CHE251 GROUP PROJECT

Group 13

Group Members:-

1. Pulkit (230809)
2. Anshika Singh (230163)
3. Shivanee Shrivas (230974)
4. Sarthak Singh (230930)
5. Sunny Kumar (230153)
6. Banavath Surya Vardhan (23082)
7. Eslavath Pinki(230399)

Topic:

STEAM REFORMING OF NATURAL GAS AND SUBSEQUENT SYNTHESIS OF METHANOL

About this Project

Methanol, a key chemical in industrial applications, is widely used in the manufacture of formaldehyde, acetic acid, and other chemical products. It can also serve as a clean-burning fuel.This project focuses on simulating the production of methanol from natural gas via steam reforming using Aspen Plus. Methanol is a critical chemical feedstock with applications in fuels, solvents, and as a precursor in chemical synthesis. This process involves two main stages:

1. Steam Reforming - Conversion of natural gas (primarily methane) into syngas (a mixture of H_2, CO, and CO_2).
2. Methanol Synthesis - Conversion of syngas into methanol.

Reference: ELEMENTARYPRINCIPLESOFCHEMICALPROCESSES-RICHARDM.FELDERandRONALDW.ROUSSEAU

Objective of the Project:

a) Analyze the chemical processes involved in the steam reforming of natural gas and the subsequent methanol synthesis.

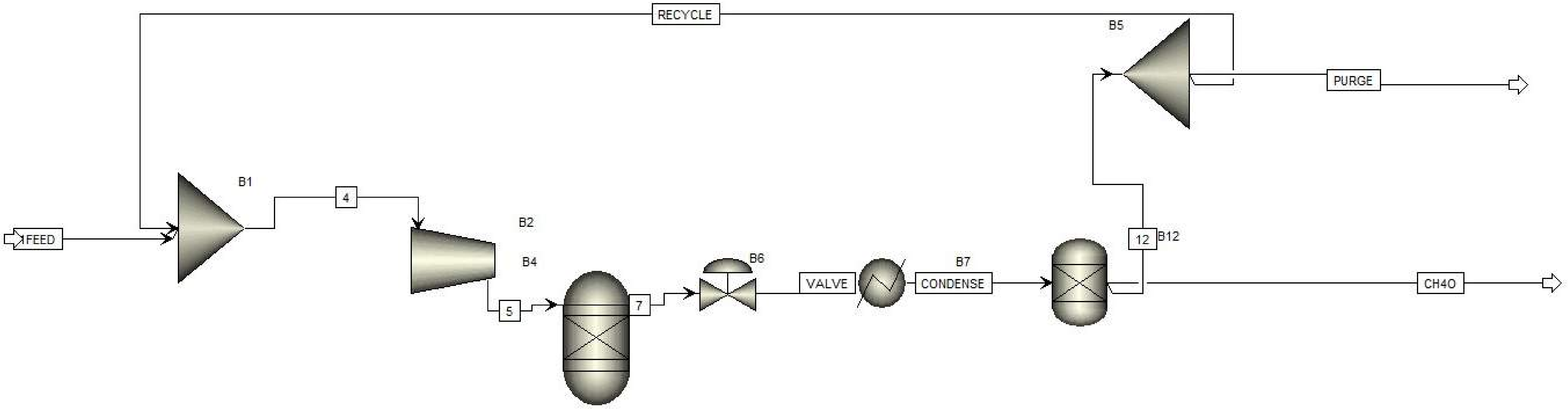
b) Evaluate the engineering design of the methanol synthesis reactor, with particular focus on the use of copper-zinc oxide catalysts.

c) Understand the impact of process variables such as temperature, pressure, and gas composition on methanol yield and production efficiency.

d) Assess the energy efficiency of the production process, particularly in terms of heat recovery and utilization of by-products.

e) Recommend optimizations for improving the overall production process, including minimizing energy consumption and reducing the formation of unwanted by-products.

