Mid-semester Term Project Report

Course: CHE251 (CHEMICAL PROCESS CALCULATIONS)

With Group members
Aditya Goel, Karan Chauhan, Krish Agrawal, Krishna Yadav,
Nishant Kumar, Rishi Gupta, Rudra Dwivedi, Saloni Kumari

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

PART A: Base Case Analysis:

Why are we doing this ?
The goal of the base case is to establish a benchmark. We simulate a simple, once through process to rigorously calculate the performance. This provides a baseline for comparing the optimized design in Part B.

1 Process Definition

1.1 Flow Diagram

The base case shows a once-through process where a single furnace provides heat to both preheating and reaction steps.

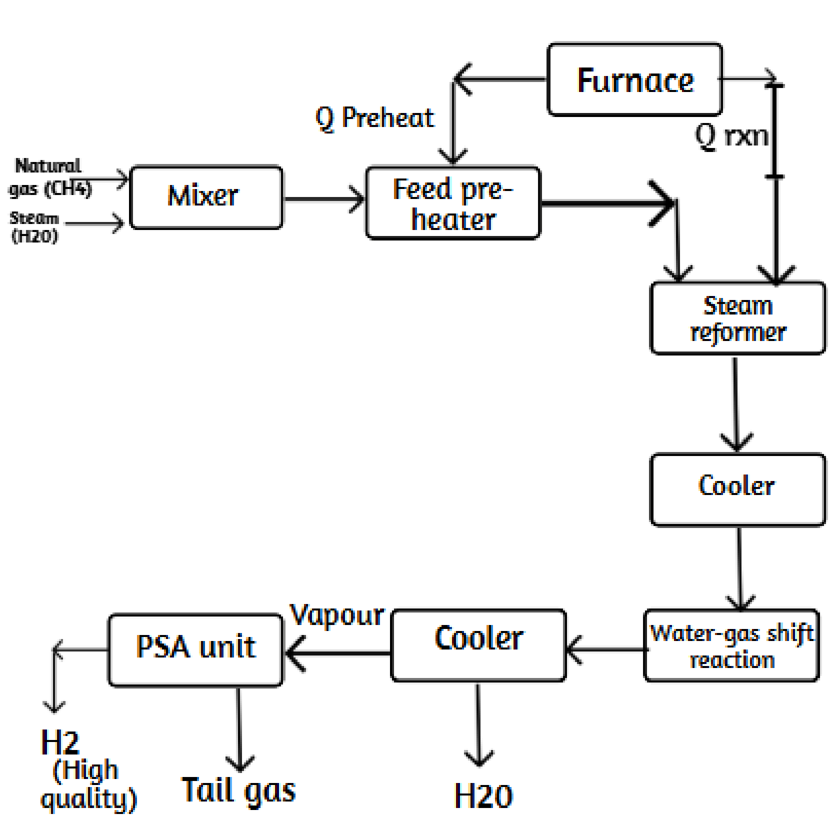


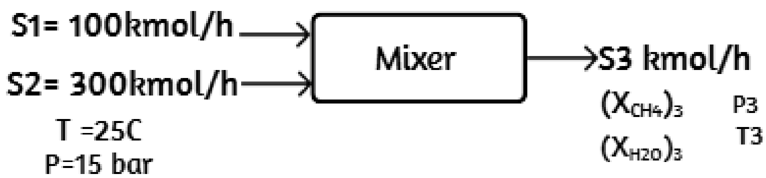
Figure 1: Process Flowchart for Base Case Process.

1.2 Basis of Calculation and Key Assumptions

- Fresh Methane (CH_4) feed (S_1) = 100 kmol/hr at 25 °C, 15 bar.
- Steam-to-carbon Ratio = 3:1 → Fresh Steam Feed (S_2) = 300 kmol/hr.
- Reformer at 800 °C WGS inlet at 400 °C, PSA inlet at 40 °C
- PSA Recovery = 90 % of Hydrogen (H_2)
- Once-Through: Tail gas (S_{10}) is vented.
- Notational Note: For non-reactive units where composition is constant (e.g., heaters, coolers), the outlet stream's composition label may retain the subscript of the inlet stream for brevity.

