CHE251 Term Project Proposal

Proposed By
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With members
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Date : 5th September 2025

Title: Process Simulation and Optimization of Hydrogen Production via MSR (Methane Steam Reforming)

1 Background and Motivation:

Hydrogen is a vital chemical and a key component of future clean energy systems. Methane Steam Reforming (MSR) is the primary industrial method for its production. While effective, this process is energy-intensive and utilizes fossil fuels, making process optimization crucial for improving efficiency and reducing its environmental footprint. This project aims to simulate a complete MSR process, implement key improvements, and analyze its performance through the lens of CHE251 (CHEMICAL PROCESS CALCULATIONS) principles.

2 Process Summary and Problems (Schematic on next page):

The process begins by mixing natural gas (methane) with steam, heating the mixture, and feeding it to a reformer where the main reactions occur:

Methane Steam Reforming (MSR): $CH_4(g) + H_2O(g) \rightarrow CO(g) + 3H_2(g)$
Water-Gas Shift (WGS): $CO(g) + H_2O(g) \rightarrow CO_2(g) + H_2(g)$

The hot syngas ($CO(g) + H_2(g)$) from the reformer is cooled and sent to a WGS reactor to maximize hydrogen yield. The stream is then further cooled, and high-purity hydrogen is separated using a **Pressure Swing Adsorption (PSA)** unit.

The Problem with the base case is that it suffers from equilibrium-limited conversion, high energy demand, and potential catalyst deactivation.

3 Objectives:

Develop a base-case process flowsheet in DWSIM/Aspen Plus and perform complete material and energy balances using an equilibrium-based Gibbs Reactor model. Design and integrate a recycle loop with a purge stream to enhance overall methane conversion and analyze its effect on process streams. Perform a heat integration analysis to reduce external utility consumption by using hot process streams to preheat the cold feed. Conduct a sensitivity analysis to identify the optimal reactor temperature for maximizing hydrogen production. Assess the environmental impact by quantifying the $CO_2(g)$ generated per kg of $H_2(g)$ produced and evaluating the energy savings from optimization.

4 Work Plan:

The team will first establish a base-case simulation of the MSR and WGS reactors. Subsequently, we will add the purification section (cooler, flash separator, PSA unit) and the recycle/purge loop. Once the complete, improved flowsheet is converged, we will perform the sensitivity analysis to find the optimal temperature and quantify the benefits of heat integration.

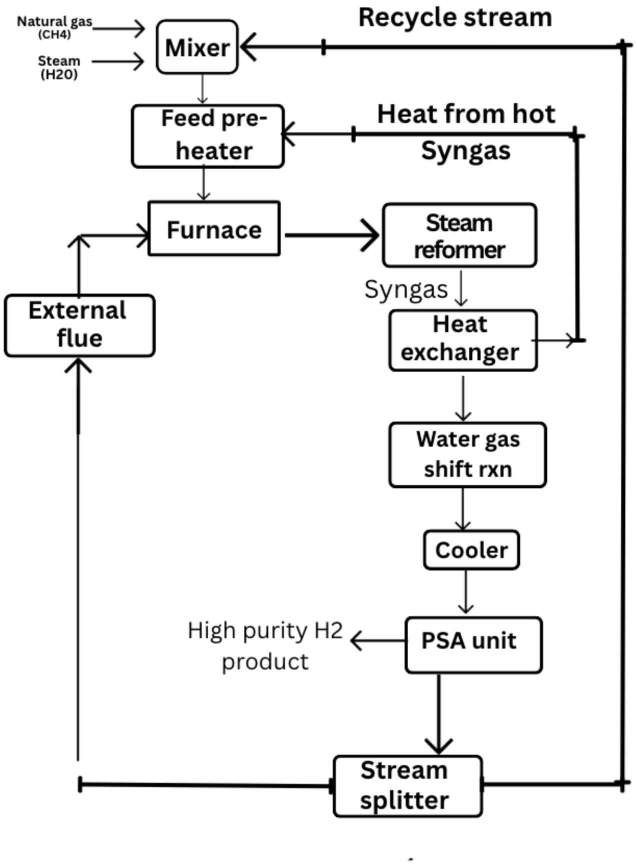

Figure 1: Schematic of our Project Proposal

5 Key References:

These are the references we utilized in creating our problem statement for our term project.

- Amran, U. I., Ahmad, A., & Othman, M. R. (2017). Kinetic based simulation of methane steam reforming and water gas shift for hydrogen production using aspen plus. Chemical Engineering Transactions, 56, 1681-1686. https://doi.org/10.3303/CET1756281
- Himmelblau, D. M., & Riggs, J. B. (2024). Basic Principles and Calculations in Chemical Engineering (9th ed.). Pearson Education.
- Felder, R. M., & Rousseau, R. W. (1986). Elementary Principles of Chemical Processes (2nd ed.). Wiley.

6 Minimum Deliverables:

A converged DWSIM or Aspen Plus simulation file for the fully integrated and optimized process. Comprehensive material and energy balance tables for the final flowsheet. A report detailing the results of the sensitivity analysis, including plots showing the effect of temperature on hydrogen production. A comparative analysis of the process before and after improvements (recycle and heat integration), focusing on conversion, $H_2(g)$ yield, and energy consumption.

7 Additional Deliverables:

An analysis of using the purge gas as a supplementary fuel in the reformer furnace, including its impact on external fuel requirements. A discussion on the role of catalysts in overall process, referencing different types of catalysts (e.g., Nickel-based) and their advantages.

8 Timeline:

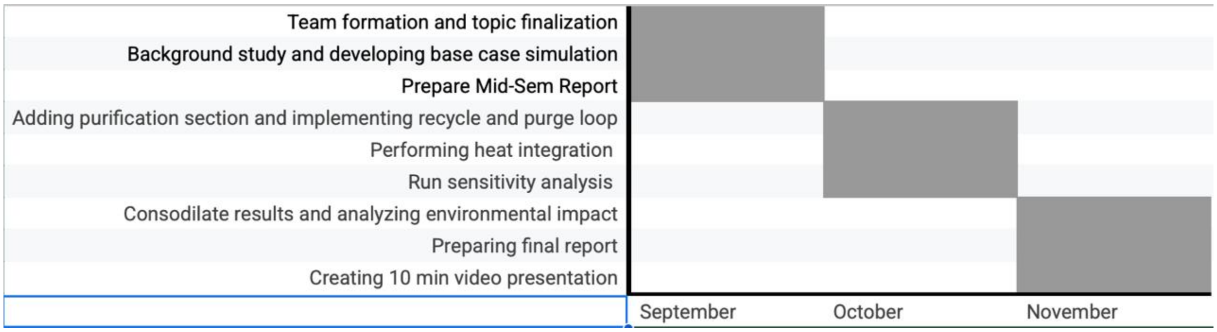

Figure 2: Timeline of Term Project