Optimisation of Methanol Synthesis by CO_2 Hydrogenation

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Background & Description:

Carbon dioxide (CO_2) is one of greenhouse gases, which can cause global warming. To combat the problem of CO_2 emissions, present day studies show that methanol show be considered as a suitable product because of its use in various petroleum based-liquid fuels.

Here, simulation carried out for a process which converts hydrogenates CO_2 into methanol. A plug flow reactor (PFR) is used to react hydrogen with the carbon dioxide in the synthesis gas to produce methanol.

The traditional syngas process has been explored exhaustively in literature and to make methanol production via CO_2 hydrogenation a competitive process, the optimal operating conditions with minimum production cost are considered. This new process can be considered a green process because it uses CO_2 obtained from thermal plants, stacks etc as the raw material contributing to the mitigation of CO_2 emissions. This thesis studied optimization of methanol production via CO_2 hydrogenation using multiple design variables. The objective function of this optimization was to maximize the profit of methanol production.

Flowsheet Description

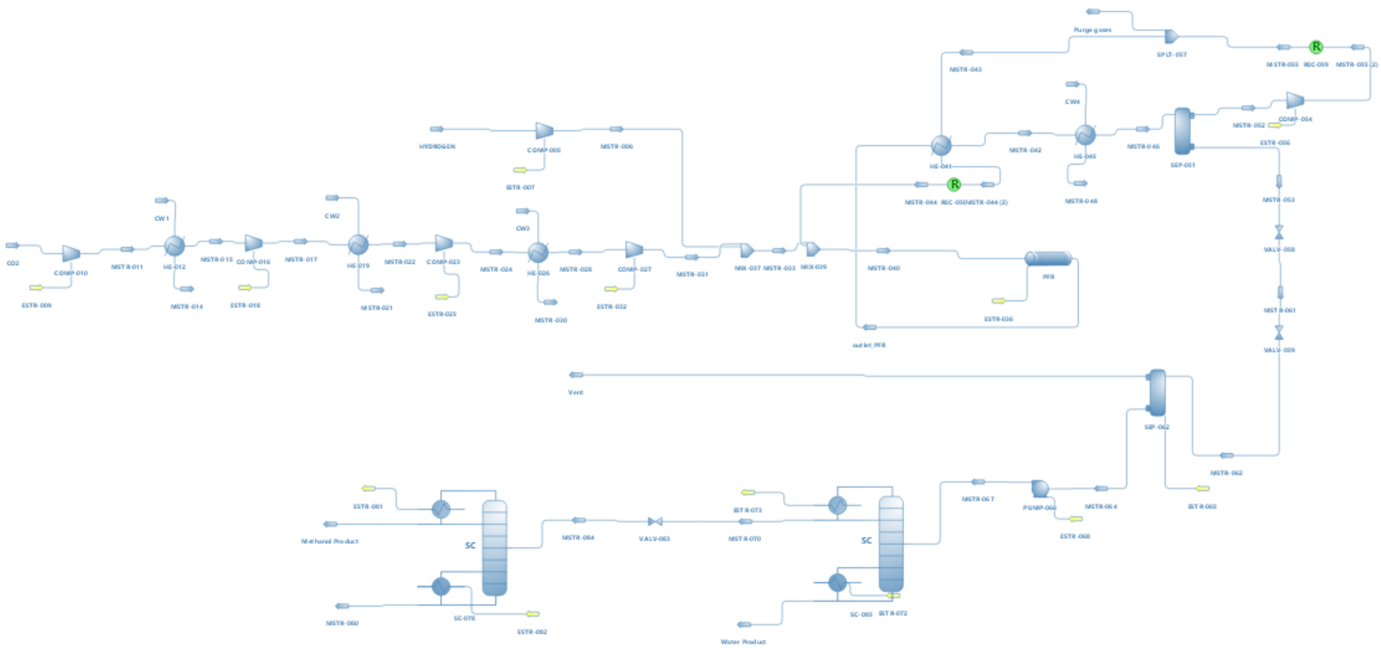
Here, fixed amounts of CO_2 and hydrogen in different streams is used for feed. In process, "Peng-Robinson" property model is used. Vanden Bussche and Froment's (Vanden Bussche, et al., 1996) kinetic model was used taking only the water-gas-shift reaction and the CO_2 hydrogenation into consideration. The process can be divided into four sections:

(1) Compression and Reactor Preheating
(2) Reactor (PFR)
(3) Separator, Recycle, and Vent
(4) Flash and Distillation

$$CO + 2H_2 \leftrightarrow CH_3OH \qquad \Delta H_{298} = -90 kJ/mol$$
$$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O \qquad \Delta H_{298} = -49.47 kJ/mol$$
$$CO_2 + H_2 \leftrightarrow CO + H_2O \qquad \Delta H_{298} = +41 kJ/mol$$

In this process, the feed of 1,000 kmoles per hour of carbon dioxide at 40◦C and 20 bar was mixed with the 3,000 kmoles per hour of hydrogen (at the same conditions). The mixture was then compressed, heated and sent to the first equilibrium reactor. The first reactor partially converted $CO_2$to methanol as liquid product. The unreacted CO_2 and H2 then entered the second equilibrium reactor to produce more methanol product. The pressure of gas phase leaving the second reactor was reduced to recover methanol as liquid phase. All liquid methanol products were sent to the first distillation column, where the light components (CO, CO_2, and H_2) leaved at the top of the column. The mixture of methanol and water leaved the column at the bottom and entered the second distillation column, where the methanol product with purity of 99.5%mole was obtained at the top of the column. The efficiency of the pumps and compressors was assumed at 75% (adiabatic). The specifications of the shortcut column were condenser temperature at 40.1◦C and reflux ratio at 0.5. The specifications of the methanol distillation column was set at 99 %mole methanol product purity.

Flowsheet:



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Results:

- From the simulation, high pure methanol is obtained about (99%) at rate of 27 kg/hr as a top
- product and water as bottom product at rate of 47.5 kg/h.
- In the plug flow reactor (PFR), about 57% and 19% conversion of carbon monoxide and carbon dioxide is achieved respectively.

The Nelder-Mead simplex constrained solving method was applied to optimize the objective function model for the maximum generated profit. In the optimal region of study, the inlet pressure of the hydrogen stream, inlet pressure and temperature to the reactor show significant impacts on the methanol production rate. The obtained maximized methanol production plant profit from a base value of Current value of $1068.65 **was $1460.12/hr of produced methanol**

The objective function is thus given as

$$Max\ P = C_{MeOH}P_{MeOH} + C_{vent}P_{Vent} + C_{purge}P_{Purge} - C_{H2}P_{H2} - C_{CO2}P_{CO2} - \sum C_{CW}\,P_{CW}$$

$$P = 0.343 * x1 + 0.24 * x2 + 8.14 * x3 - 1.88 * x4 - 3.5 * x5 - 0.1 * (cw1 + cw2 + cw3 + cw4)$$

Table 1: shows the constraints and initial value to maximize the profit ($/hr) generated from the methanol production plant via CO_2 hydrogenation.

Name	**Object**	**Lower Limit**	**Upper Limit**	**Initial Value**	**Unit**
x1	Methanol Product	40	100	48.0074	kg/h
x2	Vent	20	50	25.1293	kg/h
x3	Purge gases	400	500	453.376	kg/h
x4	HYDROGEN	100	400	105.46	kg/h
x5	CO2	200	400	258.646	kg/h
cw1	MSTR-013	3500	4000	3600	kg/h
cw2	MSTR-020	3500	4000	3600	kg/h
cw3	MSTR-029	3500	4000	3600	kg/h
cw4	MSTR-047	3500	4000	3600	kg/h

Table 2 shows the local optimal operating conditions to maximize the profit ($/hr) generated from the methanol production plant via CO_2 hydrogenation.

Parameters	Optimal values	Units
Methanol Product, x1	99.99	Kg/hr
Vent stream, x2	22.215	Kg/hr
Purge stream, x3	456.89	Kg/hr
H_2 stream, x4	105.46	Kg/hr
CO_2 stream, x5	256.646	Kg/hr
Cooling water, cw1	3600	Kg/hr
Cooling water, cw2	3600	Kg/hr
Cooling water, cw3	3600	Kg/hr
Cooling water, cw4	3600	Kg/hr