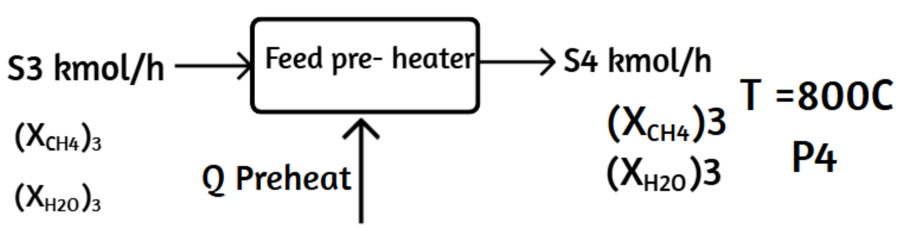
2 Step-by-Step Unit operation analysis

- **Mixer**
  - **Purpose:** Combines fresh methane and steam feeds



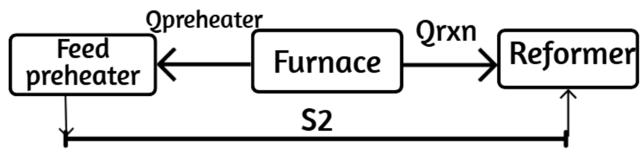
  - **Unknowns:** S_3, $(X_{CH_4})_3$, $(X_{H_2O})_3$,T_3,P_3
  - **Necessary Conditions and Calculation method:**
    - Mass Conservation: $S_3 = S_1 + S_2$
    - Energy Balance: Adiabatic mixing (Q=0)
    - Assuming Negligible Pressure drop

- **Feed Pre-Heater**
  - **Purpose:** Raises mixed feed temperature to 800 °C.



  - **Unknowns:** P_4, $Q_{preheat}$
  - **Necessary Conditions and Calculation method:**
    - Energy Balance with Specified outlet T_4 = 800 °C.
    - Assuming Negligible Pressure drop.

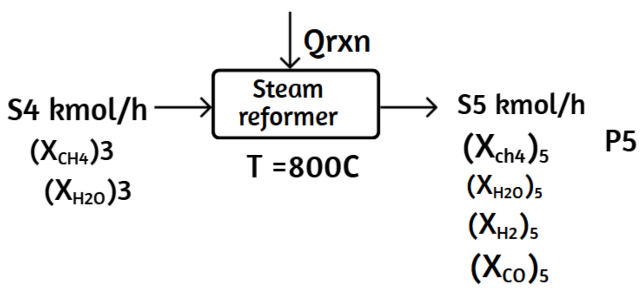
- **Furnace**
  - **Purpose:** Generates all high temperature heat by burning fuel.



– **Unknowns:** Total furnace duty, $Q_{furnace,total}$

– **Necessary Conditions and Calculation method:**
  * $Q_{furnace,total} = Q_{preheater} + Q_{reformer}$

- **Steam Reformer:**
  – **Purpose:** Drives the endothermic reforming reaction at 800 °C.

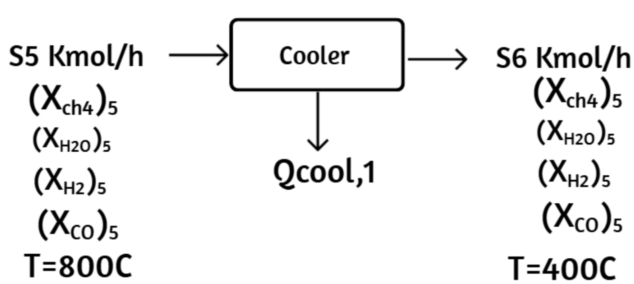


  – **Unknowns:** S_5, $(X_{CH_4})_5$, $(X_{H_2O})_5$, $(X_{CO})_5$, $(X_{H_2})_5$, P_5, Q_{rxn}

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

  – **Necessary Conditions and Calculation method:**
    * Chemical Equilibrium via Gibbs Free Energy Minimization
    * Isothermal: Q_{rxn} balances to hold 800 °C.
    * Assuming Negligible Pressure drop.

