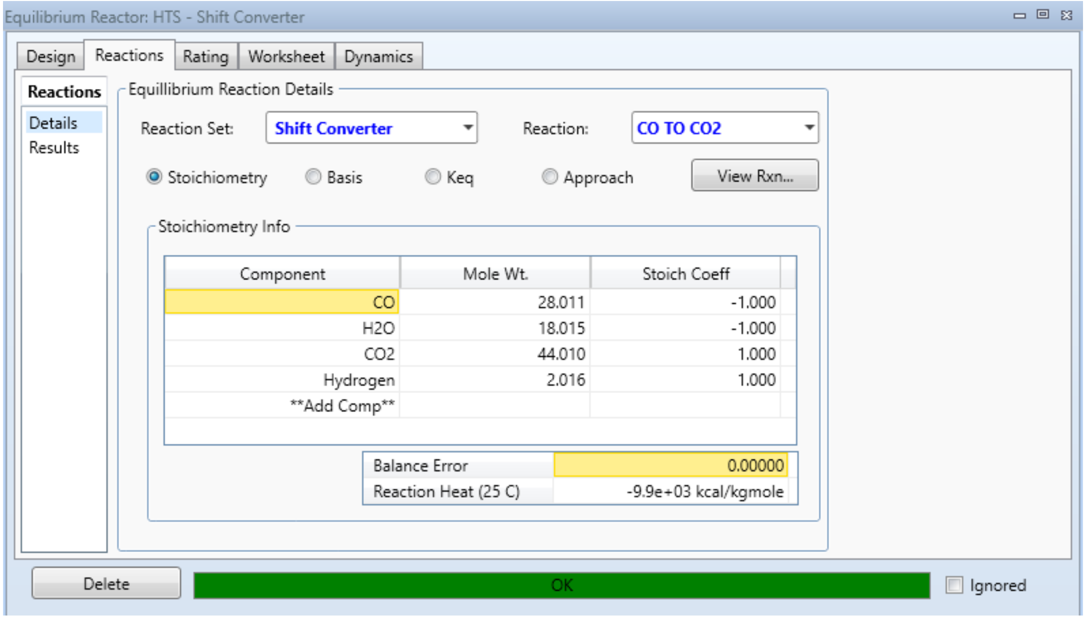
☐ Ignored

Figure 29 Secondary Reformer Specifications 2

Dynamic Tab Data for Secondary Reformer:

Height	Diameter	Volume
15.49 m	3.965 m	194. 8 m^3

High Temperature Shift Reactor:



Reaction Set: Shift Converter

Reaction: CO TO CO2

● Stoichiometry ○ Basis ○ Keq ○ Approach

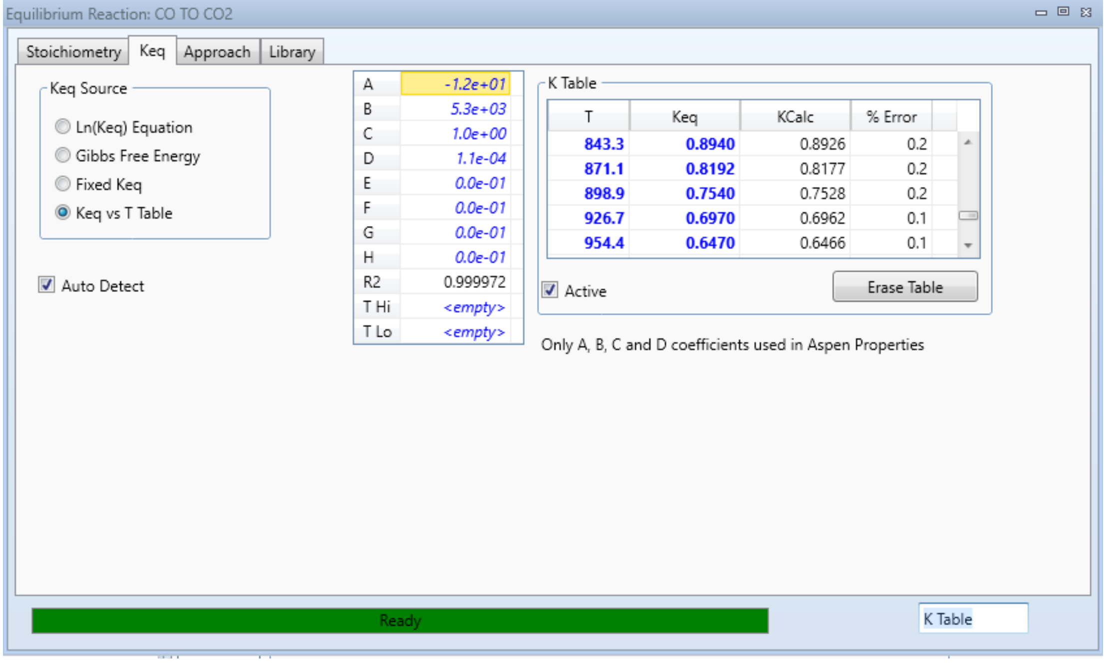
Component	Mole Wt.	Stoich Coeff
CO	28.011	-1.000
H2O	18.015	-1.000
CO2	44.010	1.000
Hydrogen	2.016	1.000
Add Comp		

Balance Error	0.00000
Reaction Heat (25 C)	-9.9e+03 kcal/kgmole

☐ Ignored

Figure 30 High Temperature Shift Reactor 1

The following Keq vs T data was used in the reaction:



Keq Source

- ○ Ln(Keq) Equation
- ○ Gibbs Free Energy
- ○ Fixed Keq
- ● Keq vs T Table

☑ Auto Detect

A	-1.2e+01
B	5.3e+03
C	1.0e+00
D	1.1e-04
E	0.0e-01
F	0.0e-01
G	0.0e-01
H	0.0e-01
R2	0.999972
T Hi	<empty>
T Lo	<empty>

K Table

T	Keq	KCalc	% Error
843.3	0.8940	0.8926	0.2
871.1	0.8192	0.8177	0.2
898.9	0.7540	0.7528	0.2
926.7	0.6970	0.6962	0.1
954.4	0.6470	0.6466	0.1

☑ Active

Only A, B, C and D coefficients used in Aspen Properties

Ready

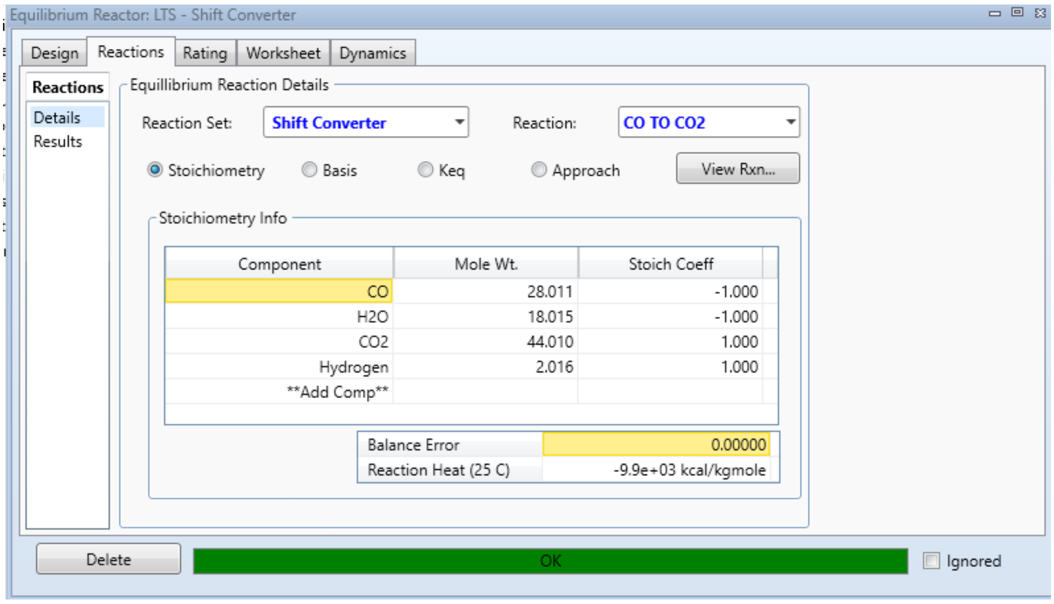
K Table

Figure 31 High Temperature Shift Reactor 2

Dynamic Tab Data for HT Shift Reactor:

Height	Diameter	Volume
4.31 m	3.966 m	53.7 m^3

Low Temperature Shift Reactor Specifications:



Equilibrium Reaction Details

Reaction Set: Shift Converter

Reaction: CO TO CO2

● Stoichiometry ○ Basis ○ Keq ○ Approach

Stoichiometry Info

Component	Mole Wt.	Stoich Coeff
CO	28.011	-1.000
H2O	18.015	-1.000
CO2	44.010	1.000
Hydrogen	2.016	1.000
Add Comp		

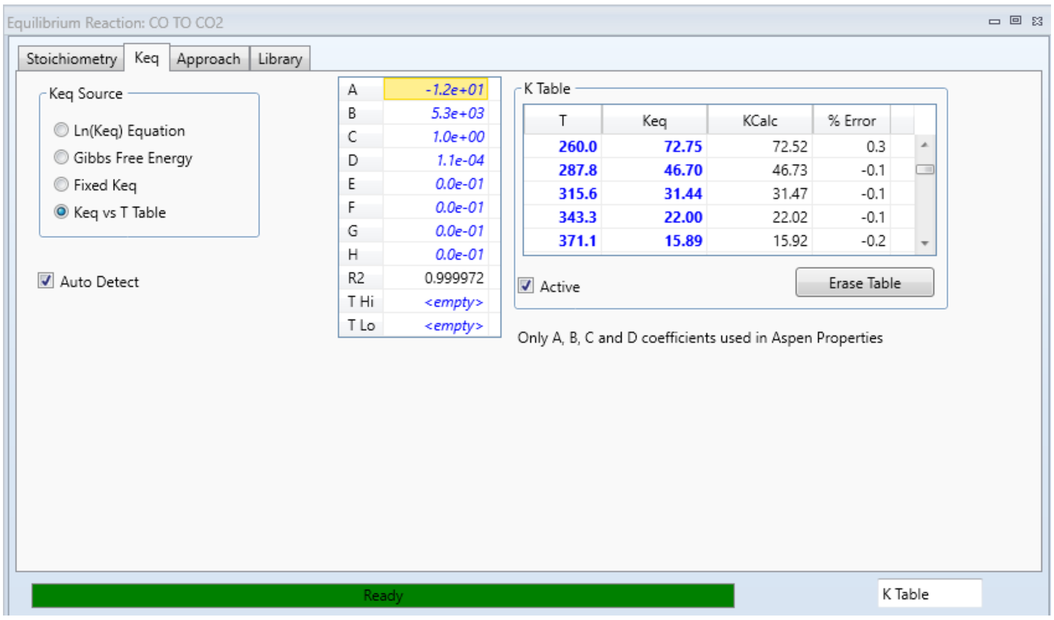
Balance Error	0.00000
Reaction Heat (25 C)	-9.9e+03 kcal/kgmole

