Indian Institute of Technology Kanpur

CHE251: Chemical Process Calculations

End-Semester Project Report

Process Simulation and Optimization of Hydrogen Production via MSR[1]

With Group members

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[1]Methane Steam Reforming

Abstract

Hydrogen is a vital chemical feedstock and a key component of future clean energy systems. Currently, Methane Steam Reforming (MSR) is the primary industrial method for its production. This process involves reacting natural gas (methane) with steam at high temperatures to produce a syngas mixture.

The main reactions governing the process are:

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 resulting syngas is then cooled, processed in a WGS[2] reactor to maximize hydrogen yield, and finally purified, typically using a Pressure Swing Adsorption (PSA) unit.

While effective, the conventional MSR[3] process is highly energy-intensive and relies on fossil fuels. A simple, "once-through" process often suffers from equilibrium-limited conversion and high energy demand. Therefore, process optimization is crucial for improving thermal efficiency, increasing methane conversion, and reducing the overall environmental footprint.

This project simulates and analyzes two configurations: a "Base Case" to establish a benchmark and an optimized "Main Case." The main case integrates key process improvements to quantify gains in efficiency and production.

[2] Water-Gas Shift
[3] Methane Steam Reforming

Contents

1 Objectives

The primary objective of this project is to perform a rigorous simulation and analysis of the MSR process using CHE251 (CHEMICAL PROCESS CALCULATIONS) principles. The key goals include:

- 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 all process streams.
- Perform a heat integration analysis to reduce external utility consumption by using the hot syngas stream to preheat the cold reactor 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 the optimization step.

2 Process Flowsheet Development

This project analyzes two distinct process flowsheets to quantify the benefits of process optimization.

2.1 Base Case: Once-Through Process

The base case establishes a benchmark for performance. It models a simple, once-through process where a single furnace provides all heat for both feed preheating and the steam reforming reaction. The tail gas from the PSA unit is vented, and there is no energy recovery. This flowsheet allows for a rigorous calculation of baseline performance, which serves as a metric for comparison against the optimized design.

2.2 Main Case: Optimized Process with Recycle and Heat Integration

The main case simulates an advanced, optimized process incorporating three key improvements:

- Recycle Loop: The tail gas from the PSA unit is split. 90% is recycled back to the mixer, increasing the overall conversion of methane.

- Heat Integration: A heat exchanger (MH-100) is added to use the hot, 800°C syngas exiting the Steam Reformer (L_1) to preheat the cold mixed feed (Stream 3).
- Purge as Fuel: The 10% purge stream, which is rich in combustible gases, is used as a supplementary fuel for the furnace, further reducing external energy demand.

3 Components and Key Reactions

The simulation involves the following primary chemical components:

- Methane (CH_4): The primary reactant in the natural gas feed.
- Water (H_2O): The steam used for the reforming process.
- Hydrogen (H_2): The desired final product.
- Carbon Monoxide (CO): An intermediate product from reforming.
- Carbon Dioxide (CO_2): The final carbon-based product after the WGS reaction.

The entire process is governed by two principal, reversible reactions:
Methane Steam Reforming (MSR):
$CH_4(g) + H_2O(g) \rightarrow CO(g) + 3H_2(g)$
This is the main endothermic reaction that produces the initial syngas mixture.

Water-Gas Shift (WGS):
$CO(g) + H_2O(g) \rightarrow CO_2(g) + H_2(g)$
This exothermic reaction converts the carbon monoxide and steam into more hydrogen, maximizing the product yield.

4 Process Unit Descriptions

The "Main Case" flowsheet integrates multiple unit operations to achieve the goals of high conversion and energy efficiency. The following is a step-by-step description of each unit's purpose in the optimized process.

4.1 Mixer

Purpose: To combine the fresh feeds (100 kmol/hr Methane and 300 kmol/hr Steam) with the recycle stream(at 40 C) coming from the PSA tail gas splitter. This unit operates adiabatically.

4.2 Heat Exchanger (MH-100)

Purpose:
This unit performs the main heat integration and has a critical dual purpose.

Syngas Cooling:
It takes the 800°C hot syngas from the Steam Reformer outlet (Stream 6) and cools it down to 400°C (Stream 7), which is the required inlet temperature for the WGS Reactor.

Feed Preheating:
It transfers this recovered heat to the cold mixed feed (Stream 3), raising its temperature from 129°C to 545°C (Stream 4). This significantly reduces the energy required from the Trim Heater.

4.3 Trim Heater and Furnace

Purpose: The furnace provides the high-temperature heat required for two endothermic processes. The Trim Heater section provides the final preheating to bring the feed (Stream F_4) to the required 800°C reaction temperature. The Furnace also supplies the main reaction heat ($Q_{reformer}$) to the steam reformer to maintain its isothermal operation.

4.4 Steam Reformer (Gibbs Reactor)

Purpose: This is the primary reactor where the heated feed is converted into syngas. It is modeled as an isothermal Gibbs Reactor operating at 800°C, where the MSR reaction ($CH_4(g) + H_2O(g) \rightleftharpoons$ CO(g)+ 3H$_2(g)$) reaches chemical equilibrium by minimizing the Gibbs free energy.

4.5 WGS Gibbs Reactor

Purpose: To maximize the hydrogen yield by converting Carbon Monoxide (CO). The syngas enters at 400°C (after cooling in the heat exchanger) and undergoes the WGS reaction ($CO(g) + H_2O(g) \rightleftharpoons$ CO$_2(g) + H_2(g)$). This unit is modeled as an adiabatic reactor, also using Gibbs free energy minimization to determine the equilibrium composition.

4.6 Cooler and Flash Separator

Purpose: This two-stage unit prepares the gas for purification. The Cooler chills the hot gas from the WGS reactor down to 40°C. The Flash Separator then removes the condensed water (Stream F_{water}) from the "dry" gas stream (Stream F_9) at 15 bar, based on vapor-liquid equilibrium principles.

4.7 PSA (Pressure Swing Adsorption unit) Unit

Purpose: To purify the final hydrogen product. It is modeled as a component splitter that recovers 90% of the H_2 from the dry gas stream (Stream F_9) to produce the high-quality hydrogen product (Stream Fp). The remaining components (CH_4, CO, CO_2, and 10% H_2) exit as the "Tail Gas" (Stream F_{10}).

4.8 Stream Splitter

Purpose: To divide the PSA tail gas (Stream F_{10}) into two streams. 90% of the flow is routed back as the Recycle Stream (Stream F_r) to the mixer. The remaining 10% is removed as the Purge Stream (Stream F_{11}) to prevent the buildup of inert components in the loop.

5 Basis of Calculations

All simulations for both the Base and Main cases are based on the following process conditions:

1. Fresh Methane Feed (S_1): 100 kmol/hr at 25°C and 15 bar.
2. Fresh Steam Feed (S_2): 300 kmol/hr.
3. Steam-to-Carbon Ratio: 3:1.
4. Reformer Temperature: 800°C.
5. WGS Inlet Temperature: 400°C.
6. PSA Inlet Temperature: 40°C (after cooling and flash).
7. PSA H_2 Recovery: 90%.
8. Recycle Split (Main Case): 90% of tail gas is recycled, 10% is purged.