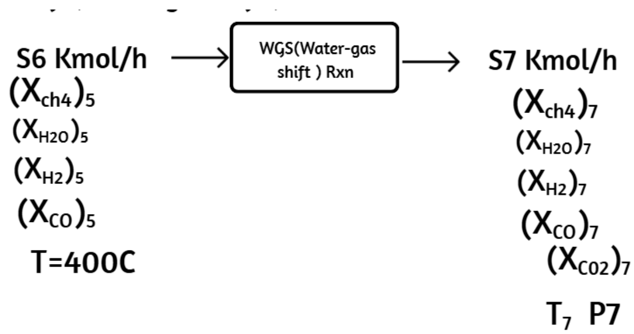
- **Cooler 1:**
  – **Purpose:** Cools syngas from 800 °C to 400 °C for WGS.



  – **Unknowns:** $Q_{cool,1}$, P_6

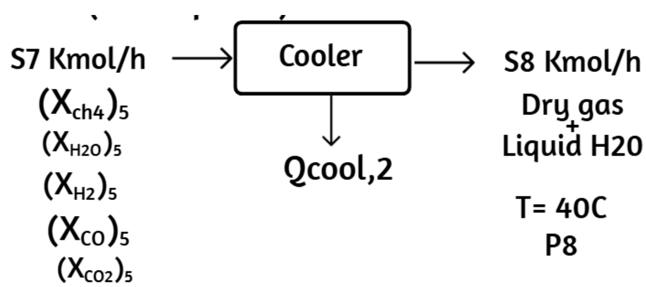
  – **Necessary Conditions and Calculation method:**
    * Energy Balance with specified outlet T = 400 °C
    * Assuming Negligible Pressure drop.

- **WGS Reactor:**



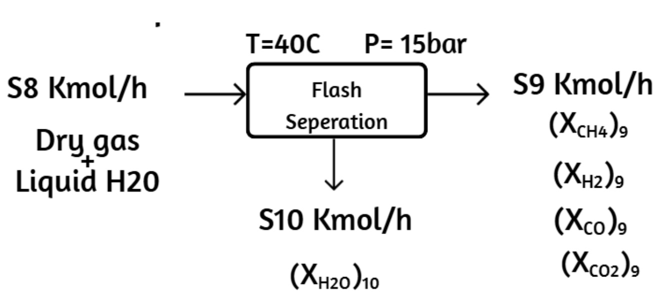
- **Purpose:** To convert CO and H2O into CO2 and H2 respectively.
- **Unknowns:** S_7, $(X_{CH_4})_7$, $(X_{H_2O})_7$, $(X_{CO})_7$, $(X_{H_2})_7$, $(X_{CO_2})_7$, P_7, T_7
- **WGS Reaction:** $CO + H_2O \rightleftharpoons CO_2 + H_2$
- **Necessary Conditions and Calculation method:**
  * Equilibrium and adiabatic assumption (Q=0)
  * Assuming Negligible Pressure drop.

- **Cooler 2:**
  - **Purpose:** Cools the input to 40 °C.



  - **Unknowns:** $Q_{cool,2}$, P_8
  - **Necessary Conditions and Calculation method:**
    * Specified outlet T = 40 °C
    * Assuming Negligible Pressure drop.

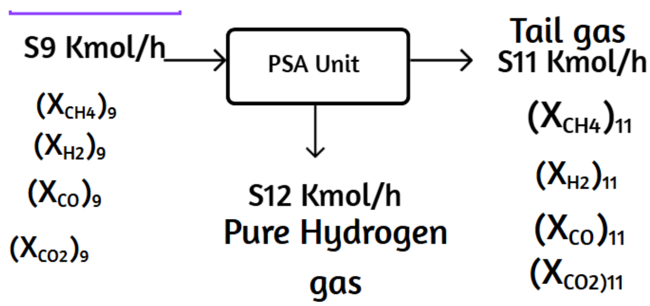
- **Flash Separation:**
  - **Purpose:** Separates dry gas and H_2O and hence removes condensed water out.



  - **Unknowns:** S_9, S_{10}, $(X_{CH_4})_9$, $(X_{CO})_9$, $(X_{H_2})_9$, $(X_{CO_2})_9$

- **Necessary Conditions and Calculation method:**
  * Principle of Vapor-Liquid Equilibrium at specific temperature and Pressure, i.e., T = 40 °C and P = 15 bar.