OK

☐ Ignored

Figure 32 Low Temperature Shift Reactor Specifications 1

Following Keq vs T data was used in the reaction:



Keq Source

○ Ln(Keq) Equation
○ Gibbs Free Energy
○ Fixed Keq
● Keq vs T Table

☑ Auto Detect

A	-1.2e+01
B	5.3e+03
C	1.0e+00
D	1.1e-04
E	0.0e-01
F	0.0e-01
G	0.0e-01
H	0.0e-01
R2	0.999972
T Hi	<empty>
T Lo	<empty>

K Table

T	Keq	KCalc	% Error
260.0	72.75	72.52	0.3
287.8	46.70	46.73	-0.1
315.6	31.44	31.47	-0.1
343.3	22.00	22.02	-0.1
371.1	15.89	15.92	-0.2

☑ Active

Only A, B, C and D coefficients used in Aspen Properties

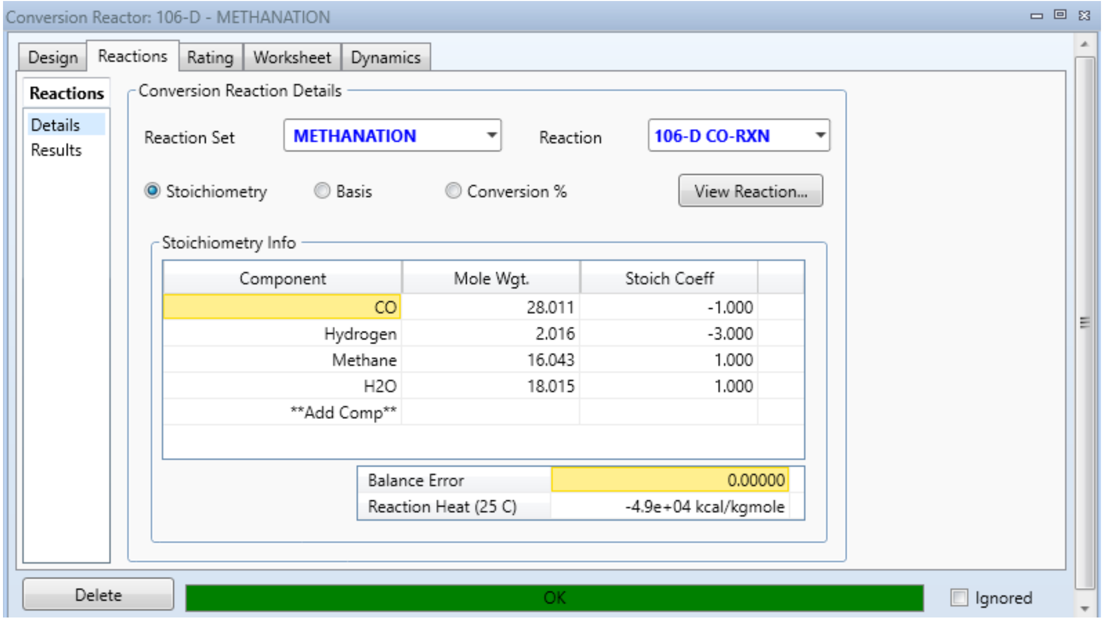
K Table

Figure 33 Low Temperature Shift Reactor Specifications 2

Dynamic Tab Data for LT Shift Reactor:

Height	Diameter	Volume
4.31 m	3.966 m	53.7 m^3

Methanator Specifications:



Conversion Reaction Details

Reaction Set: METHANATION

Reaction: 106-D CO-RXN

● Stoichiometry ○ Basis ○ Conversion %

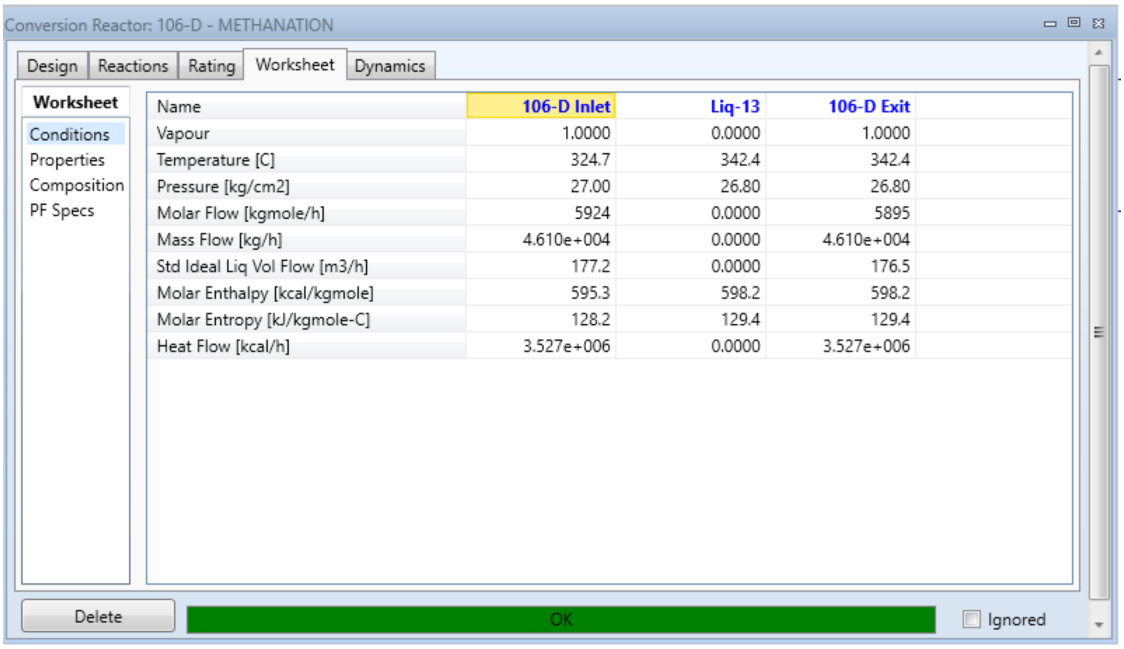
Stoichiometry Info

Component	Mole Wgt.	Stoich Coeff
CO	28.011	-1.000
Hydrogen	2.016	-3.000
Methane	16.043	1.000
H2O	18.015	1.000
Add Comp		

Balance Error	0.00000
Reaction Heat (25 C)	-4.9e+04 kcal/kgmole

☐ Ignored

Figure 34 Methanator Specifications 1



Conversion Reactor: 106-D - METHANATION

Worksheet

Name	106-D Inlet	Liq-13	106-D Exit
Vapour	1.0000	0.0000	1.0000
Temperature [C]	324.7	342.4	342.4
Pressure [kg/cm2]	27.00	26.80	26.80
Molar Flow [kgmole/h]	5924	0.0000	5895
Mass Flow [kg/h]	4.610e+004	0.0000	4.610e+004
Std Ideal Liq Vol Flow [m3/h]	177.2	0.0000	176.5
Molar Enthalpy [kcal/kgmole]	595.3	598.2	598.2
Molar Entropy [kJ/kgmole-C]	128.2	129.4	129.4
Heat Flow [kcal/h]	3.527e+006	0.0000	3.527e+006

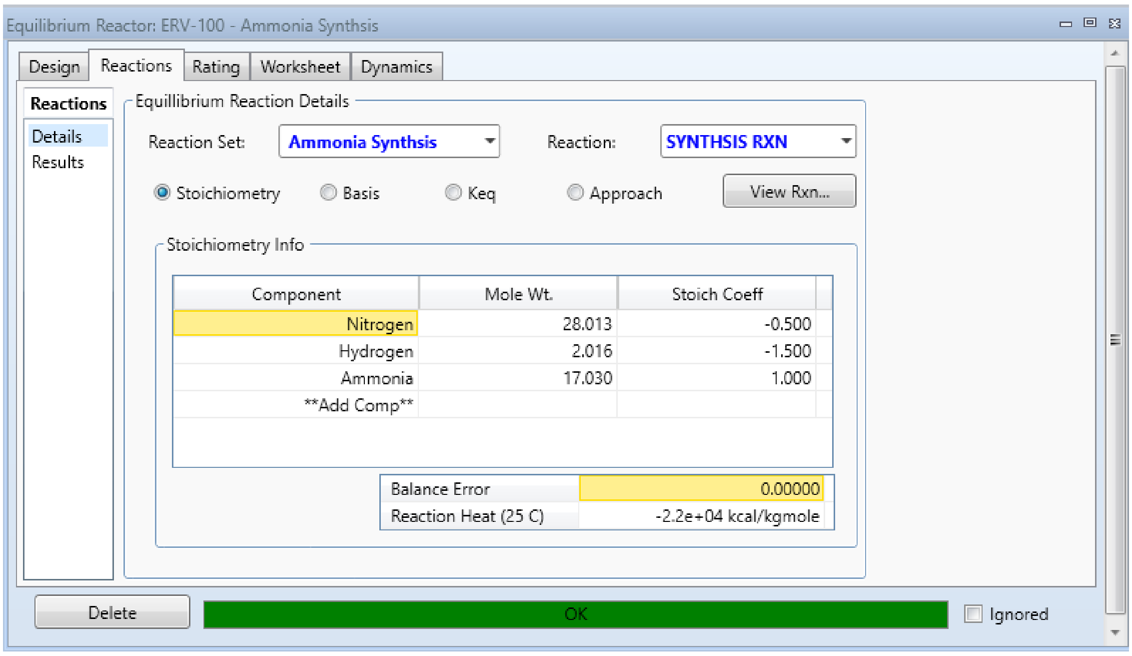
OK

Figure 35 Methanator Specifications 2

Dynamic Tab Data for Methanator Reactor:

Height	Diameter	Volume
4.31 m	3.96 m	53.7 m^3

Ammonia Synthesis Specifications:



