

FACULTY OF ENGINEERING & APPLIED SCIENCE



PROCESS OUTLINE

The ASPEN Plus simulation analyzes the feasibility of a small-scale methanol facility at remote sites in Saskatchewan's oil and gas industry. Small scale facilities can reduce capital costs while capturing carbon emissions, helping to adhere to increased regulations and societal pressures. This simulation is conducted in four key steps as follows:

1. The refrigeration loop cools the inlet gas to remove condensate containing heavy hydrocarbons.

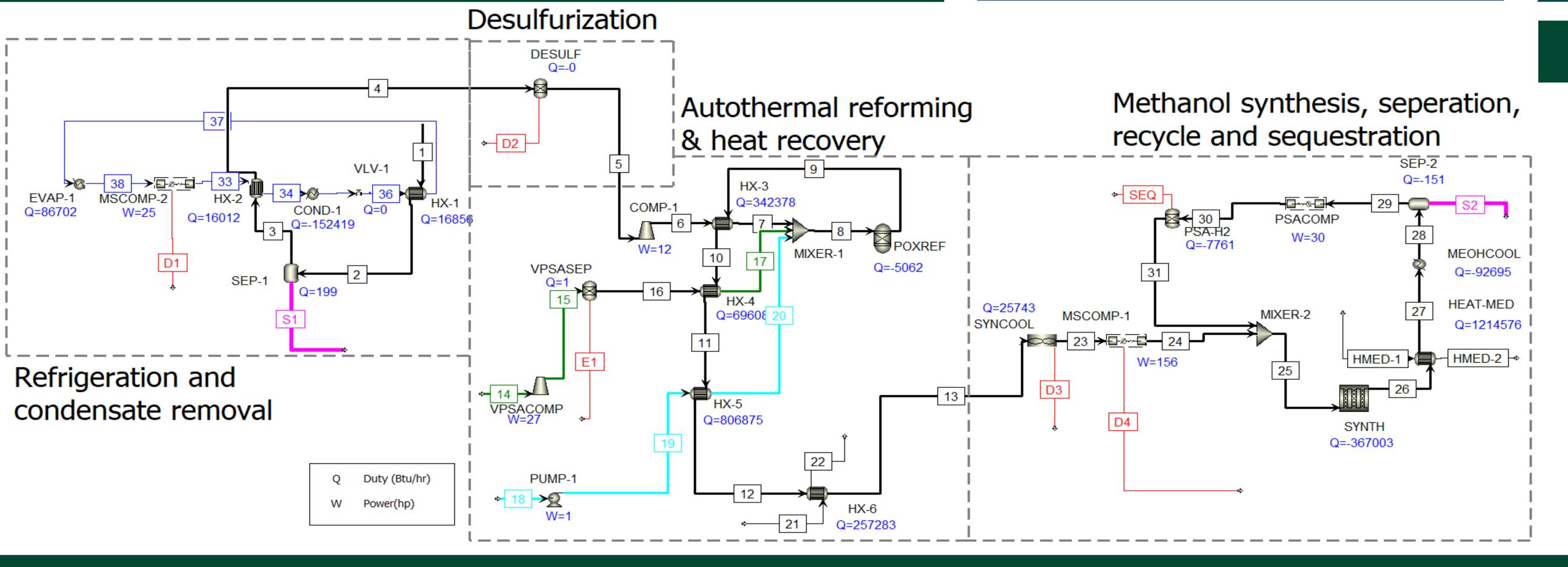
2. Desulfurization is completed through adsorption with activated carbon.

3. Autothermal reforming is completed with natural gas, 95% pure oxygen, and steam to produce syngas by partial oxidation. The syngas flows through a series of heat exchangers, pre-heating the inlet streams to the autothermal reformer.

4. The methanol synthesis reformer; converts syngas to crude methanol gas. This process stream is cooled to liquid state and separated from the recycle stream. Excess hydrogen gas is recycled into the reactor while the remaining gas stream is sequestered down hole.

This study provides important feedback on opportunities to improve the process, which can be researched further, in both catalytic and process engineering.

ASPEN PLUS PROCESS FLOWSHEET





Small Scale Modular Natural Gas to Methanol Facility

PROCESS RESULTS

<u>Parameter</u>	<u>Result</u>
Crude Methanol Production	9.25m ³ /day
Condensate	0.324m ³ /day
Natural Gas Conversion	50%
Methanol Separation	99%
CO Conversion	96%
CO ₂ Conversion	57%
CO ₂ e Conversion	5.568 Tonne/Year
Total Heat Exchanger Duty	2,721,764 BTU/hr

REACTION KINETICS

Reaction Rate (Van den Bussche and Froment, 1996)

$$r_{MeOH} = k_{MeOH} \frac{\left(p_{CO_2}H_2\right) - \left(\frac{1}{K_{p_{MeOH}}}\right) \left(\frac{p_{CH_3OH}p_{H_2O}}{p_{H_2^2}}\right)}{\left(1 + K_a \left(\frac{p_{H_2O}}{p_{H_2}}\right) + K_b \left(p_{H_2}\right)^{0.5} + K_c p_{H_2O}\right)^2}$$