SIMPLIFIED VERSION OF FLOWSHEET

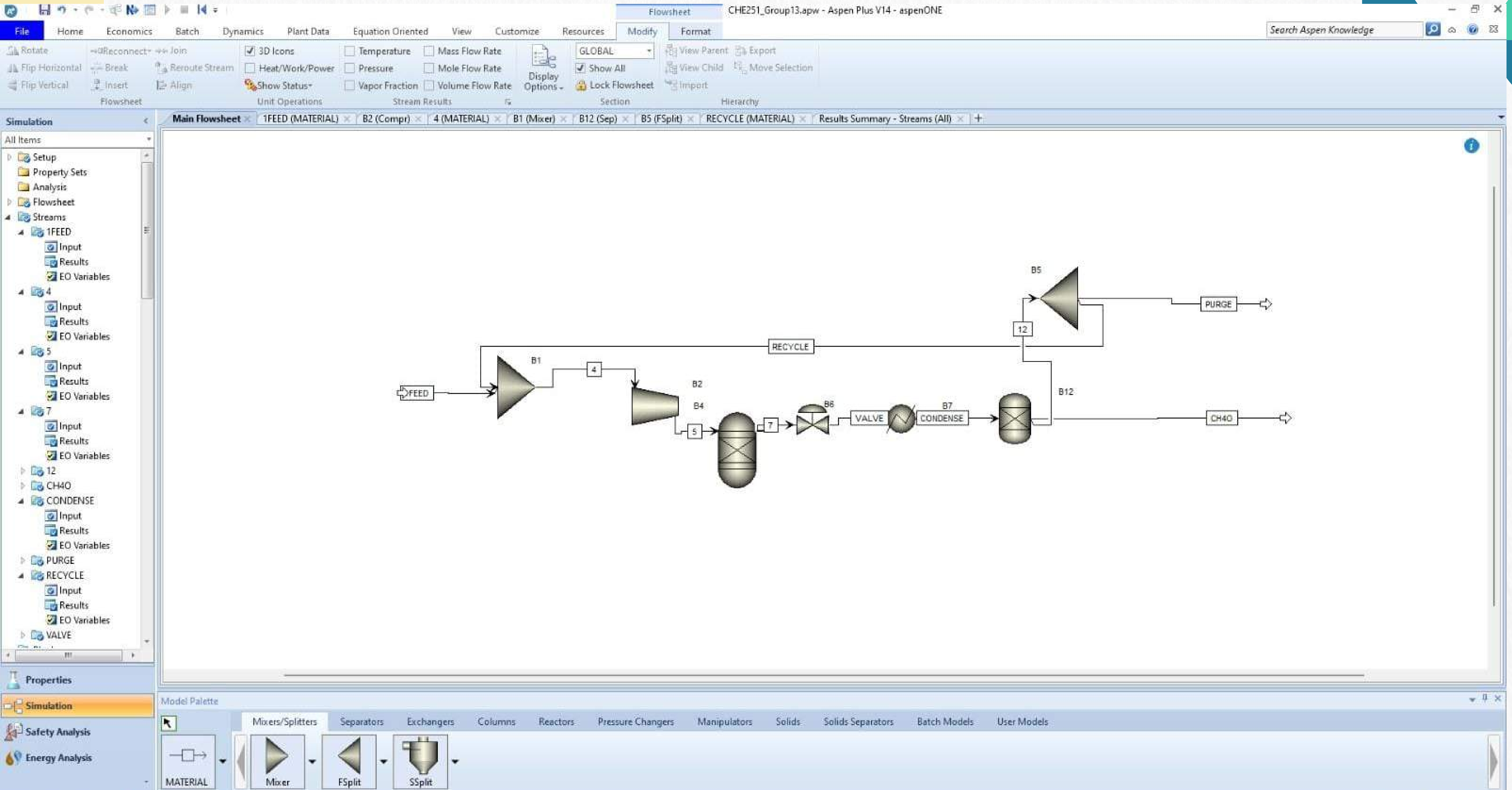


DESCRIPTION OF THE PROCESS

- First, the pure syngas stream was compressed and heated up to the operating pressure and temperature.
- Then, the stream was introduced in the reactor to accomplish the methanol production. The catalyst selected to the synthesis was Cu/ZnO due to be one of the most commercially-available catalyst for methanol production.
- The following reactions were involved during the synthesis:
- $CO+2H_2 \rightleftharpoons CH_3OH$
- $CO_2+3H_2 \rightleftharpoons CH_3OH+H_2O$