6 Material and Energy Balance Analysis

A detailed material and energy balance was performed for all unit operations in both the Base Case and Main Case using DWSIM/Aspen Plus. The full, detailed stream tables for each unit are available in Appendix A.

6.1 Key Performance Results (Summary)

Based on the converged simulations, we can compare the overall performance of the two process designs.

Parameter	Base Case Value	Main Case Value
H_2 Product Flow Rate	173.59 kmol/hr (stream 18)	267.5 kmol/hr (Pure H_2)
Tail Gas / Purge Flow	120.46 kmol/hr (Stream 19, Vented)	100.4 kmol/hr (Purge, Fuel)
Water Removed	211.35 kmol/hr	184.4 kmol/hr (F_{water})
Gross Furnace Heat Duty	12,322.68 kW	24,458.0 kW

6.2 Material Balance Analysis (Base Case)

The material flow rates for the key outlet streams were taken from the converged DWSIM simulation:

- Hydrogen Product (Stream 18):
  The final product stream has a flow rate of 173.59 kmol/hr. This stream is 100% pure hydrogen, as the PSA unit was modeled to remove all other components.

- Removed Water (Stream 16):
  The liquid stream from the flash separator (V-1) removes 211.35 kmol/hr of liquid, which is 99.25% pure water. This successfully removes the unreacted steam from the process gas.

- Tail Gas (Stream 19):
  The tail gas vented from the PSA unit has a flow rate of 120.46 kmol/hr. This stream contains all the unreacted methane (47.46 kmol/hr), CO_2, and CO byproducts, representing a significant loss of potential fuel.

6.3 Energy Balance Analysis (Base Case)

The energy duties for the Base Case were also taken directly from the DWSIM flowsheet:

- Furnace Heat Duty
  The total heat required from the furnace is the sum of the duty for the feed pre-heater (H-1) and the isothermal steam reformer (RGIBBS-1).
  - Pre-Heater Duty (E_1): 7,455.23 kW
  - Reformer Duty (E_2): 4,867.45 kW
  - $Q_{furnace,total}$ = 7,455.23 + 4,867.45 = 12,322.68 kW

- Cooling Duty
  The total cooling load is the sum of all coolers required to bring the process streams to their target temperatures.
  - Cooler 1 (E_3): 2,345.23 kW
  - Cooler 2 (E_5): 5,887.42 kW
  - Cooler 3 (E_7): 19.21 kW
  - $Q_{cooling,total}$ = 2,345.23 + 5,887.42 + 19.21 = 8,251.86 kW

6.4 Material and energy balance of main case

The Main Case analysis reflects the intensified process of the recycle loop.

Material Balance (Main Case):

- Hydrogen Product (Stream Pure H_2):
  The final product stream is $267.5 kmol/hr$, representing a 54.1% increase over the Base Case

- Removed Water (Stream F_{water}):
  The flash separator removes 184.4 kmol/hr of liquid water.

- Purge Stream (Stream Purge):
  The purge stream vents 100.4 kmol/hr of gas, which is necessary to maintain a steady state in the recycle loop.

Energy Balance (Main Case):

- Gross Furnace Heat Duty
  The total heat required from the furnace is the sum of the Trim Heater (F-101) and the Steam Reformer (L_1).
  - Trim Heater Duty (E_1): 13,889 kW
  - Reformer Duty (E_2): 10,569 kW
  - $Q_{furnace,total} = 13{,}889 + 10{,}569 = 24{,}458$ kW

  This gross energy value reflects the intensified process required to achieve the high conversion. A full analysis of the net energy requirement, including the fuel credit from the purge gas, is detailed in Section 8.

7 Process Optimization and Analysis

The objective is to enhance the Base Case process by introducing design improvements that increase conversion efficiency, optimize energy usage, and improve environmental performance.

7.1 Property Method Selection

The Peng–Robinson property package (Basis-1) was selected for the simulation. Operating at up to 800°C and 15 bar, the MSR process involves non-polar gases (CH_4, H_2, CO, CO_2) and polar water vapor (H_2O). The Peng–Robinson equation of state ensures accurate modeling for both high-temperature gas-phase reactions and lower-temperature vapor–liquid equilibrium (VLE) calculations.

7.2 Analysis of Recycle and Purge Loop

Base Case: The PSA tail gas (120.46 kmol/hr) was completely vented, containing unreacted CH_4 and unrecovered H_2, leading to major losses of reactants and product potential.

Main Case: A recycle loop was introduced where 90% of the PSA tail gas was recycled to the mixer, and 10% was purged to prevent inert buildup. This created a recycle flow of 900.9 kmol/hr. Methane conversion increased from 52.5% to 78.0%, while the 10% purge (100.4 kmol/hr) stabilized the system by removing inerts and unreacted gases.

Analysis of Results: The recycle and purge design achieved substantial methane conversion improvement and resource recovery, significantly reducing waste. The purge stream ensures steady operation, preventing CO_2 and CH_4 accumulation.

7.3 Heat Integration Analysis

Base Case: The Base Case required 12,322.68 kW of furnace heat and 8,251.86 kW of energy was spent on cooling, resulting in significant heat losses to the environment.

Main Case: A heat exchanger (MH-100) was implemented to recover 10,569 kW of heat from the 800°C reformer outlet (Stream 6), preheating the mixed feed (Stream 3) from 129°C to 545°C. The Trim Heater (F-101) supplied the remaining heat to reach 800°C. The total furnace duty became 24,458 kW (13,889 kW for the heater and 10,569 kW for the reformer).

Analysis of Results: Although total furnace load increased due to the large recycle stream, the heat exchanger improved energy efficiency by reducing external fuel needs. The recovered heat reduced overall utility consumption and enhanced process sustainability when combined with purge gas combustion.

7.4 Sensitivity Analysis: Effect of Reactor Temperature

Objective: To find the optimal steam reformer temperature, as specified in the project deliverables.

Methodology:
A sensitivity analysis was performed on the Main Case simulation. The temperature of the Steam Reformer (RGIBBS-1) was varied from 700°C to 900°C. The effect on key process variables was plotted.