Equilibrium Reactor: ERV-100 - Ammonia Synthesis

Reactions

Equillibrium Reaction Details

Reaction Set: Ammonia Synthesis

Reaction: SYNTHSIS RXN

● Stoichiometry ○ Basis ○ Keq ○ Approach

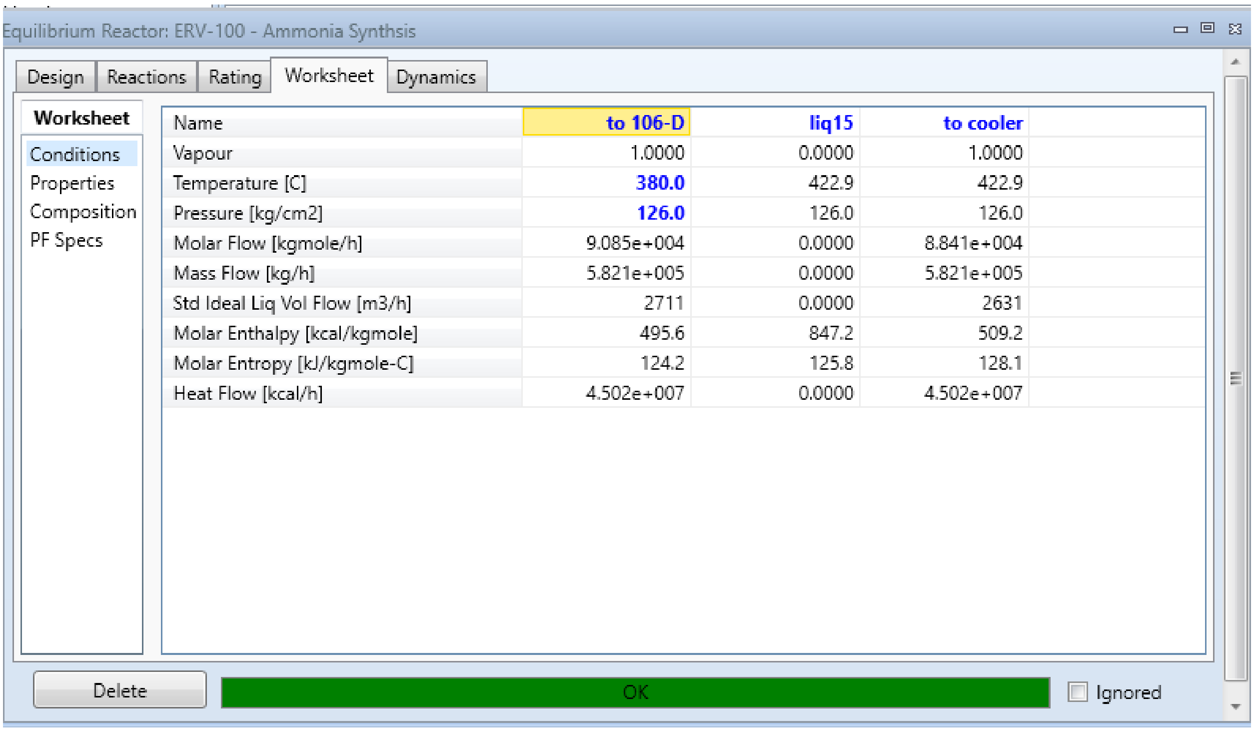
Stoichiometry Info

Component	Mole Wt.	Stoich Coeff
Nitrogen	28.013	-0.500
Hydrogen	2.016	-1.500
Ammonia	17.030	1.000
Add Comp		

Balance Error	0.00000
Reaction Heat (25 C)	-2.2e+04 kcal/kgmole

OK

Figure 36 Ammonia Synthesis Specifications 1



Name	to 106-D	liq15	to cooler
Vapour	1.0000	0.0000	1.0000
Temperature [C]	380.0	422.9	422.9
Pressure [kg/cm2]	126.0	126.0	126.0
Molar Flow [kgmole/h]	9.085e+004	0.0000	8.841e+004
Mass Flow [kg/h]	5.821e+005	0.0000	5.821e+005
Std Ideal Liq Vol Flow [m3/h]	2711	0.0000	2631
Molar Enthalpy [kcal/kgmole]	495.6	847.2	509.2
Molar Entropy [kJ/kgmole-C]	124.2	125.8	128.1
Heat Flow [kcal/h]	4.502e+007	0.0000	4.502e+007

Figure 37 Ammonia Synthesis Specifications 2

Dynamic Tab Data for Ammonia Synthesis Reactor:

Height	Diameter	Volume
8.9 m	4.8 m	248.3 m^3

Other equipment Dynamic Data:

Control Valves:

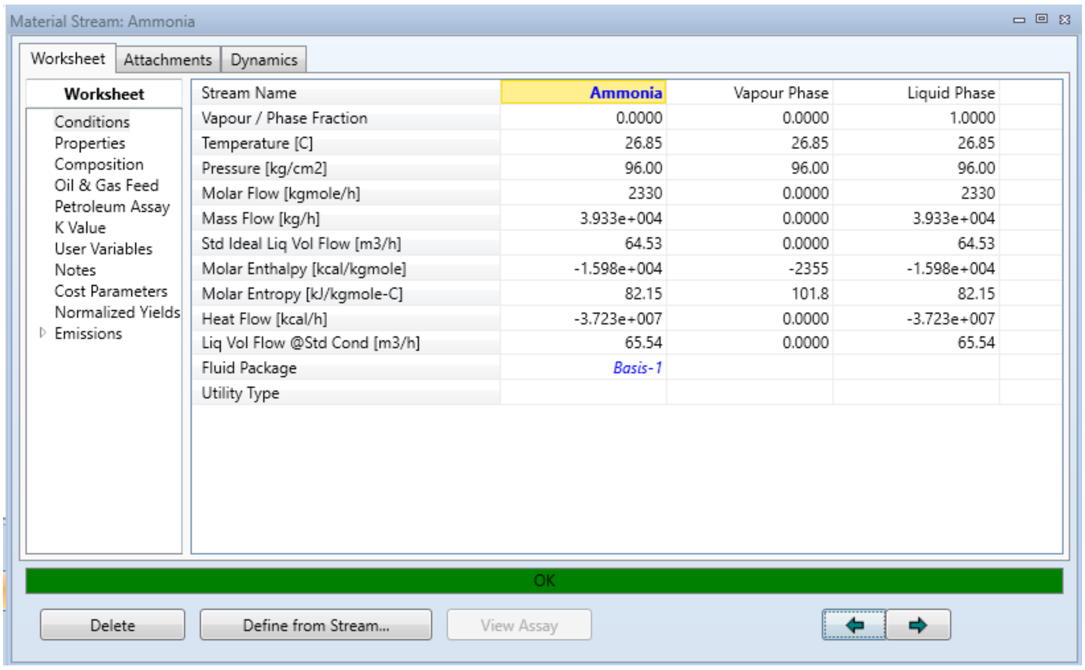
- Valve Opening: 50%
- Pressure Drop: 0.1 kg/cm2
- Valve Sizing: Auto

Compressor:

- Polytropic Efficiency: 75%
- Head: 125539 (Suction)

- Speed: 10400 rpm
- Full Load power: 14.5 MW bhp

6.3 Simulation Results and need for simulation



Stream Name	Ammonia	Vapour Phase	Liquid Phase
Vapour / Phase Fraction	0.0000	0.0000	1.0000
Temperature [C]	26.85	26.85	26.85
Pressure [kg/cm2]	96.00	96.00	96.00
Molar Flow [kgmole/h]	2330	0.0000	2330
Mass Flow [kg/h]	3.933e+004	0.0000	3.933e+004
Std Ideal Liq Vol Flow [m3/h]	64.53	0.0000	64.53
Molar Enthalpy [kcal/kgmole]	-1.598e+004	-2355	-1.598e+004
Molar Entropy [kJ/kgmole-C]	82.15	101.8	82.15
Heat Flow [kcal/h]	-3.723e+007	0.0000	-3.723e+007
Liq Vol Flow @Std Cond [m3/h]	65.54	0.0000	65.54
Fluid Package	Basis-1		
Utility Type			

OK

Figure 38 Simulation Results

**949 MET/day production with 98.07% purity of ammonia was achieved from the simulation which is in-line with required objective.*

The need for Simulation:

HYSYS is a process modelling and simulation model, i.e. whatever it calculates, is based on a mathematical model derived from various branches of chemical engineering such as thermodynamics, heat transfer, mass transfer, fluid mechanics and the list is long. During manual calculations, the very same models, or variants of the model was applied, therefore, our results should be comparable to the HYSYS simulation results, if not comparable, and there should be a logical explanation for it. It also serves as a base model to further study instrumentation and implement Dynamic mode Controller for the ammonia production unit.

CHAPTER 7

INSTRUMENTATION

A control system comprises a network of computer interfaces and controllers that are interconnected to ensure a cohesive and coordinated operation, such as in the industrial production of ammonia. Consequently, choosing an effective control system is crucial for the smooth functioning of a chemical plant.

A control loop encompasses four essential components:

- Sensor
- Transmitter
- Transducer
- Final Control element

The process begins with the sensor detecting the desired value for control. Next, the transmitter converts this value into electrical or voltage signals. These signals are then transformed by the transducer into a readable format, enabling them to control the final control element, typically a Control Valve. This control mechanism is responsible for regulating the controlled variable.

There are three types of variables in instrumentation:

- Control Variable
- Manipulated Variable
- Process Variable

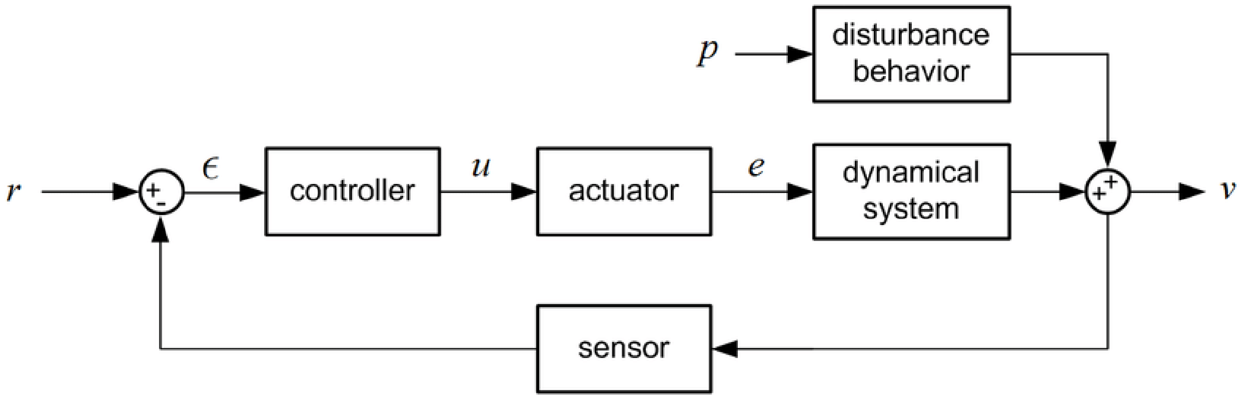


Figure 39: Components involved in a Control Loop

In a control system, various variables play essential roles in ensuring the desired operation and stability of a process. The control variable, also known as the controlled variable or process variable, is the parameter or property that needs to be regulated and maintained within a specific range or setpoint. It represents the output or the measurable quantity that the control system aims to control. Examples of control variables include temperature, pressure, flow rate, level, or composition.

The manipulated variable, also referred to as the control input or actuating variable, is the parameter that the control system actively adjusts or manipulates to influence and regulate the control variable. It is the variable that the controller can modify to achieve the desired control objective. The manipulated variable can be adjusted based on the feedback received from sensors or other control strategies. For instance, a control system may modulate the opening of a valve to regulate the flow rate or adjust the power input to a heater to control the temperature.