- **PSA unit:**
  - **Purpose:** Purifies Hydrogen Product



  - **Unknowns:** S_{12}, S_{11}, $(X_{CH_4})_{11}$, $(X_{CO_2})_{11}$, $(X_{H_2})_{11}$, $(X_{CO})_{11}$

  - **Necessary Conditions and Calculation method:**
    * 90 % H_2 Recovery via component splitter
    * Assuming Negligible Pressure drop.

PART B: Main Case Analysis:

Why are we doing this ?
This section simulates the advanced, optimized process which incorporates three key improvements: a recycle loop to increase overall conversion, heat integration to recover waste energy, and the use of the purge stream as a supplementary fuel to reduce external energy demand. The goal is to calculate the performance of this optimized design to prove and quantify these improvements in efficiency and conversion over the base case.

3 Process Definition

3.1 Flow Diagram

The full process includes recycle and heat integration, with the furnace supplying heat to both preheating and reaction steps.

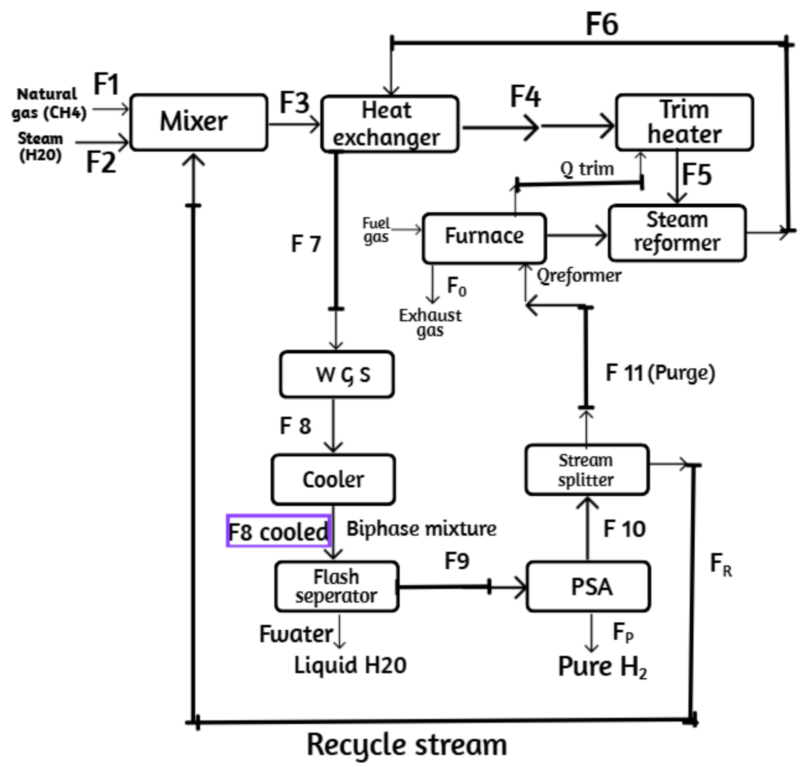


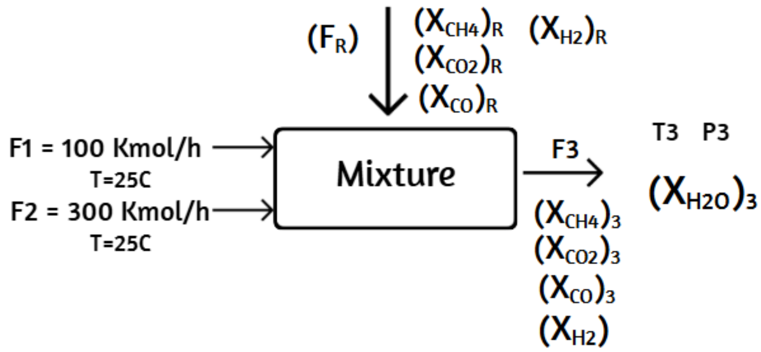
Figure 2: Process Flowchart for Main Case Process.