Analysis of results:-

Plot 1: Hydrogen Yield vs. Temperature

This plot confirms the thermodynamic principles of the endothermic MSR reaction. As the temperature increases from $700°C$ to $900°C$, the equilibrium shifts toward the

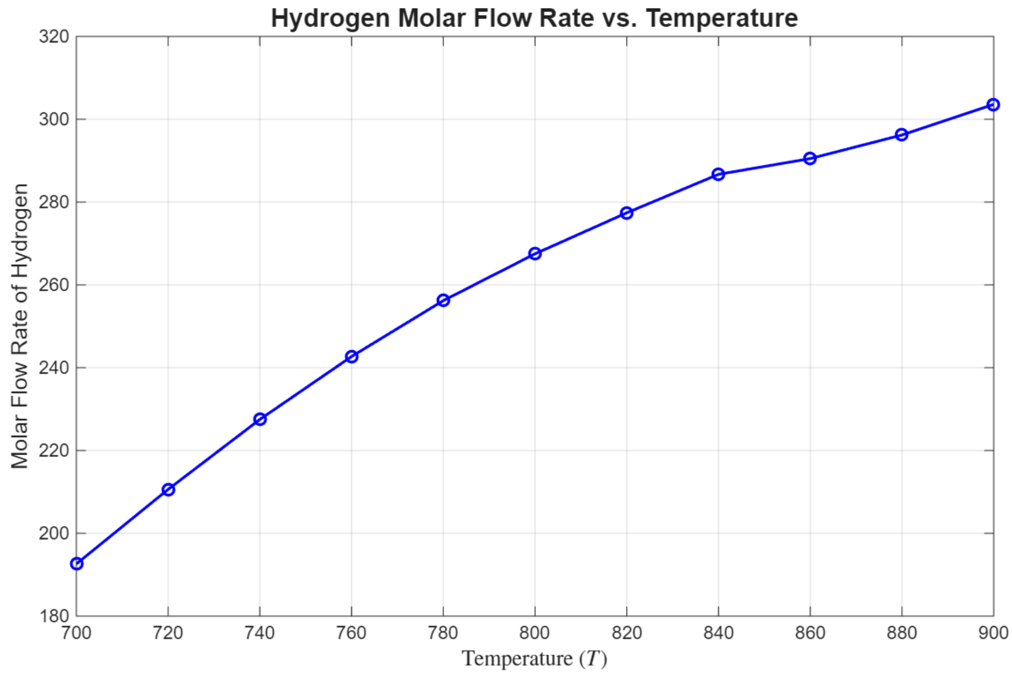


Figure 1: Hydrogen Molar Flow Rate (kmol/hr) vs. Steam Reformer Temperature (TC)

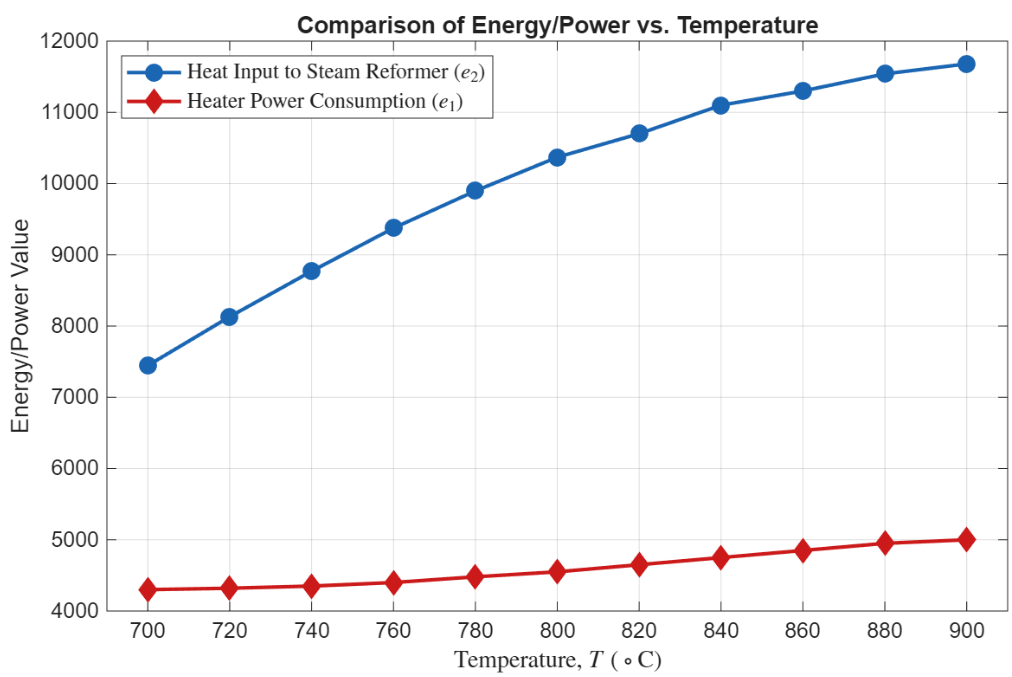


Figure 2: Comparison of Energy Duties (kW) vs. Steam Reformer Temperature (TC) showing heat input to the Reformer (E_2) and Trim Heater (E_1)

products, causing the Hydrogen Molar Flow Rate to increase from $192 kmol/hr$ to $305 kmol/hr$.

Plot 2: Total Furnace Duty vs. Temperature

This plot shows the cost associated with achieving the increased conversion:

1. **Heat Input to Steam Reformer (E_2):** Increases steadily. This is expected, as more heat is required to sustain the highly endothermic reaction at higher conversion levels.

2. **Heater Power Consumption (E_1):** This is the Trim Heater duty required to raise the temperature of the cold feed and large recycle loop to the new target temperature. It increases significantly, nearly doubling across the range.

Conclusion on Optimal Temperature

The optimal operating range is determined by finding the point where the cost of heating (Plot 2) becomes too high relative to the gain in hydrogen (Plot 1).

- **Trade-off:** Conversion increases most rapidly between $700°C$ and $800°C$. Beyond $850°C$, the curve begins to flatten (diminishing returns).

- **Optimal Range:** The simulated operating point of $800°C$ is validated as the optimal range. It provides a good balance, yielding $267.5 kmol/hr$ of H_2 without incurring the disproportionately high energy costs required to push the temperature toward $900°C$.

7.5 Analysis of Purge Gas as Fuel

Base Case: In the Base Case, the entire PSA tail gas (120.46 kmol/hr) was vented, wasting unreacted CH_4, CO, and H_2 while releasing CO_2 into the atmosphere.

Main Case: In the optimized design, 10% of the tail gas (100.4 kmol/hr) was purged and combusted in the furnace. The purge gas contained CH_4 (0.2196), CO (0.3367), and H_2 (0.0296). Combustion of these components provided a recoverable energy credit of 7,768.2 kW (CH_4: 4,912.1 kW; H_2: 199.5 kW; CO: 2,656.6 kW), reducing external fuel demand.

Analysis of Results: Using the purge gas as supplementary fuel improved the overall process energy efficiency. The energy recovered from combustion compensated part of the furnace duty, reducing operating costs and greenhouse gas emissions from venting.

7.6 Discussion on the Role of Catalysts

The simulation assumes equilibrium-based reactors, representing theoretical maximum conversion. In practical operation, catalysts are essential to approach these ideal results.

Steam Reformer Catalyst: Nickel (Ni) supported on alumina (Al_2O_3) is the industrial standard. Ni promotes C–H bond breaking in CH_4, while alumina provides high thermal stability and surface area at around 800°C. The simulated performance depends on this catalyst system under proper control.
Water–Gas Shift Catalyst: The WGS reaction typically operates in two stages:

- **High-Temperature Shift (HTS):** Fe–Cr catalyst at 350–450°C rapidly converts CO to CO_2 and H_2.
- **Low-Temperature Shift (LTS):** Cu–Zn–Al_2O_3 catalyst at 200–250°C enhances CO removal at lower temperatures.