Disturbance variables, also known as disturbances or perturbations, are external or internal factors that can affect the control system and cause deviations in the control variable. These variables are typically undesired and can arise from factors such as changes in the input conditions, fluctuations in process parameters, or external disturbances. Examples of disturbance variables include changes in feed composition, variations in ambient temperature, or sudden load changes. Control systems are designed to mitigate the impact of disturbance variables and maintain the stability and performance of the control variable by appropriately adjusting the manipulated variable in response to these disturbances.

7.1 Dynamic Mode Controller:

Dynamic Mode Controller is the design strategy that is incorporated in the plant to retify real-time fluctuations in the process.

Dynamic mode controllers differ from static controllers in that they consider more than just the current state of the system. Instead, they rely on feedback information obtained from sensors or measurements to continuously monitor and adjust the manipulated variable. These controllers analyze the system's response over time, taking into account factors such as the rate of change, stability, and accumulation of errors.

Various control algorithms and techniques, including proportional-integral-derivative (PID) control, model predictive control (MPC), adaptive control, and advanced control strategies, are employed by dynamic mode controllers. These controllers leverage mathematical models, historical data, or real-time information to determine how to adjust the manipulated variable.

The primary objective of a dynamic mode controller is to maintain the controlled variable within predefined limits while minimizing errors or deviations from the setpoint. Additionally, these controllers strive to optimize performance criteria such as stability, response time, robustness, and disturbance rejection. By continuously monitoring and adjusting the control action, dynamic mode controllers aim to achieve precise and efficient control of dynamic systems.

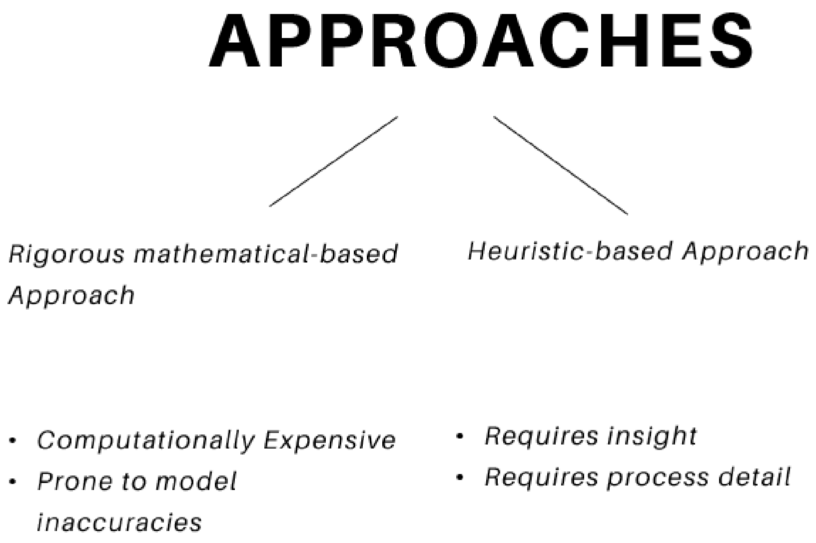


Figure 40: Types of control loop approaches

7.1.1 Our Methodology:

The growing focus on process economics in contemporary chemical plants has resulted in a heightened adoption of material recycling and energy integration practices. These practices have substantial effects on process dynamics and introduce increased complexity. Consequently, numerous plantwide control (PWC) methodologies have emerged. However, there is a scarcity of comparative studies evaluating the effectiveness of alternative methodologies. In this final year project, we develop a PWC structure for the ammonia synthesis process by employing an integrated framework of simulation and heuristics [Konda et al. Ind. Eng. Chem. Res.2005, 44, 8300–8313].

Figure 41: Our Approach

Based on the above approach following control methodology was proposed:

- Establish Plantwide Control Objectives
- Identify and analyze Disturbances affecting the entire plant and select Control Loops Accordingly
- Define Control Variables
- Determine suitable Manipulated Variables
- Select Manipulators for Less critical Controlled Variables
- Implement control strategies for Unit Operations
- Investigate integration effects
- Improve Control System performance by utilizing the remaining Control Degrees of Freedom (CDOFs)

N.I.S vs I.S controllers:

The distinction between non-intrinsic safe (N.I.S) and intrinsic safe (I.S) controllers lies in their suitability for operating in hazardous environments. Non-intrinsic safe controllers are not designed for use in areas where there may be explosive or flammable atmospheres, as they lack the requisite safety features to prevent the generation of ignition sources. In contrast, intrinsic safe controllers are purpose-built and undergo certification processes to ensure their safe operation in such hazardous areas. They incorporate safety measures that restrict electrical energy and mitigate the risk of sparks or arcs that could potentially ignite the surrounding atmosphere. Rigorous testing and certification procedures specific to hazardous environments validate the ability of intrinsic safe controllers to operate safely without posing a risk of ignition. Consequently, the key differentiation lies in the presence of safety features, certifications, and suitability for hazardous environments, with intrinsic safe controllers offering the necessary protection in such settings.

2/4 wire controllers:

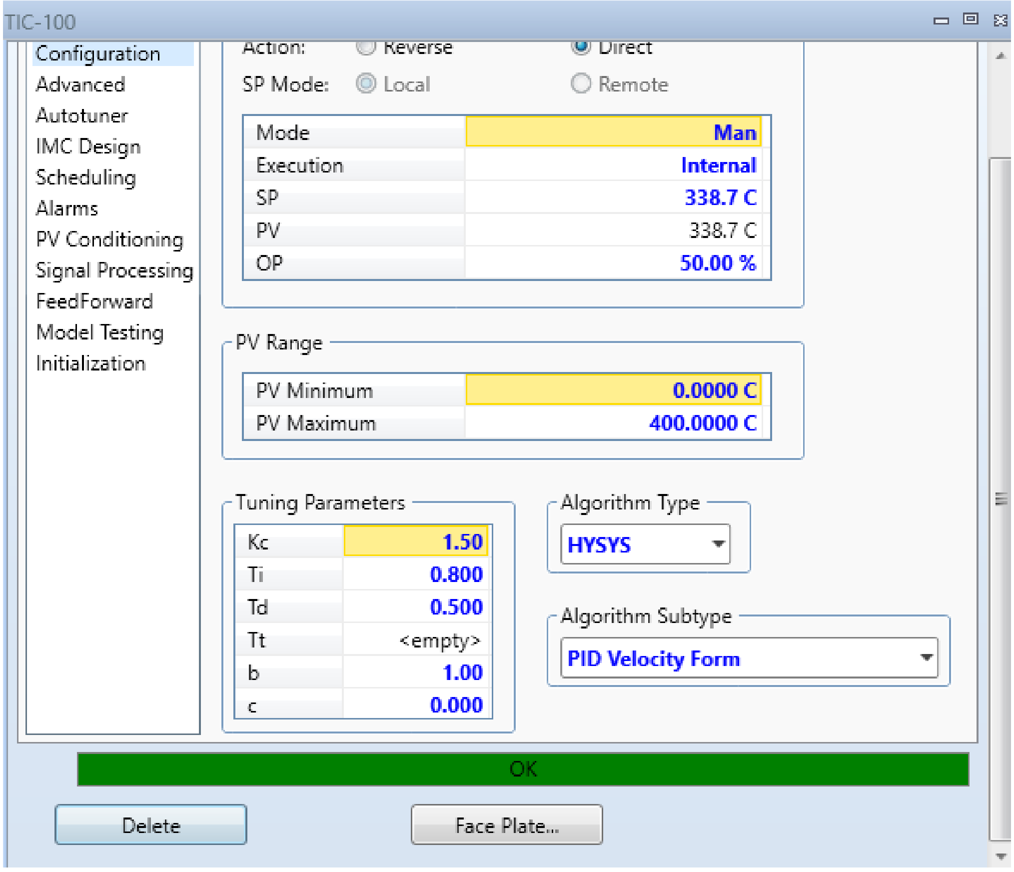
The primary distinction between 2-wire and 4-wire control systems resides in the quantity of wires employed for transmitting control signals. In 2-wire control systems, a mere two wires serve the dual purpose of carrying both the power supply and control signals. These systems find application in straightforward control scenarios that prioritize cost-effectiveness and wiring simplicity. By utilizing the same wires for power supply and control signals, however, the effective transmission distance of the control signals may be limited.

Conversely, 4-wire control systems utilize distinct wires for power supply and control signals. Two wires are specifically allocated to the power supply, ensuring a stable and reliable source of electrical energy. The remaining two wires facilitate the transmission of control signals, enabling greater separation between the controller and the controlled devices. This segregation of power and control signals fosters enhanced signal integrity, reducing interference and facilitating accurate and efficient control.

While 2-wire control systems offer simplicity and cost efficiency, they may encounter limitations in terms of the distance over which control signals can be effectively transmitted. In contrast, 4-wire control systems, characterized by separate power and control lines, yield improved signal quality, and prove more suitable for applications necessitating extended transmission distances and precise control.

7.1.2 Method for tuning the controller:

The method employed for tuning the controller was “Hit and Trial Method” on Aspen HYSYS. In this method educated guesses are made for the Proportional, Integral and Derivative values until the offshoot value is offset.



