CHE654 Design Project #2

Semester 1, 2026

Problem Statement

Project Title

Design, Simulation, and Economic Evaluation of Hydrogen Production via Steam Methane Reforming (SMR)

Background

Hydrogen is one of the most important industrial chemicals and plays a critical role in petroleum refining, ammonia production, methanol synthesis, hydrocracking, hydrogenation processes, and the emerging hydrogen economy. As global demand for cleaner fuels and low-carbon energy systems continues to grow, the need for efficient, reliable, and economically competitive hydrogen production technologies has become increasingly important.

Currently, more than 70% of the world's hydrogen is produced from natural gas through the Steam Methane Reforming (SMR) process due to its high efficiency, technological maturity, and relatively low production cost. The process involves the catalytic reaction of methane with steam at high temperatures to produce synthesis gas (hydrogen and carbon monoxide), followed by the water-gas shift reaction to maximize hydrogen production and pressure swing adsorption (PSA) for high-purity hydrogen recovery. However, SMR is an energy-intensive process and is associated with significant carbon dioxide emissions. Therefore, improving process efficiency, maximizing hydrogen yield, minimizing energy consumption, and reducing production costs remain major engineering challenges.

The objective of this project is to design a commercial hydrogen production plant based on Steam Methane Reforming using Aspen Plus process simulation software. The proposed process will include natural gas pretreatment, feed compression, steam generation, steam methane reforming, high- and low-temperature water-gas shift reactors, process cooling, condensate separation, hydrogen purification using Pressure Swing Adsorption (PSA), and appropriate utility systems. Suitable thermodynamic models, reactor models, and operating conditions will be selected based on published industrial data and engineering practice.

The project will include complete material and energy balance calculations, equipment sizing, utility requirement estimation, and process optimization to improve thermal efficiency and hydrogen recovery. Heat integration strategies will be investigated to recover waste heat from the reformer flue gas and process streams, thereby reducing fuel consumption and operating costs.

A comprehensive techno-economic evaluation will be performed to determine the commercial feasibility of the proposed hydrogen production plant. Capital investment, annual operating costs, utility costs, catalyst replacement, maintenance expenses, and product revenues will be estimated. Financial performance will be assessed using Net Present Value (NPV), Internal Rate of Return (IRR), Payback Period (PBP), Return on Investment (ROI), and profitability index. Sensitivity analyses will be conducted to evaluate the effects of fluctuations in natural gas prices, electricity costs, plant capacity, hydrogen selling price, and carbon pricing on overall project profitability.

The final design should demonstrate technical feasibility, economic viability, energy efficiency, operational safety, and environmental sustainability while identifying opportunities for future improvements, including carbon capture and storage (CCS), carbon capture, utilization and storage (CCUS), and integration with renewable energy sources to support the transition toward low-carbon hydrogen production.

Objective

The primary objective of this project is to develop a technically feasible, energy-efficient, and economically viable process for the commercial production of high-purity hydrogen from natural gas using the Steam Methane Reforming (SMR) process.

The specific objectives are to:

1. Develop a complete process flow diagram (PFD) for hydrogen production using Steam Methane Reforming.
2. Simulate the entire process using Aspen Plus, including natural gas pretreatment, steam reforming, water-gas shift reactors, hydrogen purification, and utility systems.
3. Perform complete material and energy balance calculations for all process units.
4. Select appropriate thermodynamic property methods and reactor models based on industrial practice and published literature.
5. Design and size the major process equipment, including desulfurization units, reformer furnace, reforming reactor, shift reactors, heat exchangers, waste heat recovery systems, compressors, separators, and Pressure Swing Adsorption (PSA) unit.
6. Optimize key operating variables such as steam-to-carbon ratio, reformer temperature, reactor pressure, and hydrogen recovery to maximize process efficiency.
7. Investigate heat integration opportunities to improve thermal efficiency and reduce fuel consumption.
8. Estimate utility requirements, including fuel gas, steam, cooling water, electricity, and instrument air.
9. Estimate capital investment and annual operating costs using accepted chemical engineering economic methods.
10. Evaluate project profitability using Net Present Value (NPV), Internal Rate of Return (IRR), Payback Period (PBP), Return on Investment (ROI), and Profitability Index (PI).
11. Conduct sensitivity analyses to determine the effects of variations in natural gas price, hydrogen selling price, electricity cost, plant capacity, and carbon pricing on project profitability.