In the simulation, the WGS reactor (L_2) operates at 400°C, consistent with HTS operation. The Fe–Cr catalyst ensures high CO conversion and minimizes side reactions such as methanation.

Conclusion: Effective catalysts—Ni/Al_2O_3 for the reformer and Fe–Cr (optionally Cu–Zn–Al_2O_3) for the WGS reactor—are crucial to achieving simulated conversions. Without them, actual conversion and efficiency would fall short of equilibrium predictions.

8 Comparative Analysis: Base Case vs. Main Case

This section provides a direct comparison of the key performance indicators for both process designs. The Base Case results are taken from the converged simulation, while the Main Case results are left blank to be filled in after that simulation is complete.

8.1 Key Performance Indicator Comparison

Category	Parameter	Base Case Value	Main Case Value
INPUTS	Fresh Methane Feed	100.00 kmol/hr	100.00 kmol/hr
	Fresh Steam Feed	300.00 kmol/hr	300.00 kmol/hr
OUTPUTS	High-Purity H_2 Product (S_{19}/F_p)	173.59 kmol/hr	267.50 kmol/hr
	Tail Gas / Purge Flow (S_{18}/F_{11})	120.46 kmol/hr (Vented)	100.40 kmol/hr
	Water Removed (Liquid) (S_{16} / F_{water})	211.35 kmol/hr (Vented)	184.40 kmol/hr
PERFORMANCE	Overall Methane Conversion	52.5%	78.0%
ENERGY	Gross Furnace Duty ($Q_{furnace,total}$)	12,322.68 kW	$24,458.00$ KW
	Purge Gas Energy Credit	0.00 kW	$7,768.20$ kW
	Net External Energy Required	$12,322.68$ kW	$16,689.80$ kW

8.2 Analysis of Results

1. Hydrogen Yield Methane Conversion (The Primary Success):

   - H_2 Production:
     The Main Case produced 267.5 kmol/hr of hydrogen, a 54.1% increase over the Base Case (173.59 kmol/hr).
   - Methane Conversion:
     The increase in H_2 yield is primarily due to improved reactant utilization via recycling. Overall Methane Conversion (calculated as (CH_{4in} - $CH_{4out-purge}$) / CH_{4in}) rose from 52.5% (Base) to 78.0% (Main).

2. Energy Consumption Analysis (Net vs. Gross):

   - Gross Energy:
     The Main Case gross furnace duty (24,458.0 kW) is significantly larger than the Base Case (12,322.68 kW), because the furnace must heat the additional recycle flow in the Main Case.
   - Purge Credit:
     The Main Case recovers energy by combusting the purge stream; Section 7.5 calculated a purge gas credit of 7,768.2 kW.
   - Net External Energy: Subtracting the purge credit gives a Main Case net external energy of 16,689.8 kW. Compared to the Base Case (12,322.68 kW), this is a net increase of 35.4% in external energy for a 54.1% increase in H_2 output.
     This trade-off is favorable: sizeable production gain for a moderate net energy penalty, with improved environmental performance.

3. Environmental and Operational Advantages:

   - The Main Case eliminates direct venting of CH_4 and CO (see Section 9), improving regulatory compliance and site safety.
   - Product purity and yield improvements make downstream utility and separation units more effective.
   - The recovered purge energy reduces purchased fuel and operating cost compared to a design that vents tail gas.

8.3 Overall Conclusion

- The Main Case is clearly superior from the standpoint of process intensification: it achieves a 54.1% increase in H_2 production and raises methane conversion from 52.5% to 78.0%.

- Although gross furnace duty increases substantially in the Main Case, the purge gas energy credit (7,768.2 kW) reduces net external energy demand to a realistic figure (16,689.8 kW).
- When environmental improvements (100% elimination of vented CH_4 and CO) and improved resource utilization are considered, the Main Case represents a more complete, efficient, and industrially viable design than the Base Case.

9 Environmental Impact Analysis

A key objective of this project is to assess the environmental impact. This analysis must include not only Carbon Dioxide (CO_2) but also other highly potent greenhouse gases like Methane (CH_4) and toxic pollutants like Carbon Monoxide (CO).

9.1 Base Case Analysis

In the Base Case, the tail gas (Stream 19) is vented directly to the atmosphere. This is an environmentally irresponsible design, as it releases unburnt fuel and toxic gases.

- Tail Gas Flow (Stream 19): 120.46 kmol/hr
- Vented Pollutants:
  - CH_4 Vented: (120.46 kmol/hr * 0.39387) = 47.46 kmol/hr (A potent greenhouse gas)
  - CO Vented: (120.46 kmol/hr * 0.15759) = 18.98 kmol/hr (A toxic pollutant)
  - CO_2 Vented: (120.46 kmol/hr * 0.28044) = 33.78 kmol/hr

The Base Case is not a viable process as it vents large quantities of toxic CO and potent CH_4.

9.2 Main Case Analysis: Combustion of Purge Gas

In the Main Case, the purge stream (Stream 10) is routed to the furnace, where its combustible components are burned. This is a form of waste gas treatment, which destroys the most harmful pollutants.

- Purge Gas Flow (Stream 10): 100.4 kmol/hr
- Pollutants before Combustion:
  - CH_4: 22.05 kmol/hr
  - CO: 33.80 kmol/hr
  - CO_2: 38.93 kmol/hr

- Pollutants after Combustion:
  - The furnace converts all CH_4 and CO into CO_2:
    - $CH_4 \rightarrow CO_2$: 22.05 kmol/hr of CH_4 becomes 22.05 kmol/hr of CO_2
    - $CO \rightarrow CO_2$: 33.80 kmol/hr of CO becomes 33.80 kmol/hr of CO_2
  - Total CO_2 Emitted: 38.93 (original) + 22.05 (from CH_4) + 33.80 (from CO) = 94.78 kmol/hr

9.3 Environmental Conclusion

A direct comparison of the final atmospheric emissions shows the clear superiority of the Main Case.

Atmospheric Emission	Base Case (Vented)	Main Case (Burned)	Environmental Impact
CO (Toxic Gas)	18.98 kmol/hr	0.00 kmol/hr	100% Reduction (SUCCESS)
CH_4 (Potent GHG)	47.46 kmol/hr	0.00 kmol/hr	100% Reduction (SUCCESS)
CO_2 (GHG)	33.78 kmol/hr	94.78 kmol/hr	(Increase)

Analysis: The Main Case is an unambiguously superior environmental design. **It completely eliminates 100% of toxic Carbon Monoxide and potent Methane emissions.**

While the CO_2 emissions are higher, this is a direct consequence of proper environmental treatment. The Main Case correctly converts all pollutants into CO_2, which is the industry-standard and environmentally required practice for handling such a waste stream. The Base Case's lower CO_2 value is misleading, as it comes at the cost of venting highly toxic and potent pollutants

10 Deliverables

This project successfully satisfies the objectives outlined in the proposal.
The key deliverables provided include:

1. **Converged Simulation Files:**
   - DWSIM simulation files for the Base Case and Aspen file for the fully integrated Main Case.
2. **Comprehensive Report:**
   This document includes detailed analysis and results covering the following:
   - Complete material and energy balances for both flowsheets (Section 6)
   - Comparative analysis of the process before and after improvements (Section 8)

- Sensitivity analysis on the reactor temperature (Section 7.4)
- Analysis of using purge gas as supplementary fuel (Section 7.5)
- A discussion on the role of catalysts in the process (Section 7.6)
- Environmental impact analysis of CO_2 generation (Section 9)

11 Timeline

The project was carried out according to the proposed semester plan. It covered three main months of work — from initial research and simulation setup to optimization, environmental evaluation, and final report submission.