- The conversions were 35% and 17% for CO and CO2, respectively. Then, reaction product was depressurized to 1 atm and cooled down to 25 °C to condense and separate the crude methanol from the gas-phase in the METSEP flash, getting by the bottom pure methanol as the final product.
- Finally, top stream, which contained unconverted H2, was recycled to the combustion chamber to reduce the amount of char necessary to reach the gasification temperature.

Simplified version of flowsheet that we made in Aspen



RESULTS WE GET IN ASPEN

	Units	1FEED	4	5	7	12	CH4O	CONDENSE	PURGE	RECYCLE	VALVE
Mass Vapor Fraction		0.0194018	0.643144	1	1	0.78862	0	0.78862	0.78862	0.788618	1
Mass Liquid Fraction		0.980598	0.356856	0	0	0.21138	1	0.21138	0.21138	0.211382	0
Mass Solid Fraction		0	0	0	0	0	0	0	0	0	0
Molar Enthalpy	J/kmol	-2.20722e+08	-1.7515e+08	-1.68297e+08	-1.56112e+08	-1.73729e+08	-2.384e+08	-1.73729e+08	-1.73729e+08	-1.74346e+08	-1.56112e+08
Mass Enthalpy	J/kg	-7.35953e+06	-8.6448e+06	-8.3066e+06	-7.77381e+06	-8.65106e+06	-7.44019e+06	-8.65106e+06	-8.65106e+06	-8.67866e+06	-7.77381e+06
Molar Entropy	J/kmol-K	-214054	-93966	-90972.1	-51815.7	-66310.2	-240245	-66310.3	-66310.2	-66334.1	-51815.7
Mass Entropy	J/kg-K	-7137.18	-4637.84	-4490.08	-2580.23	-3302.01	-7497.78	-3302.01	-3302.01	-3302.01	-2580.23
Molar Density	kmol/cum	9.18692	2.91909	5.52758	1.85341	0.0533863	24.7462	0.0533863	0.0533863	0.0533671	1.85341
Mass Density	kg/cum	275.528	59.1428	111.993	37.2198	1.07209	792.921	1.07209	1.07209	1.07209	37.2198
Enthalpy Flow	Watt	-6.13117e+06	-2.80633e+08	-2.69653e+08	-2.52358e+08	-2.80836e+08	-68.089	-2.80836e+08	-5.61671e+06	-2.74501e+08	-2.52358e+08
Average MW		29.9914	20.2607	20.2607	20.0818	20.0818	32.0422	20.0818	20.0818	20.089	20.0818
− Mole Flows	**kmol/hr**	**100**	**5768.08**	**5768.08**	**5819.46**	**5819.46**	**0.00102819**	**5819.46**	**116.389**	**5668.08**	**5819.46**
H2	kmol/hr	7.2	545.738	545.738	554.891	554.891	0	554.891	11.0978	538.538	554.891
CO	kmol/hr	1.4	142.154	142.154	145.767	145.767	0	145.767	2.91534	140.754	145.767
CO2	kmol/hr	1.4	928.746	928.746	950.825	950.825	0	950.825	19.0165	927.346	950.825
CH4	kmol/hr	0	2607	2607	2671.31	2671.31	0	2671.31	53.4262	2607	2671.31
CH4O	kmol/hr	90	90	90	0.00102819	0	0.00102819	0.00102819	0	0	0.00102819
H2O	kmol/hr	0	1454.44	1454.44	1496.67	1496.67	0	1496.67	29.9333	1454.44	1496.67
− Mole Fractions											
H2		0.072	0.0946136	0.0946136	0.095351	0.095351	0	0.095351	0.095351	0.0950125	0.095351
CO		0.014	0.024645	0.024645	0.0250482	0.0250482	0	0.0250482	0.0250482	0.0248328	0.0250482
CO2		0.014	0.161015	0.161015	0.163387	0.163387	0	0.163387	0.163387	0.163609	0.163387
CH4		0	0.451971	0.451971	0.459031	0.459031	0	0.459031	0.459031	0.459945	0.459031
CH4O		0.9	0.0156031	0.0156031	1.76681e-07	0	1	1.76681e-07	0	0	1.76681e-07
H2O		0	0.252153	0.252153	0.257183	0.257183	0	0.257183	0.257183	0.256601	0.257183