 $CO_2 + H_3 \leftrightarrow CH_3OH + H_2O$ $\Delta H_{298}^{o} = -87 \frac{kJ}{mol}$

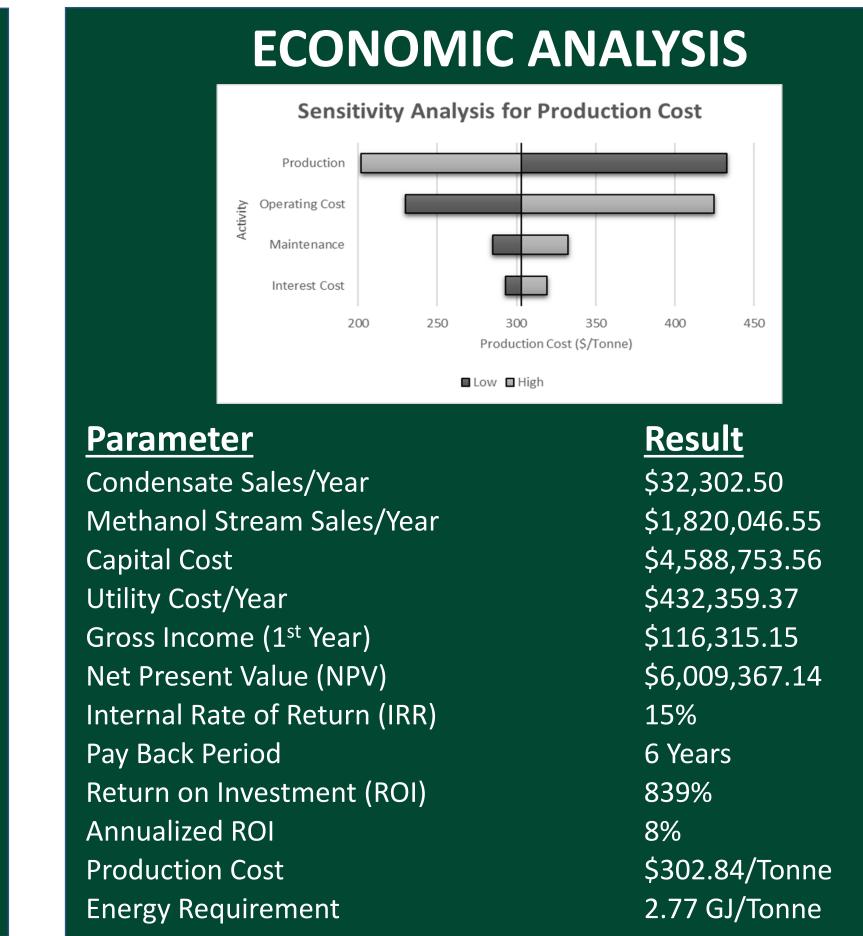
Expression

$$r_{RWGS} = k_{RWGS} \frac{p_{CO_2} - \left(\frac{1}{K_{p_{RWGS}}}\right) \left(\frac{p_{CO} p_{H_2}}{p_{H_2}}\right)}{\left(1 + K_a \left(\frac{p_{H_2O}}{p_{H_2}}\right) + K_b \left(p_{H_2}\right)^{0.5} + K_c p_{H_2O}\right)}$$

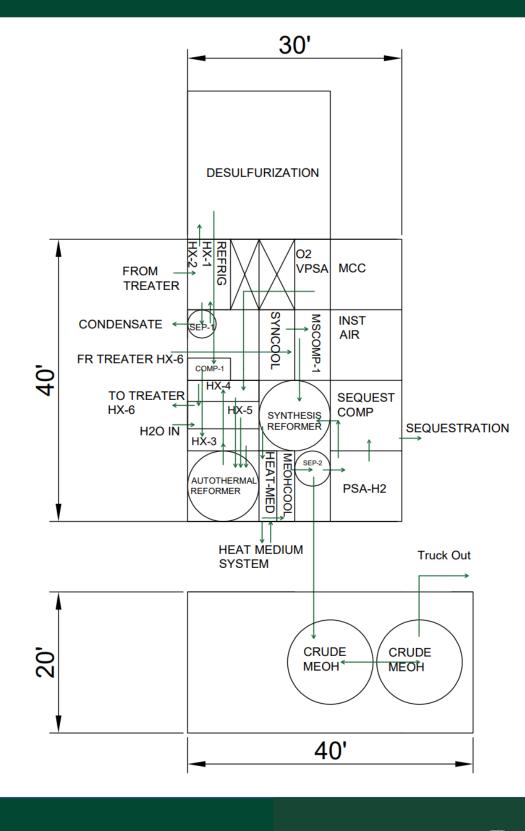
 $CO_2 + H_2 \leftrightarrow CO + H_2O$ $\Delta H_{298}^o = 41 \frac{kJ}{mol}$

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FACILITY LAYOUT



Cern