3.2 Basis of Calculation and Key Assumptions

- Basis: CH_4 and H_2O are supplied at a rate of 100 kmol/hr and 300 kmol/hr, respectively at a temperature of 25 °C
- At the Stream splitter, the streams are divided into two parts:
  - 90 % Recycled Stream (F_R)
  - 10 % Purge Stream (F_{11})
- Notational Note: For non-reactive units where composition is constant (e.g., heaters, coolers), the outlet stream's composition label may retain the subscript of the inlet stream for brevity. .

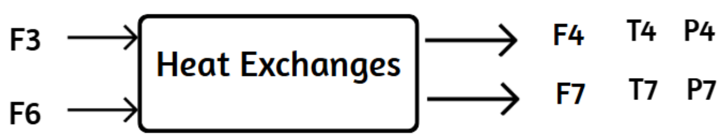
4 Step-by-Step Unit operation analysis

- **Mixer**
  - **Purpose:** Combines fresh feed and recycled stream



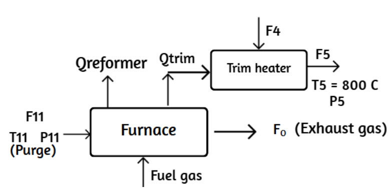
  - **Unknowns:** F_3, $(X_{CH_4})_3$, $(X_{CO_2})_3$, $(X_{H_2})_3$, $(X_{CO})_3$, $(X_{H_2O})_3$, T_3, P_3
  - **Necessary Conditions and Calculation method:**
    * No chemical reaction is taking place in the mixer (requires significantly high temperature)
    * Energy Balance: Adiabatic mixing (Q=0)
    * Minimal Pressure drop across the mixer.
    * Mass Balance.

- **Heat Exchanger**
  - **Purpose:** Preheats feed by recovering waste heat from syngas.



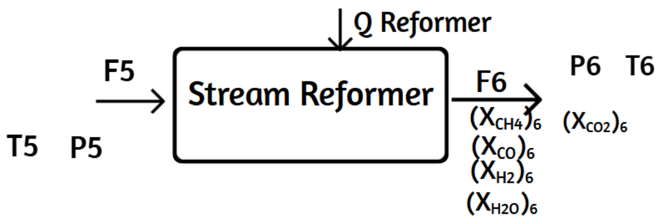
  - **Unknowns:** T_4, P_4, P_7
  - **Necessary Conditions and Calculation method:**
    * Outlet Temperature $T_7 = 400\,°C$
    * Energy Balance: $Q_{lost,hot} = Q_{gained,cold}$
    * Assuming Negligible Pressure drop

- **Furnace and Trim heater**
  - **Purpose:** Provides final heat to reach 800 °C (required temperature for MSR).



- **Unknowns:** F_5, Q_{trim}(heat given by furnace to rise the temperature of mixture to 800C), P_5,F_0,F_g(flow rate of fuel gas), $Q_{Furnace,total}$
- **Necessary Conditions and Calculation method:**
  - $T_5 = 800\,°\mathrm{C}$
  - Conservation of mass is obeyed
  - Assuming Negligible Pressure drop
  - $Q_{furnace,total} = Q_{Trim} + Q_{reformer}$

- **Steam Reformer:**
  - **Purpose:** To convert the heated feed into a syngas mixture at chemical equilibrium.

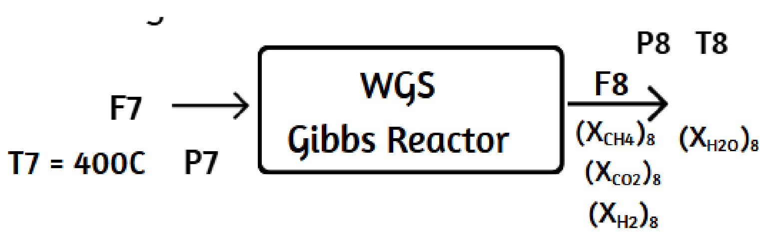


  - **Unknowns:** F_6, $(X_{CH_4})_6$,$(X_{H_2O})_6$, $(X_{H_2})_6$, $(X_{CO})_6$, P_6,$Q_{reformer}$,$(X_{CO_2})_6$