Task	**Month**
Team formation and topic finalization	September
Background study and developing base case simulation	September
Prepare Mid-Sem Report	October
Adding purification section and implementing recycle/purge	October
Performing heat integration	November
Running sensitivity analysis	November
Consolidating results and analyzing environmental impact	November
Preparing final report	November
Creating 10-minute video presentation	November

12 Results and Simulation Files

The complete, converged simulation files for both the Base Case and the Main Case are available for review.

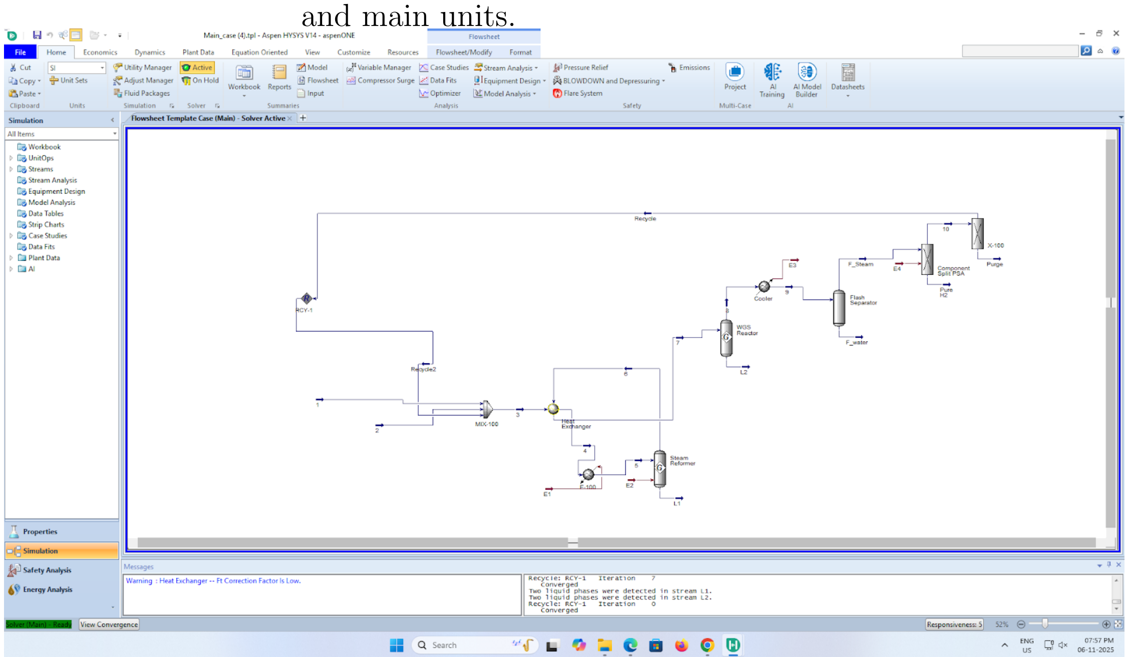
These files contain:

- All stream data
- Unit operation configurations
- Sensitivity analysis data used to generate the results presented in this report