Action: ○ Reverse ● Direct

SP Mode: ● Local ○ Remote

Mode	Man
Execution	Internal
SP	338.7 C
PV	338.7 C
OP	50.00 %

PV Range

PV Minimum	0.0000 C
PV Maximum	400.0000 C

Tuning Parameters

Kc	1.50
Ti	0.800
Td	0.500
Tt	<empty>
b	1.00
c	0.000

Algorithm Type: HYSYS

Algorithm Subtype: PID Velocity Form

Figure 42: Controller parameter tab

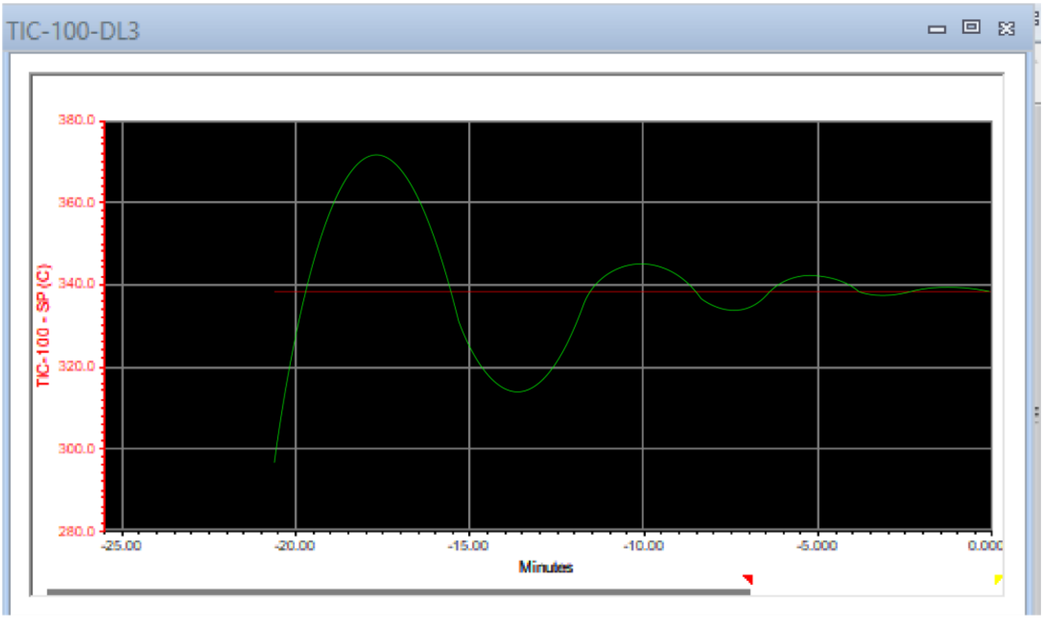


Figure 43: Controller Tuning

7.2 Flow, Pressure, Level and Temperature Controllers:

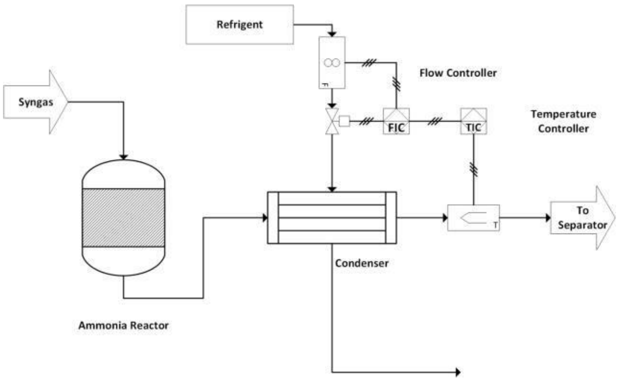


Figure 44: Cascade control loop for ammonia refrigeration

Function: To adjust the refrigerator flow rate

Gain	1.93
Ti	0.21
TD	0

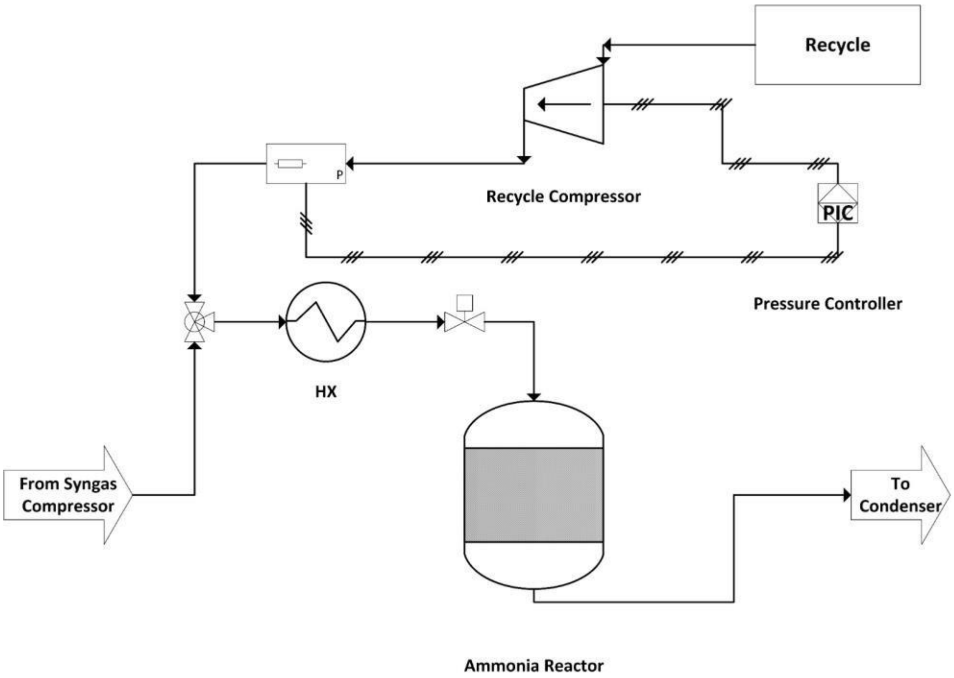


Figure 45: Pressure control loop for recycle compressor.

Function: To maintain the required pressure condition for ammonia reaction

Here the PIC controller (Pressure controller) measures the outlet of the Ammonia recycle compressors through a sensor and sends it to the transmitter. Transducer is further used to convert the signal into required output i.e. adjusting the rpm of the compressor.

Following PID values were calibrated for the for the controller:

Gain	0.8
Ti	0.15
TD	0

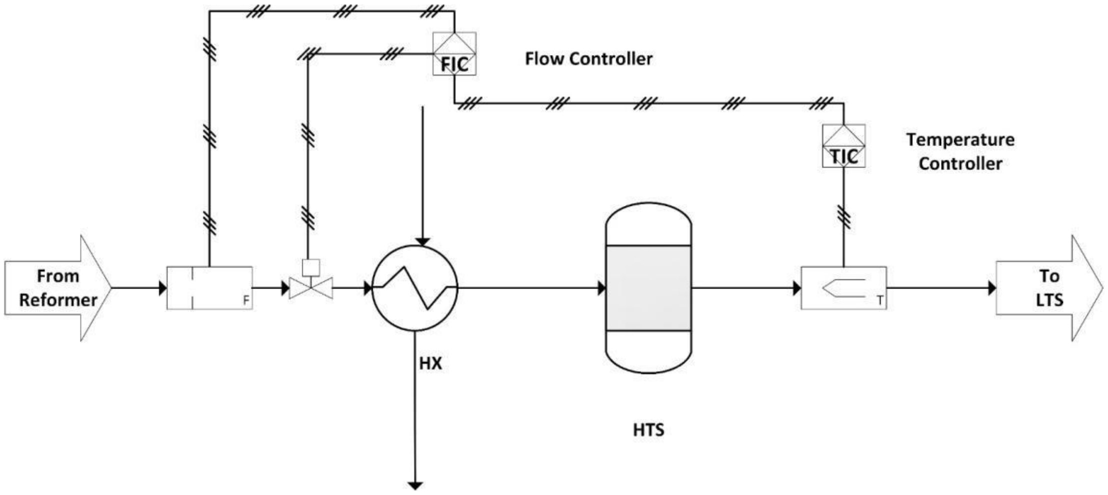


Figure 46: Cascade loop for HTS

Function: To tackle the effect of catalytic poisoning in High-Temperature Shift reactor.

Here a cascade controller is used for a quick response action. Following PID values were obtained for the controller.

Gain	1
Ti	0.22
TD	0.1

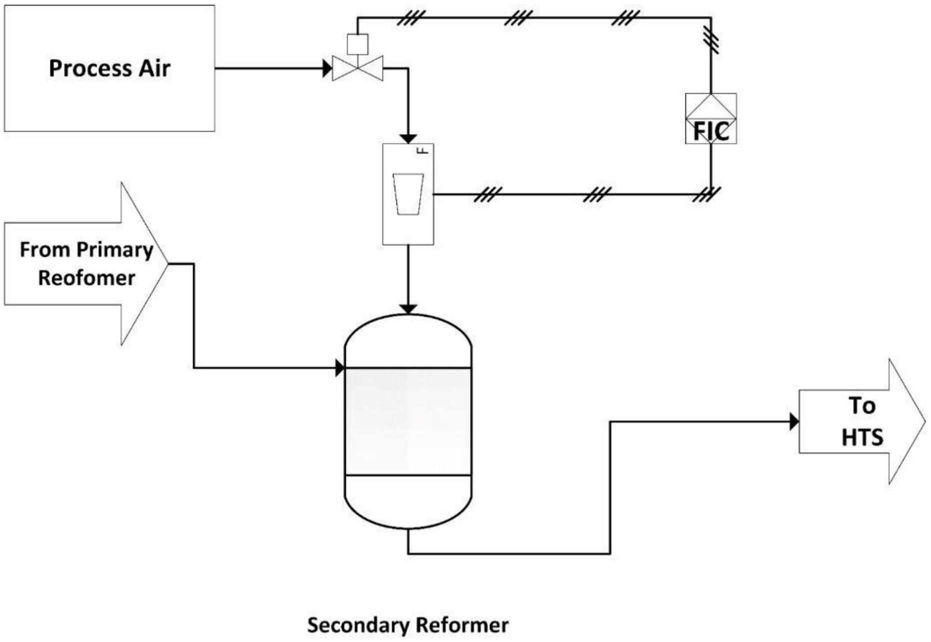


Figure 47: Flow control loop for Secondary reformer inlet

Function: To maintain the air flowrate

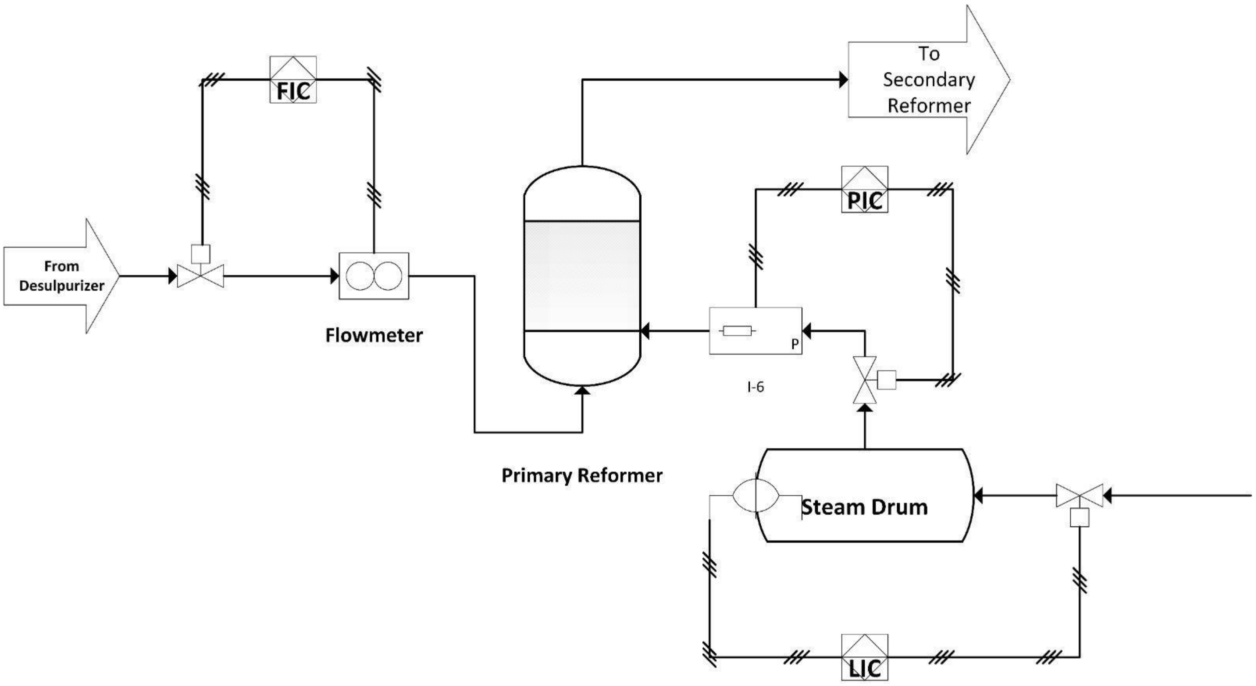


Figure 48: Multiple control loops in steam drum section

Function: Here three controllers are installed a flow controller for the inlet of Primary reformer, a pressure controller for the inlet of the steam drum and a level controller for the steam drum.