12. Assess process safety, environmental performance, and opportunities for future implementation of Carbon Capture and Storage (CCS) or Carbon Capture, Utilization and Storage (CCUS).

Scope of Work

This project focuses on the conceptual process design and simulation of a commercial hydrogen production plant based on Steam Methane Reforming (SMR) using natural gas as the primary feedstock.

The scope of work includes:

- Review of industrial hydrogen production technologies and selection of Steam Methane Reforming as the preferred production route.
- Development of the overall Process Flow Diagram (PFD).
- Selection of thermodynamic property methods suitable for high-temperature gas-phase reactions.
- Process simulation using Aspen Plus.
- Modeling of the major process sections, including:
    - Natural gas desulfurization
    - Feed compression and steam generation
    - Steam methane reforming
    - High-temperature water-gas shift reactor
    - Low-temperature water-gas shift reactor
    - Waste heat recovery
    - Gas cooling and condensate separation
    - Pressure Swing Adsorption (PSA) hydrogen purification
    - Hydrogen product compression (if required)
- Material and energy balance calculations.
- Design and sizing of major equipment.
- Utility consumption estimation.
- Heat integration and energy recovery analysis.
- Capital cost estimation using equipment cost correlations.
- Estimation of annual operating costs, including feedstock, utilities, catalyst replacement, labor, maintenance, and overhead.
- Cash-flow analysis and profitability evaluation.
- Sensitivity analysis of major technical and economic parameters.
- Discussion of process safety, environmental impacts, and recommendations for future improvements.

The project does not include detailed mechanical design, piping design, instrumentation and control system design, civil engineering, plant layout, construction scheduling, or detailed hazard analysis beyond conceptual process safety considerations.

Design Basis

The process is designed for the continuous commercial production of high-purity hydrogen using Steam Methane Reforming (SMR) of natural gas.

The principal design assumptions are as follows:

- **Plant Capacity:** 100,000 Nm^3/h of hydrogen (approximately 78,000 tonnes/year), or another specified design capacity.
- **Operating Schedule:** 8,000 operating hours per year.
- **Feedstock:** Pipeline-quality natural gas.
- **Steam Source:** High-pressure steam generated through waste heat recovery and auxiliary boilers.
- **Main Product:** Hydrogen with a purity of 99.99% or higher.
- **Hydrogen Recovery:** Greater than 85% through Pressure Swing Adsorption (PSA).
- **Desulfurization:** Zinc oxide guard bed for sulfur removal.
- **Steam-to-Carbon Ratio:** Typically between 2.5 and 3.5.
- **Primary Reformer Operating Temperature:** 800–900°C.
- **Primary Reformer Pressure:** 20–30 bar.
- **High-Temperature Shift Reactor:** Approximately 350–400°C.
- **Low-Temperature Shift Reactor:** Approximately 200–250°C.
- **Hydrogen Purification:** Pressure Swing Adsorption (PSA).
- **Process Simulation Software:** Aspen Plus.
- **Thermodynamic Property Method:** Peng–Robinson Equation of State or another appropriate property package for gas-phase hydrocarbon systems.
- **Plant Lifetime:** 20 years.
- **Construction Period:** 2 years.
- **Discount Rate:** 10–12%.
- **Corporate Income Tax:** According to the selected country or regional regulations.
- **Economic Base Year:** Clearly specified and applied consistently throughout the analysis.

Where industrial operating data are unavailable, engineering assumptions supported by published literature and industrial practice will be adopted.

Economic Evaluation Methodology

The economic feasibility of the proposed hydrogen production plant will be assessed using standard chemical engineering economic evaluation techniques.

The economic analysis includes:

- Estimation of purchased equipment costs based on equipment sizing and published cost correlations.
- Determination of installed equipment costs using appropriate installation factors.