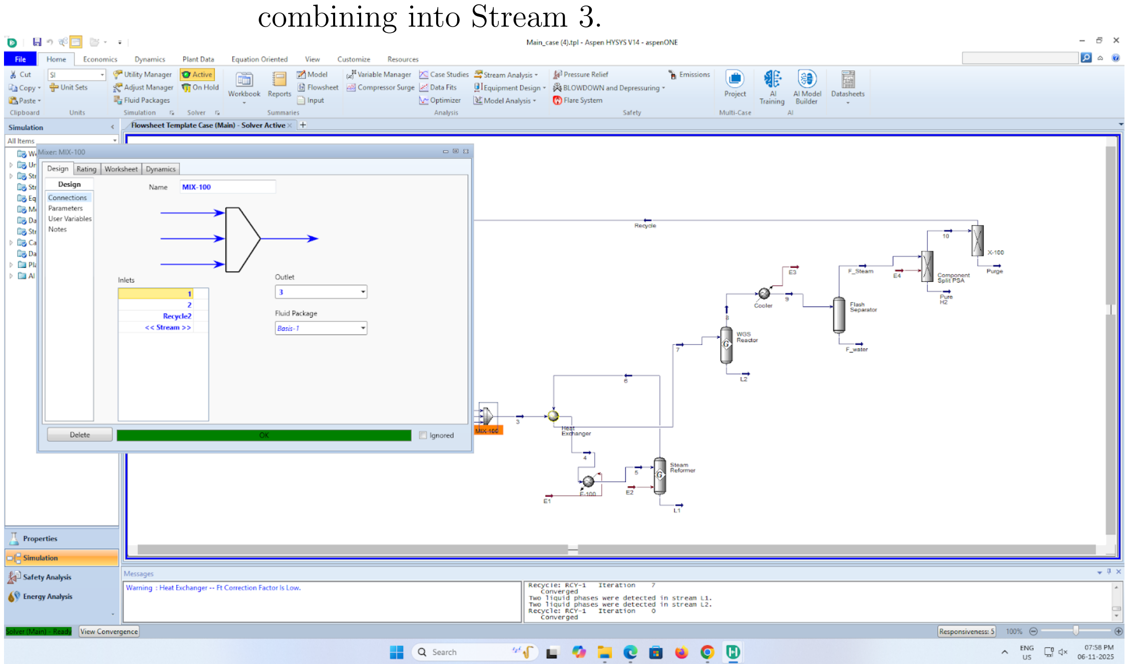
Google Drive Link to Simulation Files

13 Appendices

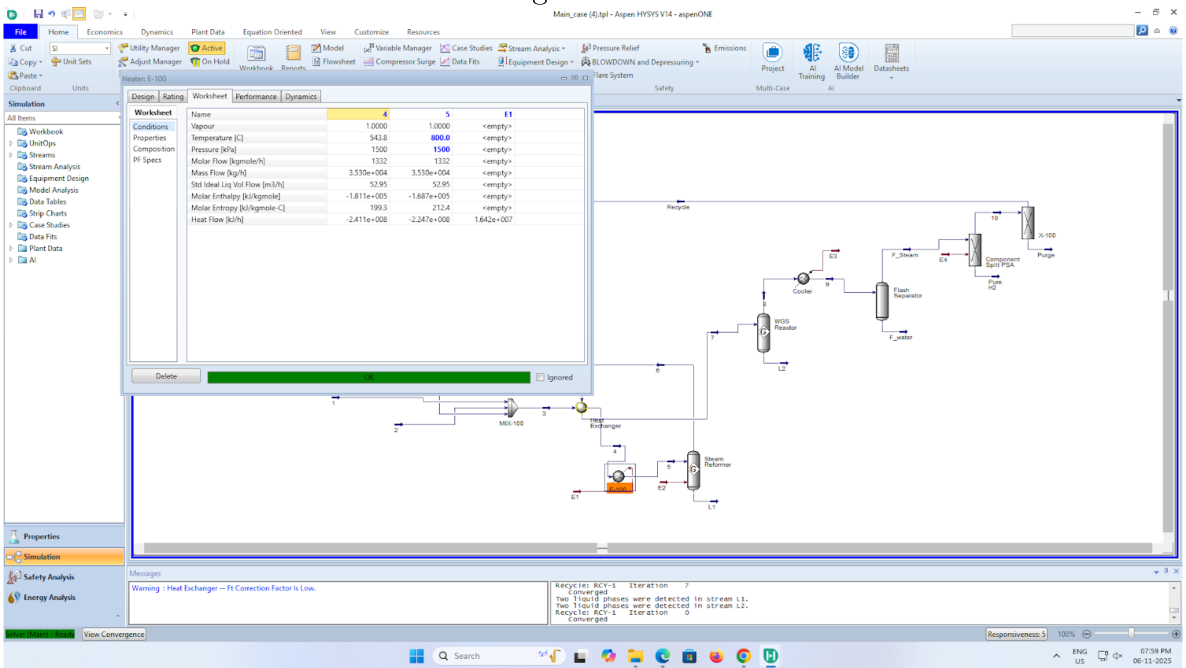
Main Case Flowsheet. Overview of the optimized process showing the recycle loop and main units.



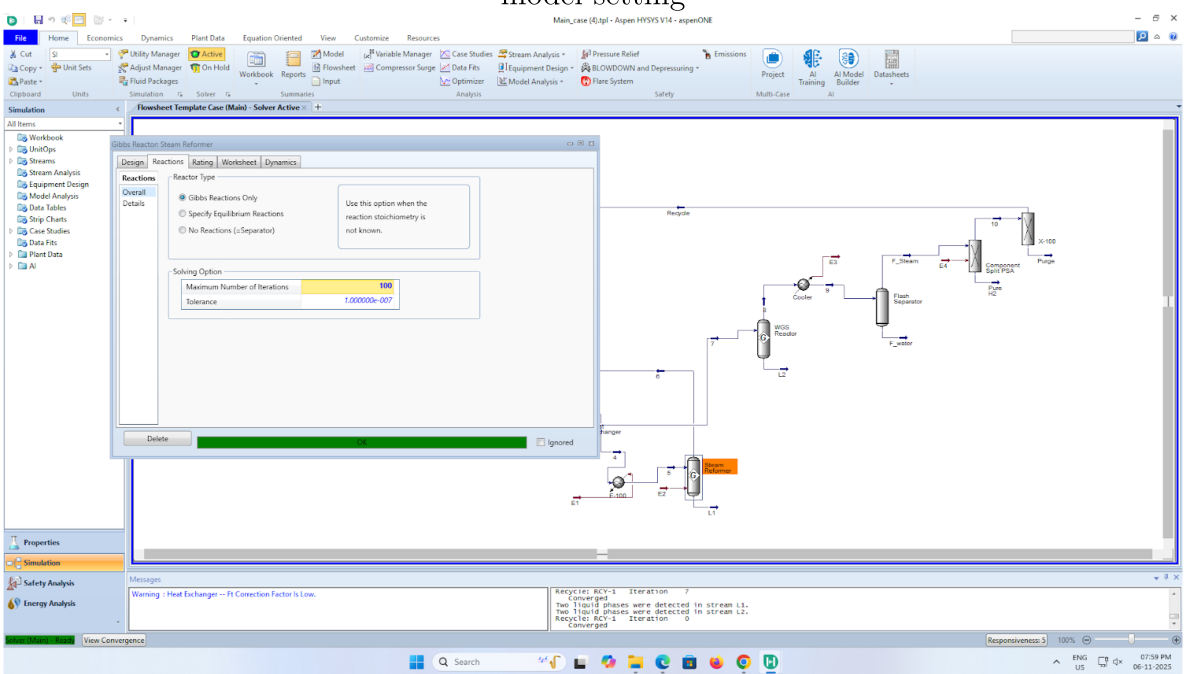
Mixer (MIX-100) Connections. Shows the three inlets (Fresh Feeds, Recycle) combining into Stream 3.



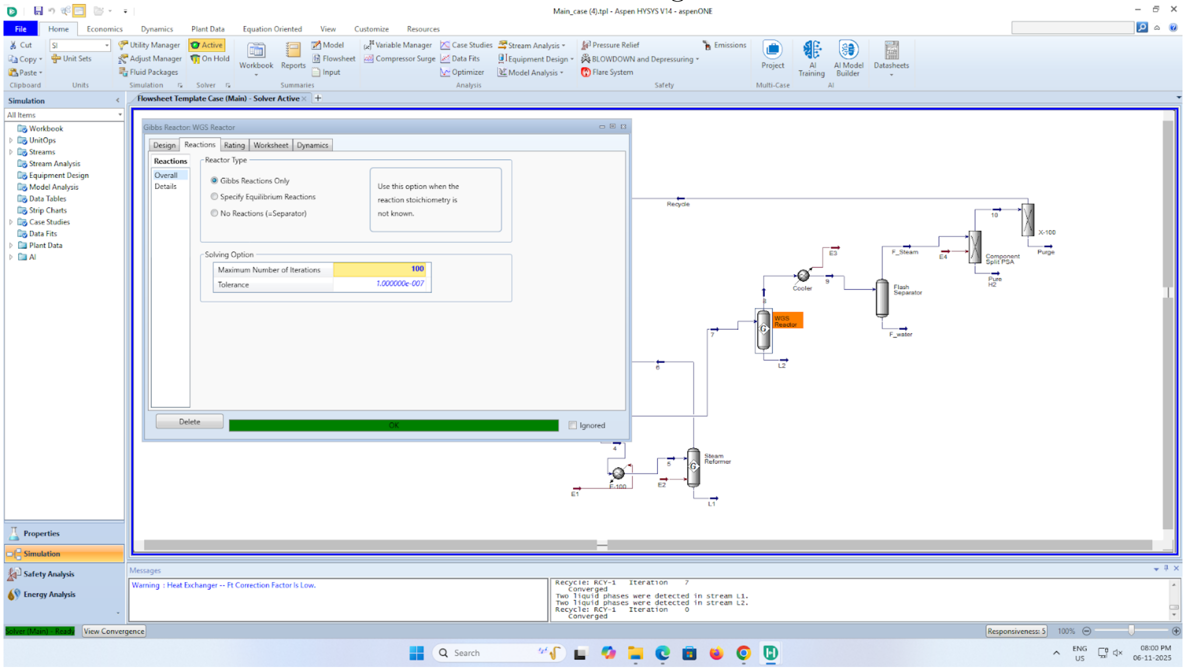
Trim Heater (E-100) Worksheet. Confirms outlet Stream 5 temperature is 800 degree celsius