MATERIAL BALANCE

- F_CO_in=140 kmol/hr
- F_CO2_in = 140 kmol/hr
- F_H2_in =172 kmol/hr

Reactions Involved :-

- $CO + 2H_2 = CH_3OH$
- $CO_2 + 3H_2 = CH_3OH + H_2O$

So **CO Conversion** :- 35 % of F_CO_in is converted to methanol.
and **CO2 Conversion** :- 17% of F_CO2_in is converted to methanol

=> F_CO_out = F_CO_in * (1- 0.35) = 140 * 0.65 = 91 kmol/hr
F_CO2_out = F_CO2_in * (1- 0.17) = 140 * 0.1 = 116.2 kmol/hr

So **H2 CONSUMPTION =** (2*0.35*F_CO_in) + (3*0.17*F_CO2_in)
=(2* 0.35 * 140) + (3*0.17*140)
= 169.4 kmol/hr

MATERIAL BALANCE

=> F_H2_out = F_H2_in - H2 consumption

= 172 - 169.4 = 2.6 kmol / hr

So F_CH3OH = (0.35 * F_CO_in) + (0.17 *F_CO2_in)

= (0.35 * 140) + (0.17 * 140)

= 72.8 kmol/hr

RESULT

Based on the simulation in Aspen, the following results were observed:

a) Yield Optimization: By adjusting reforming and synthesis parameters, the yield of methanol was maximized.

b) Energy Efficiency: Heat integration and recycling strategies were explored to improve overall process efficiency.

c) Environmental Impact: The simulation identified opportunities to reduce CO_2 emissions through optimized reaction conditions and recycling of unreacted syngas.

Discussion

The simulation results highlight several key aspects of the process:

1. Process Efficiency: The integration of a heat recovery system contributed to significant energy savings. By recycling heat from the reformer, the process minimized energy losses, making the production of methanol more sustainable and cost-effective.

2. Catalyst Performance: The copper-zinc oxide catalyst performed optimally in the synthesis reactor, providing efficient conversion of CO and CO2 to methanol. Maintaining high catalyst activity is crucial for sustaining methanol yield; potential catalyst poisoning from impurities requires regular monitoring and possible regeneration.

3. Optimization Opportunities:

Enhanced Heat Recovery: Using advanced heat exchangers could further increase steam production, improving energy utilization.
PurgeStream Management: The 10% purge from the MSR could be further minimized by optimizing separation technologies, which would also reduce methane losses.
By-product Control: Improved separation techniques for dimethyl ether (DME) and water could enhance methanol purity, thereby reducing downstream purification costs.