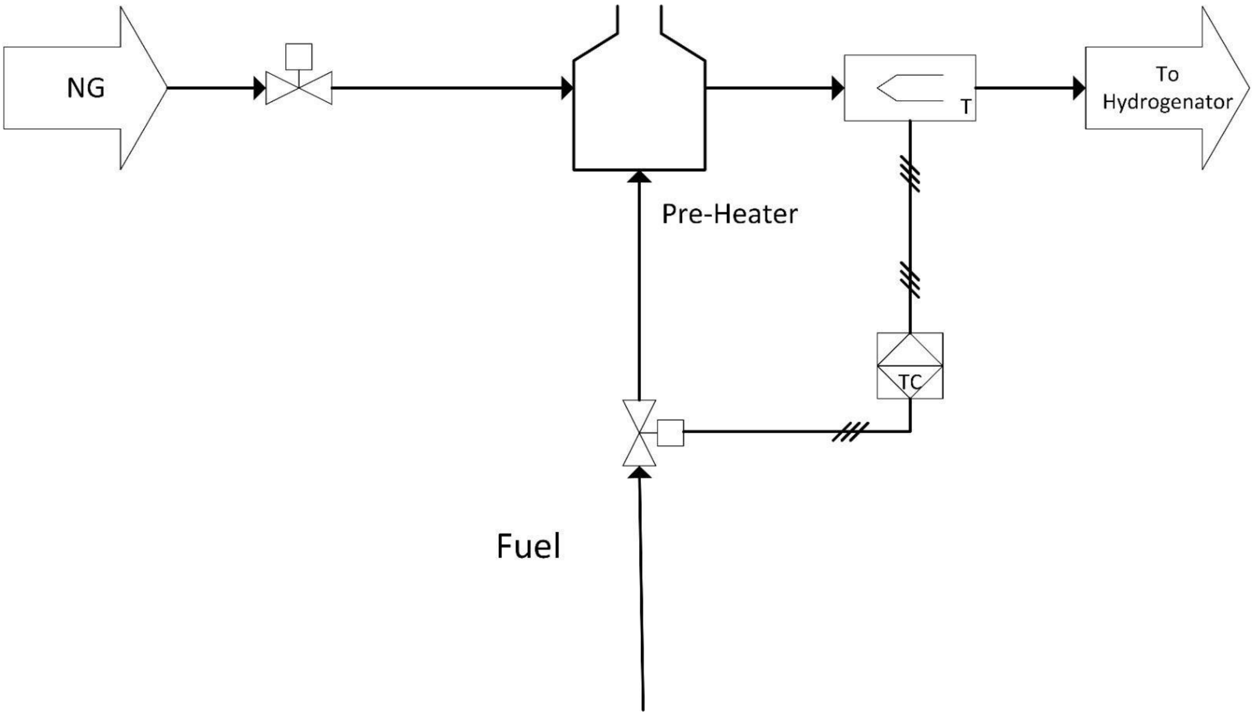


Figure 49 Pre-heater temperature control loop

Function: Incase of a failure in pre-heater tube or any disturbance and may reduce the outlet temperature, this controller will increase the fuel supply to the pre-heater burners.

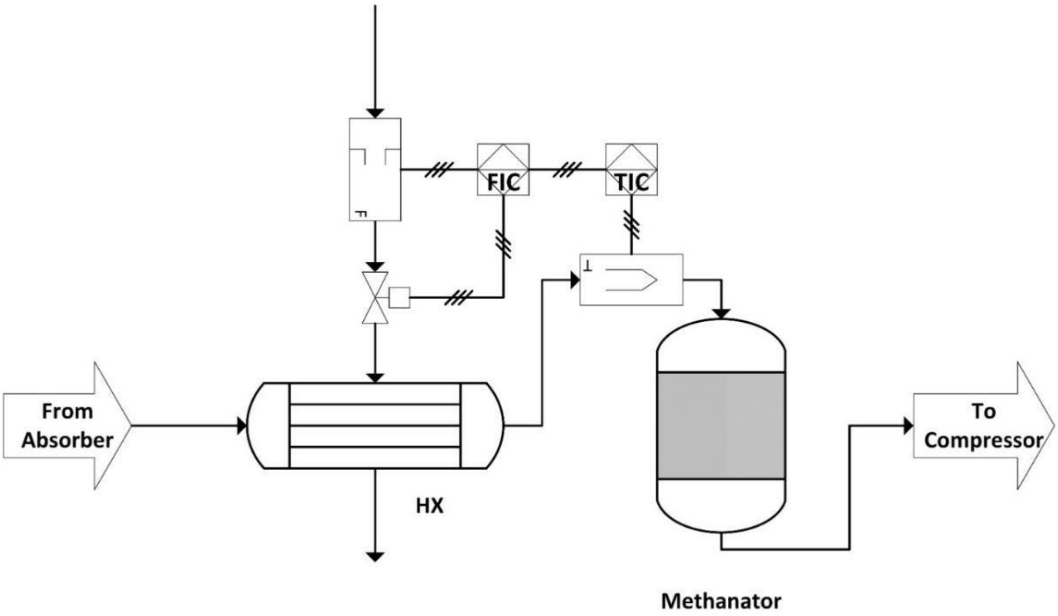


Figure 50: Cascade loop for methanator

Function: A cascade controller is installed to adjust the flow of heat exchanger shell side to maintain a steady temperature at the inlet of the methanator.

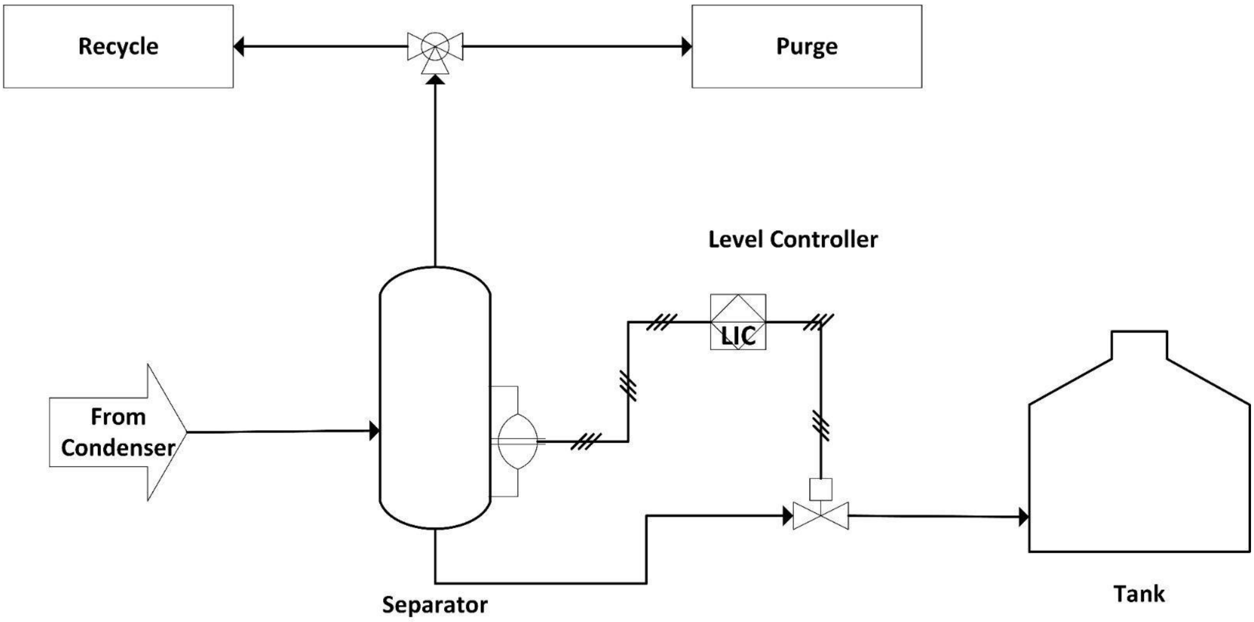


Figure 51: Level control loop for ammonia separator

Function: To achieve the safe liquid level percentage in ammonia separator.

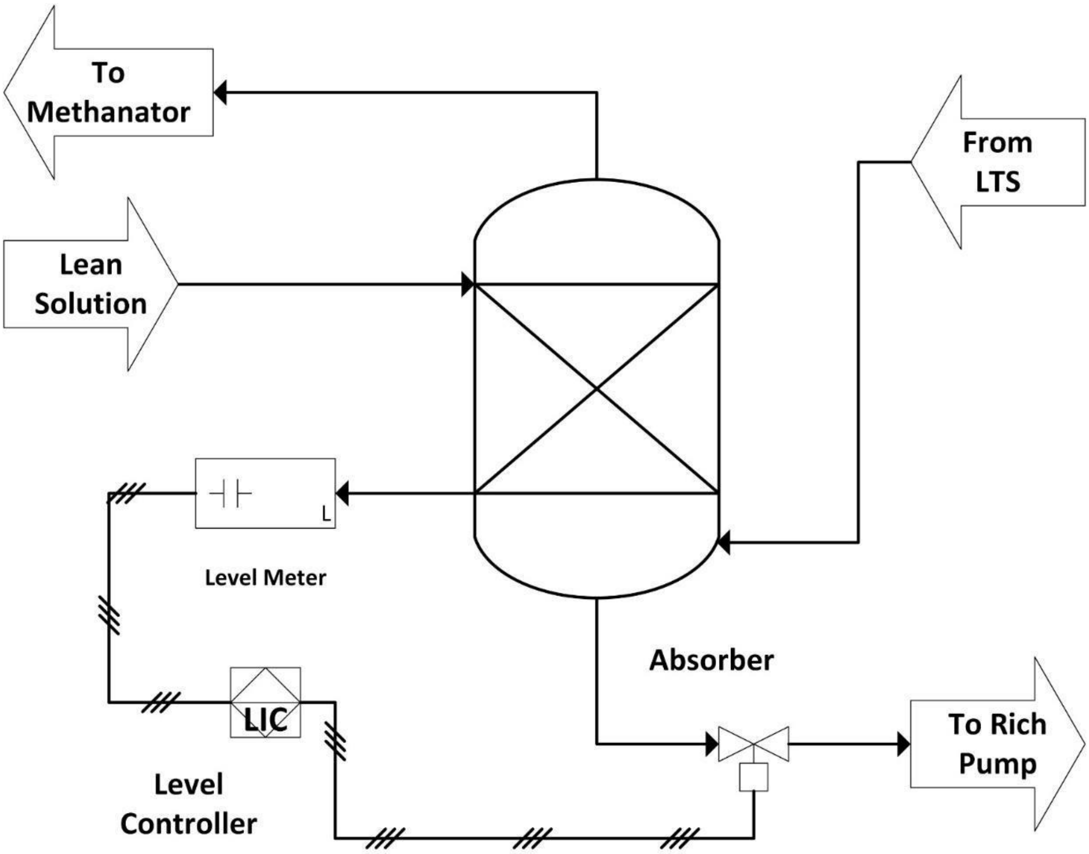


Figure 52: Level control loop for absorber

Function: The level of the absorption column is to be maintained to a definite level. If a required level was not achieved, then the efficiency of absorber is affected. Hence a particular level was to be maintained. For this level controller was installed to maintain the level at the bottom of absorber. Here the level of the column was the controlled variable, the rich solution flow rate was the manipulated variable, and the lean and semi lean solution flow rate was the disturbance variable.