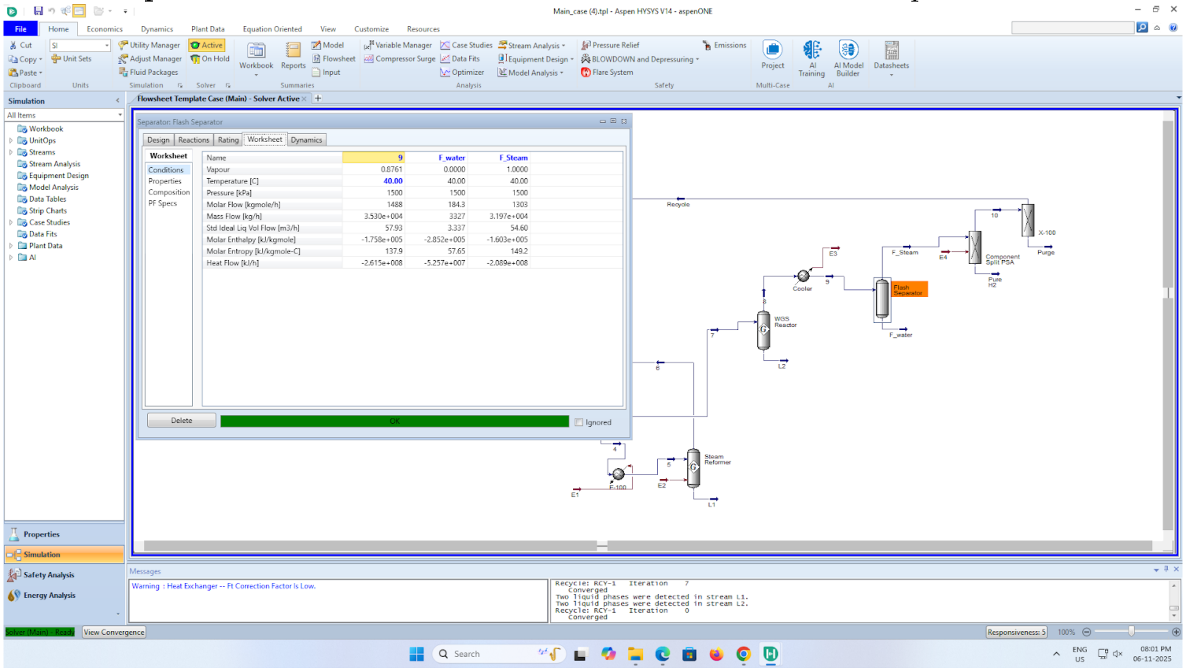
Steam Reformer (L_1) Reactions. Confirms the Gibbs Reactions Only equilibrium model setting



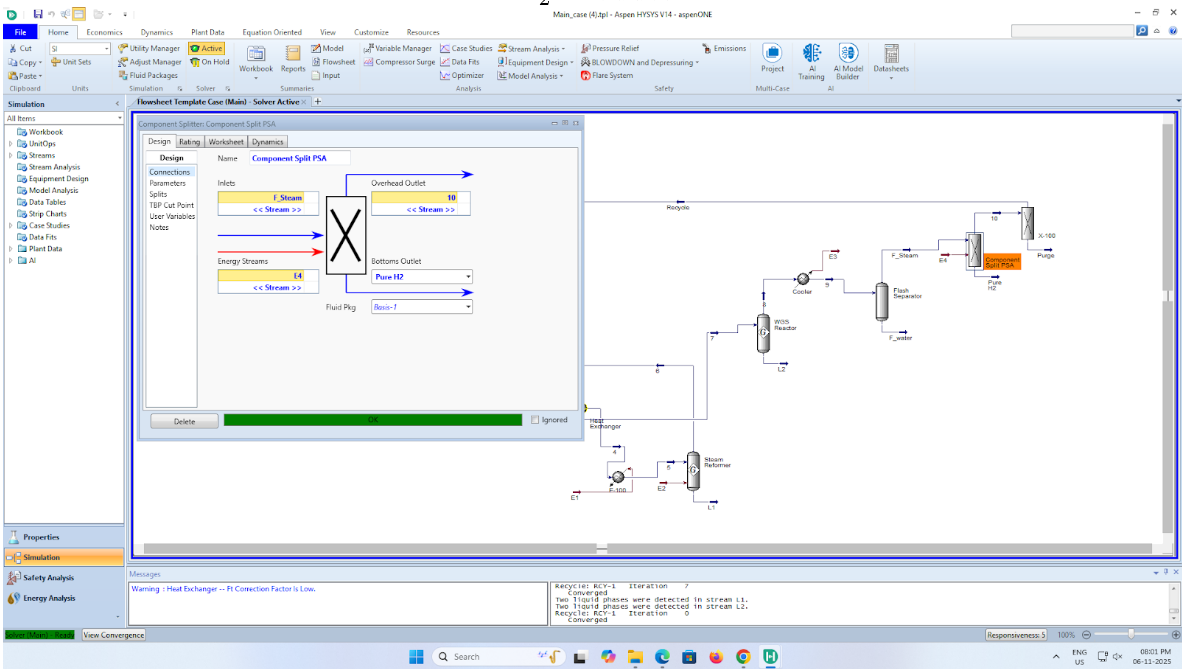
WGS Reactor (L_2) Reactions. Confirms the Gibbs Reactions Only equilibrium model setting



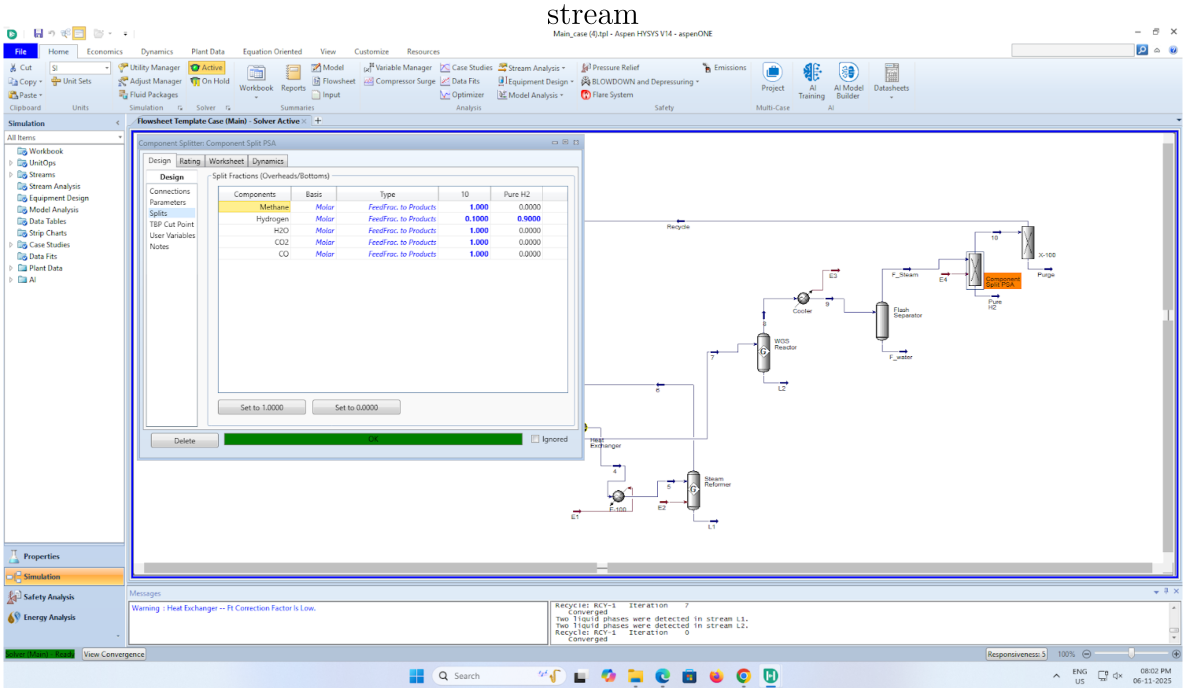
Flash Separator Worksheet. Shows the 40°C and 1500 kPa separation conditions