- Estimation of Fixed Capital Investment (FCI), Working Capital Investment (WCI), and Total Capital Investment (TCI).
- Calculation of annual operating costs, including:
    - Natural gas feedstock
    - Fuel gas consumption
    - Steam generation
    - Cooling water
    - Electricity
    - Catalyst replacement
    - Labor
    - Maintenance
    - Plant overhead
    - Waste treatment and environmental compliance
- Estimation of annual hydrogen production and product sales revenue.
- Development of discounted cash-flow statements over the plant lifetime.
- Evaluation of project profitability using:
    - Gross Profit
    - Net Profit
    - Return on Investment (ROI)
    - Payback Period (PBP)
    - Net Present Value (NPV)
    - Internal Rate of Return (IRR)
    - Profitability Index (PI)
    - Break-even Analysis
- Sensitivity analyses to evaluate the impact of changes in:
    - Natural gas price
    - Hydrogen selling price
    - Electricity price
    - Steam cost
    - Plant capacity
    - Carbon tax or carbon pricing
    - Discount rate

The proposed project will be considered economically feasible if the Net Present Value is positive at the selected discount rate, the Internal Rate of Return exceeds the company's minimum acceptable rate of return, and the Payback Period falls within an acceptable industrial investment horizon. The results of the sensitivity analyses will be used to identify the key economic drivers and assess the robustness of the project under different market conditions.

Detailed Design of a Heat Exchanger

You are to pick one heat exchanger in your process to carry out its detailed design. You should use ASPEN Exchanger Design & Rating (EDR) in the ASPEN Plus simulator to carry out the detailed design. For this heat exchanger design, the following information should be provided:

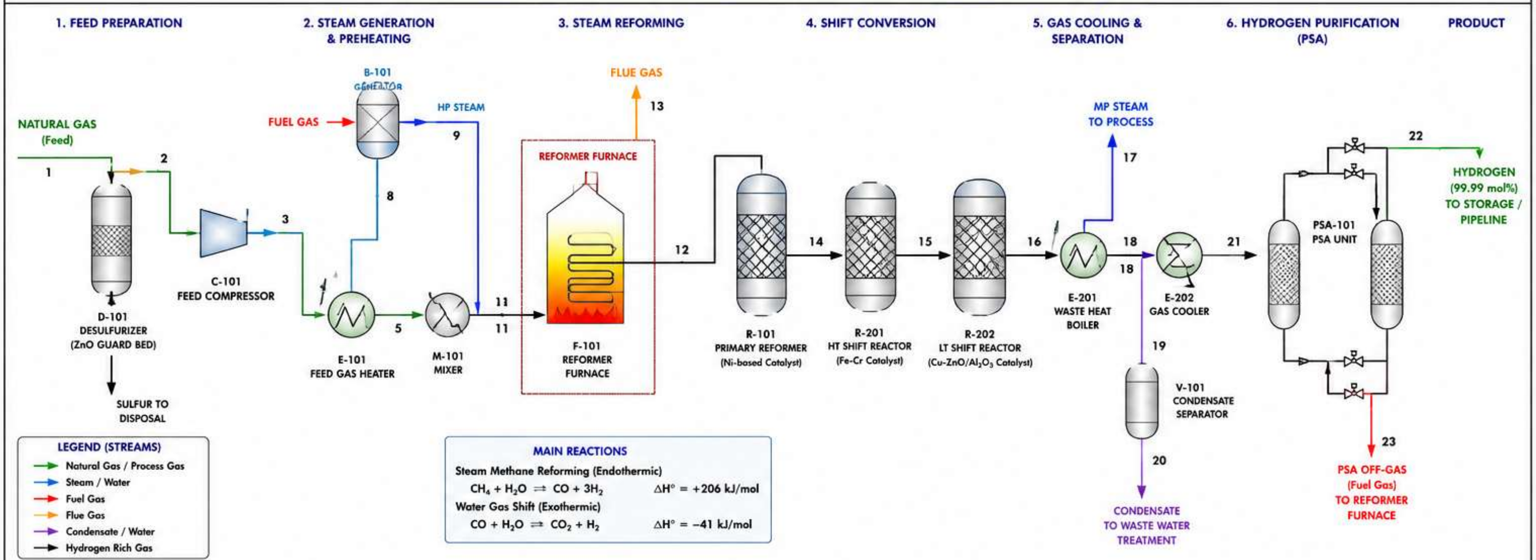
- Diameter of shell
- Number of tube and shell passes
- Number of tubes per pass
- Tube pitch and arrangement (triangular/square/..)
- Number of shell-side baffles, if any, and their arrangement (spacing, pitch, type)
- Diameter, tube-wall thickness, shell-wall thickness, and length of tubes
- Calculation of both shell- and tube-side film heat transfer coefficients
- Calculation of overall heat transfer coefficient (you may assume that there is no fouling on either side of the exchanger)
- Heat transfer area of the exchanger
- Shell-side and tube-side pressure drops (calculated, not estimated)
- Materials of construction
- Approximate cost of the exchanger

A detailed sketch of the exchanger should be included along with a set of comprehensive calculations in an appendix for the design of the chosen heat exchanger.