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7.3 Dynamic Mode Controllers Database:

Dynamic mode controllers play a crucial role in control systems as they continuously monitor and adjust the control action based on feedback from sensors or measurements. Unlike static controllers that only consider the current state of the system, dynamic mode controllers analyse the system's response over time, considering factors such as rate of change, stability, and error accumulation. By incorporating feedback information, these controllers make real-time adjustments to the manipulated variable, resulting in improved control performance and enhanced system efficiency. Dynamic mode controllers employ various control algorithms and techniques, including proportional-integral-derivative (PID) control, model predictive control (MPC), adaptive control, and advanced control strategies. They utilize mathematical models, historical data, or real-time information to make informed decisions regarding adjustments to the manipulated variable. The primary objective of dynamic mode controllers is to maintain the controlled variable within desired limits, minimize errors or deviations from the setpoint, and optimize key performance criteria such as stability, response time, robustness, and disturbance rejection. By continuously monitoring and adjusting the control action, dynamic mode controllers strive to achieve precise and efficient control of dynamic systems.

Given its sheer importance, we have prepared a database of **more than 250** tuned controllers.

Table 35 Dynamic Mode Controllers Database

Sr. No.	**Description**	**Process Area**		**Signal Type**						**Calib Range**		**Unit**	**Unit**	**Controller Action**	**Gain (K)**	**KI**	**KD**
				Level	**I.S / N.I.S**	**2/4 Wire**	**Equipment**	**From**	**To**	**Min**	**Max**						
1	FUEL GAS Pressure TO Aux boiler Fuel Header	Front End	Fuel Gas	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.000	6.000	kg/cm^2	kg/cm2	Direct	1.8	0.2	0
2	Flow of HYDROGEN RICH GAS TO 103-B Feed Gas PRE-HEATER	Front End	Sulphur Removal	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0	1250	mm H2O	Nm3/hr	Reverse	0.8	0.2	0
3	Flow of NATURAL GAS FEED TO 103-B Feed Gas PRE-HEATER	Front End	Sulphur Removal	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0	2500	mm H2O	Nm3/hr	Direct	0.75	0.35	0
4	PURGE GAS (from 126-C and 139-C) VENT Pressure INDICATOR	Front End	Fuel Gas	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.00	20.00	kg/cm^2	kg/cm2	Direct	2	0.5	0
5	Desulphurized GAS Pressure INDICATOR TO 101-B Primary Reformer	Front End	Sulphur Removal	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.00	60.00	kg/cm^2	kg/cm2	Direct	2	0	0

6	101-B AUX. BOILER RADIANT SECTION DRAFT Pressure INDICATOR	Front End	Fuel Gas	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.00	25.00	mm H_2O	mm H20	Direct	0.93	0	0
7	Fuel Gas Pressure INDICATOR to 101-B PRIMARY REFORMER Arch,Superheater and Tunnel Burners (ByPass INDICATOR of PIC-149)	Front End	Fuel Gas	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.00	14.00	kg/cm^2	kg/cm^2	Direct	2	0.2	0
8	Pressure Indicator 101-B Convection Section DRAFT Before ID Fan	Front End	Reforming	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	-250	250.00	mm H_2O	mm H_2O	Direct	0.97	0.25	0
9	Fuel Gas Pressure INDICATOR to 101-B PRIMARY REFORMER Arch,Superheater and Tunnel Burners	Front End	Fuel Gas	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.00	10.00	kg/cm^2	kg/cm2	Direct	1.74	0.1	0

10	FUEL GAS Pressure TO 101-B ARCH BURNERS Row-1	Front End	Fuel Gas	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.000	6.000	kg/cm^2	kg/cm2	Direct	2.1	0.24	0
11	FUEL GAS Pressure TO 101-B ARCH BURNERS Row-2	Front End	Fuel Gas	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.000	6.000	kg/cm^2	kg/cm2	Reverse	1.93	0,22	0
12	FUEL GAS Pressure TO 101-B ARCH BURNERS Row-3	Front End	Fuel Gas	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.000	6.000	kg/cm^2	kg/cm2	Direct	1.37	0.2	0
13	FUEL GAS Pressure TO 101-B ARCH BURNERS Row-4	Front End	Fuel Gas	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.000	6.000	kg/cm^2	kg/cm2	Reverse	2	0.25	0
14	FUEL GAS Pressure TO 101-B ARCH BURNERS Row-5	Front End	Fuel Gas	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.000	6.000	kg/cm^2	kg/cm2	Direct	2	0.24	0
15	FUEL GAS Pressure TO 101-B ARCH BURNERS Row-6	Front End	Fuel Gas	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.000	6.000	kg/cm^2	kg/cm2	Direct	2	0.21	0
16	FUEL GAS Pressure TO 101-B ARCH BURNERS Row-7	Front End	Fuel Gas	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.000	6.000	kg/cm^2	kg/cm2	Reverse	2	0,22	0

17	FUEL GAS Pressure TO 101-B ARCH BURNERS Row-8	Front End	Fuel Gas	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.000	6.000	kg/cm^2	kg/cm2	Reverse	2	0	0
18	FUEL GAS Pressure TO 101-B ARCH BURNERS Row-9	Front End	Fuel Gas	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.000	6.000	kg/cm^2	kg/cm2	Reverse	2	0.2	0
19	FUEL GAS Pressure TO 101-B ARCH BURNERS Row-10	Front End	Fuel Gas	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.000	6.000	kg/cm^2	kg/cm2	Direct	2	0.25	0
20	Pressure Indicator and INDICATOR of 101-B RADIANT SECTION DRAFT	Front End	Reforming	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	-25	25.00	mm H2O	mm H20	Reverse	1	0.1	0
21	FUEL GAS Pressure TO 101-B SUPERHEATER BURNERS	Front End	Fuel Gas	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.000	6.000	kg/cm^2	kg/cm2	Direct	2	0	0
22	Level INDICATOR of 101-C WATER JACKET	Front End	Reforming	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.0	356.0	mm	%	Direct	1.01	0,22	0
23	NG Pressure INDICATOR to Main	Front End	Fuel Gas	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.00	20.00	kg/cm^2	kg/cm2	Reverse	2	0.2	0

	FUEL GAS Header																
24	HS Steam Pressure INDICATOR at 101-F STEAM DRUM	Front End	STEAM GENERATION	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.0	200.0	kg/cm^2	kg/cm2	Direct	2	0.19	0
25	Pressure Letdown INDICATOR from HP to M.P. STEAM	Front End	STEAM GENERATION	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.00	60.00	kg/cm^2	kg/cm2	Reverse	2	0.24	0
26	Process GAS flow TO 101-B PRIMARY REFORMER	Front End	Reforming	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0	2500	Nm3/h	Nm3/hr	Direct	0.8	0.21	0
27	PROCESS STEAM flow TO 101-B PRIMARY REFORMER	Front End	Reforming	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0	2500	Nm3/h	kg/hr	Direct	0.74	0,22	0
28	Level INDICATOR for 119-F STEAM DRUM BLOW DOWN	Front End	STEAM GENERATION	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.0	356.0	mm	%	Reverse	0.98	0.5	0
29	FUEL GAS Pressure TO 101-B TUNNEL BURNERS	Front End	Fuel Gas	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.000	6.000	kg/cm^2	kg/cm2	Reverse	2	0	0
30	Level INDICATOR for SECOND	Front	Reforming	AIC (4-20	I.S	2 Wire	Transmitter	Field	DCS	0.0	356.0	mm	%	Reverse	1	0.53	0

	ARY REFORMER 103-D WATER JACKET	End		mA)													
31	Level INDICATOR for STEAM DRUM 101-F	Front End	STEAM GENERATION	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.0	813.0	mm	%	Direct	1	0.57	0
32	H.P. STEAM Flow FROM 101-F STEAM DRUM	Front End	STEAM GENERATION	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0	5000	mm H2O	kg/hr	Reverse	0.71	0.62	0
33	Level INDICATOR for STEAM DRUM 101-F	Front End	STEAM GENERATION	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.0	813.0	mm	%	Direct	1	0.52	0
34	SEMI LEAN SOLUTION Flow TO 101-E ABSORBER	Front End	CO2 Removal	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0	2500	mm H2O	m3/hr	Direct	0.69	0.18	0
35	Level INDICATOR CO2 ABSORBER 101-E	Front End	CO2 Removal	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0	5221.5	mm H2O	%	Reverse	1	0.25	0
36	Level INDICATOR for K.O. DRUM 117-F	Front End	CO2 Removal	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.0	356.0	mm	%	Direct	1	0.1	0
37	Level INDICATOR of SURFACE CONDENSER 104-L	Front End	STEAM GENERATION	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.0	356.0	mm	%	Reverse	1.02	0.24	0

38	Pressure Transmitter for 101-U DEAERATOR	Front End	STEAM GENERATION	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.000	4.000	kg/cm^2	kg/cm2	Direct	1.94	0,22	0
39	Level Transmitter for DEAERATOR 101-U	Front End	STEAM GENERATION	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0	2130	mm	%	Reverse	1	0.2	0
40	Flow Transmitter for BFW PUMP 104-JA Kick Back	Front End	STEAM GENERATION	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.0	950.0	mm H2O	m3/hr	Reverse	0.8	0.25	0
41	Flow Transmitter forBFW PUMP 104-JB Kick Back	Front End	STEAM GENERATION	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0	2500	mm H2O	m3/hr	Reverse	0.82	0.24	0
42	Flow Transmitter for BFW PUMP 104-JS Kick Back	Front End	STEAM GENERATION	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.0	950.0	mm H2O	m3/hr	Reverse	0.78	0.21	0
43	Pressure Transmitter for CO2 REFLUX DRUM 113-F	Front End	CO2 Removal	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.000	0.500	kg/cm^2	kg/cm2	Reverse	2	0,22	0
44	Pressure Transmitter for H.P. FLUSHING WATER	Front End	CO2 Removal	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.0	100.0	kg/cm^2	kg/cm2	Reverse	2	0	0
45	Pressure Transmitter for	Front	CO2 Removal	AIC (4-20	I.S	2 Wire	Transmitter	Field	DCS	0.00	16.00	kg/cm^2	kg/cm2	Direct	2	0.2	0