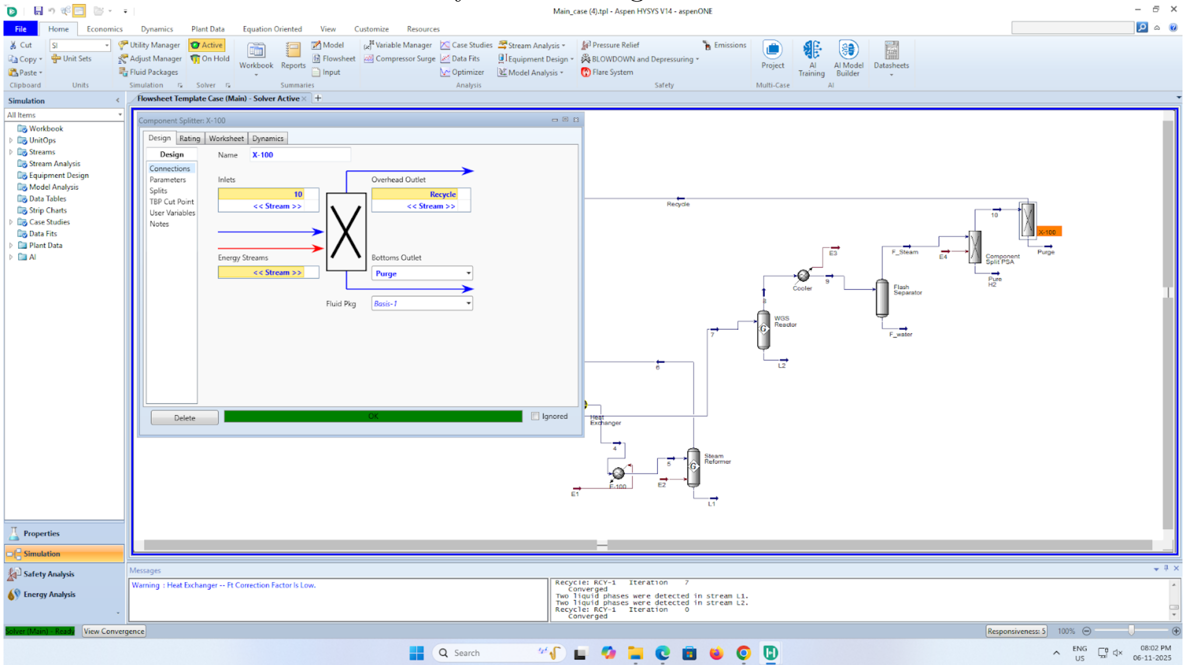
PSA Unit Connections. Shows Stream F_{Steam} splitting into Tail Gas (10) and Pure H_2 Product



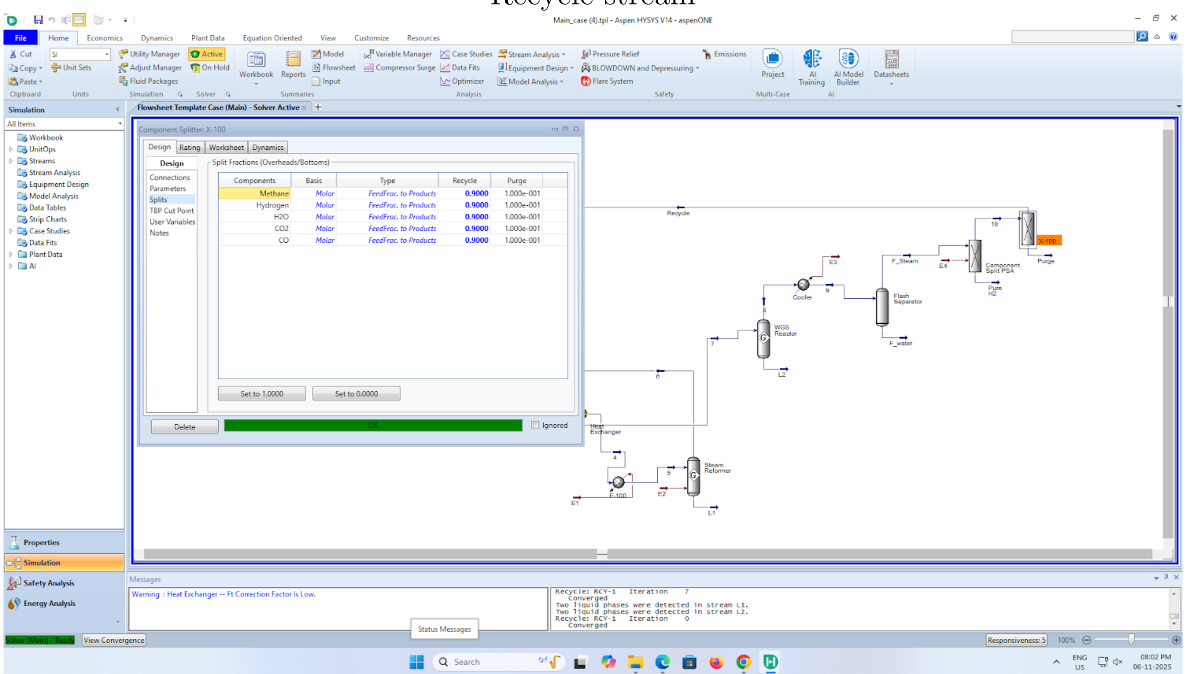
PSA Unit Split Parameters. Confirms the 90% recovery of H_2 to the product stream



Stream Splitter (X-100) Connections. Shows Tail Gas (10) being split into Recycle and Purge streams.



Stream Splitter (X-100) Parameters. Confirms the 90% split fraction to the Recycle stream



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