Process Flow Diagram

STEAM METHANE REFORMING (SMR) PROCESS

HYDROGEN PRODUCTION PLANT – PROCESS FLOW DIAGRAM (PFD)



STREAM TABLE

No.	DESCRIPTION	PHASE	T (°C)	P (bar)	MAIN COMPONENTS (mol%)
1	Natural Gas Feed	G	25	20	CH_4, C_2H_6, C_3+, H_2O, CO_2, N_2
2	Desulfurized Gas	G	25	19.5	CH_4, C_2H_6, C_3+, H_2O, CO_2, N_2
3	Compressed Feed Gas	G	40	21	"
4	Preheated Feed Gas	G	250	20	"
5	Hot Feed Gas	G	350	20	"
8	Boiler Feed Water	L	105	25	H_2O
9	HP Steam	G	500	25	H_2O
10	Steam to Mixer	G	500	20	H_2O
11	Reformer Feed	G	550	20	CH_4, H_2O
12	Reformer Outlet	G	850	20	H_2, CO, CO_2, H_2O, CH_4
13	Reformer Flue Gas	G	350	1.2	CO_2, H_2O, N_2, O_2
14	To HT Shift	G	380	19.5	H_2, CO, CO_2, H_2O, CH_4
15	To LT Shift	G	220	19.2	H_2, CO, CO_2, H_2O, CH_4
16	To WHB	G	200	19.0	H_2, CO_2, H_2O, CH_4, N_2
17	Process Steam (MP)	G	250	18.5	H_2O
18	Cooled Gas	G	40	18.5	H_2, CO_2, H_2O, CH_4, N_2
19	Liquid Condensate	L	40	18.5	H_2O
20	Condensate Out	L	35	1.5	H_2O
21	Dry Syngas to PSA	G	40	18.5	H_2, CO_2, CH_4, N_2
22	Product Hydrogen	G	40	18.0	H_2 (≥ 99.99 mol%)
23	PSA Off-gas	G	35	1.2	H_2, CH_4, CO, CO_2, N_2

EQUIPMENT LIST

No.	DESCRIPTION
D-101	Desulfurizer (ZnO Guard Bed)
C-101	Feed Gas Compressor
E-101	Feed Gas Heater
B-101	Steam Generator
M-101	Mixer
F-101	Reformer Furnace (Radiant Section)
R-101	Primary Reformer (Ni-based Catalyst)
R-201	High Temperature Shift Reactor
R-202	Low Temperature Shift Reactor
E-201	Waste Heat Boiler
E-202	Gas Cooler
V-101	Condensate Separator
PSA-101	Pressure Swing Adsorption Unit

UTILITY SUMMARY (Typical)

UTILITY	REMARKS
Fuel Gas	Used in reformer furnace and interheater as required
Steam	Generated in waste heat boiler and auxiliary boiler
Cooling Water	Used in gas cooler and other exchangers
Electricity	For compressors, PSA blowers, pumps, controls, lighting
Instrument Air	For instrumentation and valves
Demineralized Water	For boiler feed make-up

ECONOMIC EVALUATION METRICS

METRIC	DESCRIPTION
CAPEX	Total Capital Investment (Installed)
OPEX	Annual Operating Cost
NPV	Net Present Value
IRR	Internal Rate of Return
PBP	Payback Period
ROI	Return on Investment
PI	Profitability Index
BEP	Break-even Point (Capacity)

DESIGN CAPACITY (Base Case)

- Hydrogen Production : 100,000 Nm^3/h (99.99 mol%)
- Plant Availability : 8,000 h/yr
- Feedstock : Natural Gas
- Plant Life : 20 years
- Basis : 1 atm = 1.01325 bar, 25 °C

Note: Temperatures and pressures are typical design values and may be adjusted during detailed design and process optimization.