	L.P. FLUSHING WATER	End		mA)													
46	LEAN SOLUTION Flow TO 101-E ABSORBER	Front End	CO2 Removal	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0	2500	mm H2O	m3/hr	Reverse	0.78	0.25	0
47	Flow Transmitter for CO2 VENT AT STRIPPER 102-E	Front End	CO2 Removal	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.0	735.0	mm H2O	Nm3/hr	Direct	0.78	0.1	0
48	Flow Transmitter for 120-J Kick Back	Front End	CO2 Removal	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.0	635.0	mm H2O	Nm3/hr	Direct	0.78	0	0
49	Level Transmitter for REFLUX DRUM 103-F	Front End	CO2 Removal	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.0	356.0	mm	%	Direct	1	0,22	0
50	Level Transmitter for CO2 BLOWER KO DRUM 121-F	Front End	CO2 Removal	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.0	356.0	mm	%	Reverse	1	0.2	0
51	Level Transmitter for RAW GAS SEPARATOR 102-F	Front End	CO2 Removal	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.0	813.0	mm	%	Direct	1	0.19	0
52	Level Transmitter for PROCESS CONDENSATE STRIPPER 103-E	Front End	CO2 Removal	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0	1219	mm	%	Reverse	1	0.24	0

53	Level Transmitter for 111-C REBOILER POT	Front End	CO2 Removal	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0	1219	mm	%	Reverse	1	0.21	0
54	Level Transmitter for 146-C REBOILER POT	Front End	CO2 Removal	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0	3337	mm H2O	%	Reverse	1	0,22	0
55	Pressure Transmitter for RECYCLE HYDROGEN COMPRESSOR 121-J DISCHARGE	Front End	Sulphur Removal	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.00	60.00	kg/cm^2	kg/cm2	Direct	2	0.5	0
56	Process Gas Vent at Methanator 106-D INLET	Front End	CO2 Removal	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.00	50.00	kg/cm^2	kg/cm2	Reverse	2	0	0
57	Level Transmitter for SYN GAS COMPRESSOR SUCTION KOD 104-F	BACK END	SYNTHESIS	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.0	356.0	mm H2O	%	Direct	1	0.53	0
58	Pressure Transmitter for H2 FROM PGRU	BACK END	PGRU	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.0	100.0	kg/cm^2	kg/cm^2	Reverse	2	0.57	0
59	SYN GAS COMPRESSOR 103-J SUCTION VENT	BACK END	SYNTHESIS	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.00	50.00	kg/cm^2	kg/cm2	Reverse	1.99	0.62	0

60	Level Transmitter for SYN.GAS COMP IST STAGE SEP. 105-F	BACKEND	SYNTHESIS	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.0	356.0	mm H2O	%	Reverse	0.96	0.52	0
61	Level Transmitter for 103-J S-O L.P STAGE O.H TANK	BACKEND	SYNTHESIS	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS				%	Direct	1	0.18	0
62	Level Transmitter for 103-J S-O H.P STAGE O.H TANK	BACKEND	SYNTHESIS	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS				%	Direct	1	0.25	0
63	Level Transmitter for 103-J S-O HP Trap	BACKEND	SYNTHESIS	AIC (4-20 mA)	I.S	2 Wire	Transmitter	Field	DCS	0.0	356.0	mm	%	Reverse	1	0.1	0

Complete Controller database file is available on the following link:

https://drive.google.com/drive/folders/11mCmkNPpM73aaffr_GUQf5Vk1d69lia9?usp=sharing

or:

SCAN ME

Figure 53: Dynamic Mode Controller Database QR Code

CHAPTER 8

HAZOP ANALYSIS

8.1 Background

HAZOP or Hazard and Operability Study is a research tool used to find out potential hazards which might lead to a disaster. There is a wide use of HAZOP as a tool in all types of industries such as chemical and otherwise to study the possibility of a problem or hazard occurring on a stream or unit of operation. It is done by a multidisciplinary team which employs a critical and analytical approach on the unit or stream being studied. This team consists of between 6 to 12 members normally and usually requires weeks of work to be concluded [10]. These members normally include the operations engineer, mechanical engineer, process engineer, electrical engineers, chemical engineers, HSE consultant and a project manager as well. For the discussion of all records and parameters that may lead the process of the track, all the members are needed to meet multiple times in a week. Full HAZOP study requires several PFDs and P&IDs which are not easy to understand and require lot of collective effort to be sorted out, and this needs to be done for each unit separately. It is a laborious process and takes more than a month to complete. Although this is a very tough technique to perform but it is considered as the best possible method or study for having a hands-on approach to any sort of problem that might occur in a process. So, performing a HAZOP analysis of a chemical plant is the most important step in making it safe.

The main reason for a HAZOP analysis is to study the core possible reasons of failure and take steps to prevent them. Each unit or process is broken down into the minutest detail and then the guide words are applied on the node in question. Deviations are then checked for in terms of temperature, pressure, flow and composition and they are applied on every guide word that is applicable to them.

8.2 Methodology:

The HAZOP study was performed using the following steps:

- Prepare a point-to-point flow sheet and map out the various units within it.
- Select a unit for study, like an absorber or stripper
- Describe the reasoning for choosing that unit
- Choose a process parameter
- Apply the guide words on the process parameters and find out potential deviations from those words introduced in the below tables.
- Determine the potential causes and any systems required to prevent the disaster
- Evaluate deviation outcomes
- Recommend possible preventive measures.
- Record all associated data and present it

8.3 Low Temperature Shift Reactor

Table 36 HAZOP of LTS

Deviation	Possible Causes	Consequences	Suggested Actions
No Flow	Valve not functioning properly or failed	- Loss of reaction and buildup of unreacted materials.	- Investigate and repair/replace faulty valves.
	Feed line having blockages of any sort	- Disruption of the reaction, loss of productivity.	- Clear blockages.
Reverse Flow	Extreme Backpressure from downstream	- Disruption of the chemical reaction, low product	- Review valve configuration and designing system of pipes.
	Incorrect valve positions	- Contamination or blockages on the beds of catalyst.	- Make sure there is correct valve positioning.
High Temperature	Reduction in cooling	- Catalyst deactivation	- Increase in the cooling capacity.
	Failure of digital control system	- Vulnerable operating conditions, chances of potential accidents.	- Add temperature alarms, sensor and interlocks.
High Pressure	Reactor overpressure	- Failure of equipment, explosion, concerns related to safety.	- Add pressure relief valves.
Composition Change	Decrease of feedstock quality	- Change of reaction kinetics, issues related to quality of product.	- keep tabs on the feedstock quality.

8.4 Ammonia Reactor

Table 37 HAZOP of Ammonia Reactor

Deviation	Possible Causes	Consequences	Suggested Actions
No/Low Flow	Valve not functioning properly or failed	- Reduced ammonia production, decreased efficiency.	- Replace malfunctioned valves with new ones.
	Pump not functioning properly or failed	- Reduction in conversion rates, no complete mixing.	- Replace malfunctioned pumps with new ones.
High Temperature	Insufficient cooling	- Catalyst deactivation, reduction in ammonia production.	- Increase the cooling by increasing flow rated of CFW
High Pressure	Valve not functioning properly or failed	- Equipment damage, safety risks, potential explosion.	- Inspect and repair/replace faulty valves.
	Reactor overpressure	- Reactor failure, safety hazards, release of toxic gases.	- Install pressure relief devices.
Low Pressure	Valve not functioning properly or failed	- Inadequate reactant supply, reduced ammonia output.	- Inspect and repair/replace faulty valves.
	Leakage in the equipment	- Decrease in efficiency loss of valuable feedstock.	- Inspect and repair leaks
Composition Change	Variation in feedstock quality	- Altered reaction kinetics, issues related to product quality.	- Check feedstock quality periodically

8.5 Compressor:

Table 38 HAZOP of Compressor

Deviation	Possible Causes	Consequences	Suggested Actions
Low Concentration	Leakage in suction line of the compressor	- Insufficient compression, reduction in the purity.	- Identification of leakage area and repair those leaks in suction line.
	Contamination	- Impurities in output, decreased product quality.	- Implement proper filtration and purification systems.
Low Flow	Suction pressure lower than average	Insufficient output pressure, compressor efficiency decreased	- Adjust suction pressure in accordance to required levels.
High Flow	Valve not functioning properly or failed	- Issues related to safety.	- Replace malfunctioned valves with new ones.
Low Pressure	Valve not functioning properly or failed	- Insufficient output pressure, compressor efficiency decreased	- Replace malfunctioned valves with new ones.
	Restriction in the flow of inlet stream	- Reduction in flow rate of stream, not enough compression ratio	- Remove blockages, clean the filters of compressor and screens.
High Pressure	Valve not functioning properly or failed	- Loss in pressure, compressor efficiency decreased.	- Replace malfunctioned valves with new ones.

CONCLUSION

The dynamic mode simulation serves as **an excellent comprehensive tool** to study any steady and dynamic state case for rectifications both in steady state and real-time, in the plant. A comprehensive instrumentation model provides a roadmap for day-to-day plant safety while considering product profitability and purity and shows an estimation of **7%** saving in annual energy savings.

Implementing a dynamic mode controller on an ammonia production unit yielded positive results and led to significant improvements in control performance. The dynamic mode controller continuously monitored the system's response and made real-time adjustments to the manipulated variables based on feedback information from sensors or measurements. This approach resulted in tighter control over the ammonia production process and enhanced stability.

The implementation of the dynamic mode controller improved the control of critical variables such as ammonia synthesis temperature, pressure, and flow rates. The controller effectively maintained these variables within desired ranges, minimizing deviations from the setpoints and reducing process variability. This led to increased process efficiency, improved product quality, and reduced waste or off-spec production.

Furthermore, the dynamic mode controller demonstrated its ability to respond quickly to changes in operating conditions or disturbances. It efficiently adjusted the manipulated variables to counteract any fluctuations or disturbances, thereby ensuring the stability of the ammonia production process. The controller's responsiveness and adaptability contributed to faster process stabilization and reduced downtime due to process upsets.

In conclusion, the implementation of a dynamic mode controller in the ammonia production unit resulted in significant improvements in control performance, stability, and efficiency. The controller's continuous monitoring, real-time adjustments, and responsiveness to changes in operating conditions contributed to tighter control over critical variables, improved product quality, and reduced process variability. The successful implementation of the dynamic mode controller highlights its effectiveness in optimizing the ammonia production process and showcases its potential for enhancing control systems in similar industrial applications.

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