- In order to optimize the process, the pressure and temperature influence on the methanol production was evaluated. Different studies reported that typical operation conditions of the synthesis were in the ranges from 220 to 280 °C and 50 to 100 atm.
- At higher temperatures, the catalyst could be damaged, producing its sintering and fusion. On the other hand, lower temperatures could reduce the reaction rate . For this reason, the model proposed was simulated at standard temperatures and pressures ranges.
- Below fig shows the methanol production at different temperatures and pressures studies. It was observed that the methanol yield was improved at **high pressures and lower temperatures.** Although the methanol production is favoured at high pressures, a pressure of 55 atm was selected in order to avoid operational issues observed at higher pressures.
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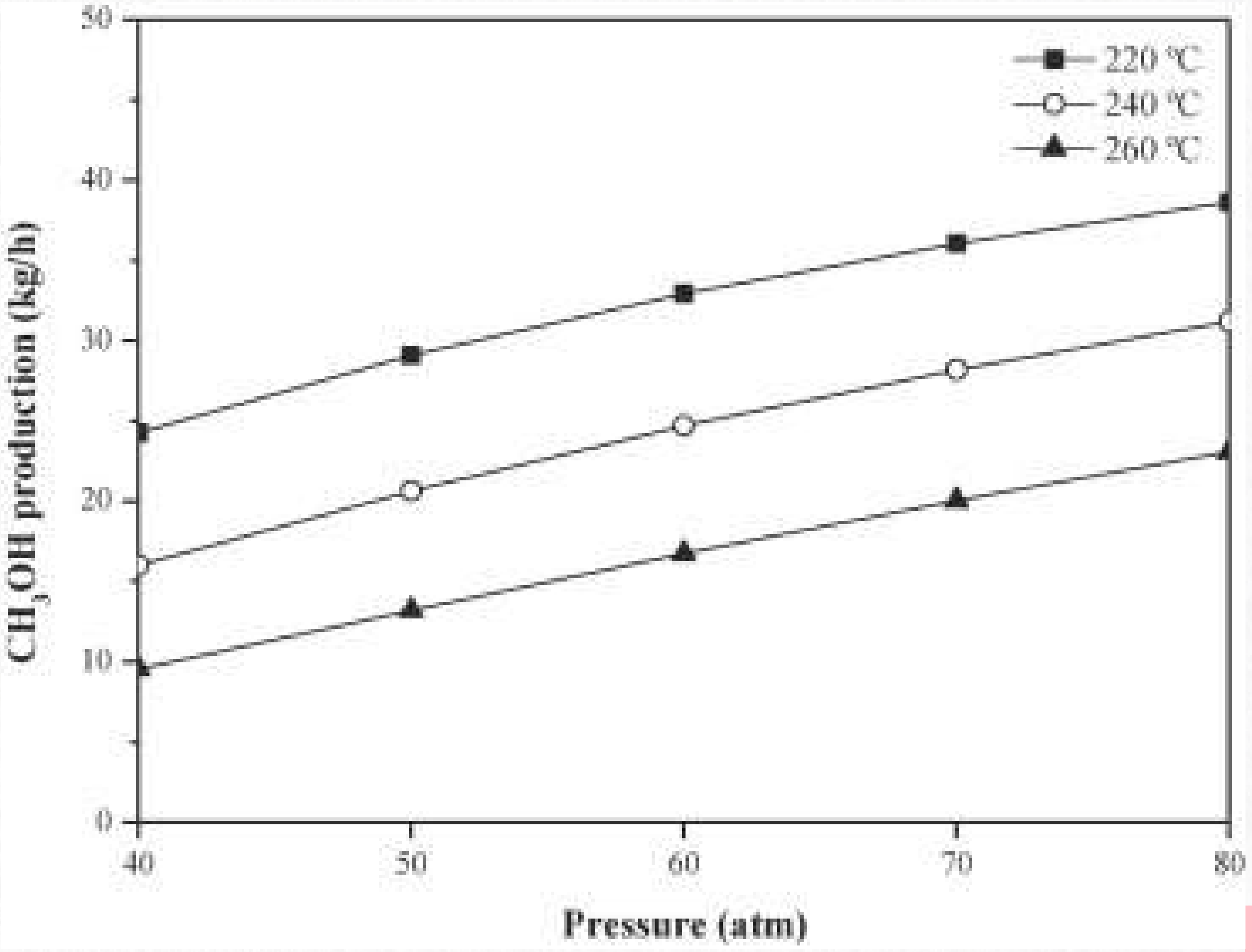

Conclusion

The simulation of the methanol production process through steam reforming and methanol synthesis highlights an effective, energy-conscious methodology for methanol production.

This Aspen Plus simulation provides a comprehensive model for methanol production from natural gas, highlighting process efficiency, yield, and environmental considerations. The project demonstrates the feasibility and optimization techniques for large-scale methanol production using steam reforming and subsequent synthesis.

THANK YOU