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

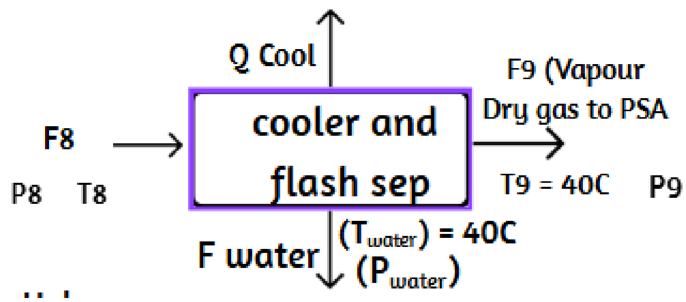
  - **Necessary Conditions and Calculation method:**
    - Equilibrium is reached when the thermodynamically most stable product is formed, minimizing Gibbs free energy.
    - Isothermal operation so that the equilibrium is not disturbed(T6=800C).
    - Assuming a Negligible Pressure Drop.

- **WGS Gibbs Reactor:**
  - **Purpose:** Converts CO to $CO2$ and increases H_2 yield



  - **Unknowns:** F_8, $(X_{CH_4})_8$, $(X_{H_2O})_8$, $(X_{CO_2})_8$, $(X_{H_2})_8$, $(X_{CO})_8$, T_8, P_8
  - **WGS Reaction:** $CO + H_2O \rightleftharpoons CO_2 + H_2$
  - **Necessary Conditions and Calculation method:**
    - Equilibrium is reached when the thermodynamically most stable product is formed, minimizing Gibbs free energy.
    - Adiabatic reactor ($Q_{net} = 0$)
    - Assuming Negligible Pressure drop.

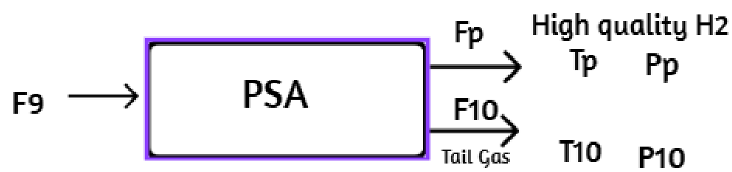
- **Cooler and Flash:**
  - **Purpose:** Cooler cools the feed to $40\,°\mathrm{C}$ and removes condensed water via flash distillation



- **Unknowns:** F_9, F_{water}, $(X_{CH_4})_9$, $(X_{CO_2})_9$, $(X_{H_2})_9$, $(X_{CO})_9$, Q_{cool}, P_9, P_{water}

- **Necessary Conditions and Calculation method:**
  * The specified outlet temperature, $T_9 = 40$ and Pressure (P) is equal to 15 bar.
  * The vapor-liquid equilibrium is reached.
  * Assuming a Negligible Pressure Drop.

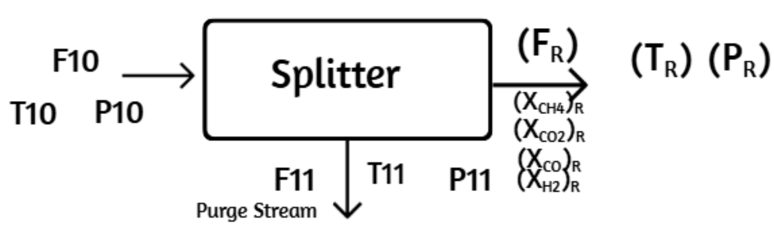
- **PSA unit:**
  - **Purpose:** Purifies Hydrogen Product



  - **Unknowns:** F_{10}, F_P, , $(X_{CH_4})_{10}$, $(X_{CO_2})_{10}$, $(X_{H_2})_{10}$, $(X_{CO})_{10}$, P_{10}, P_P, T_P, T_{10}

  - **Necessary Conditions and Calculation method:**
    * 90 % H_2 Recovery
    * Assuming Negligible Pressure and Temperature drop.
    * Temperature Will remain constant.

- **Stream Splitter:**
  - **Purpose:** Divides PSA tail gas into recycle and purge streams.



  - **Unknowns:** F_{11}, F_R, P_{11}, P_R, T_{11}, T_R

  - **Necessary Conditions and Calculation method:**
    * The splitter divides the feed stream (F_{10}) into recycle (90 %) and purge (10 %) streams.
    * Assume a negligible pressure and temperature drop across the splitter.
    * Temperature will remain constant in separation process