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Annex 4 Methanol synthesis

This file calculates the costs of methanol synthesis.

Get libraries

- Include << .\Libraries\multVecMat.mcdx
- Include << .\Libraries\Units.mcdx
- Include << .\Libraries\CEPCI.mcdx
- Include << .\Generic data.mcdx
- Include << .\Libraries\Mw.mcdx
- Include << .\Libraries\Molecular formulas.mcdx

Data were taken from: Rajaei et al. (2024)

$$\tau := 7884 \cdot \frac{hr}{yr}$$
 operating hours

From Table 2

- S14 Syngas to synthesis
- S15 MeOH to purification
- S17 Light gas
- S18 Purge to ICE

<i>Comp</i>	$f^{(S14)}$ (1%)	$f^{(S15)}$ (1%)	$f^{(S17)}$ (1%)	$f^{(S18)}$ (1%)	<i>StreamNr</i>	ϕ $\left(\frac{kmol}{hr}\right)$
<i>H2O</i>	0.07	30.27	0.08	0.07	<i>S14</i>	17386
<i>H2</i>	73.05	0.24	73.52	64.35	<i>S15</i>	1170
<i>CO2</i>	5.07	1.22	3.52	12.04	<i>S17</i>	14622
<i>CO</i>	3.42	0.01	1.04	0.92	<i>S18</i>	157
<i>methanol</i>	0.34	68.03	0.41	2.87		
<i>methane</i>	4.73	0.14	5.61	5.77		

Calculate molar flows

$$\phi_{comp} := multVecMat(\phi, f^T)^T = \begin{bmatrix} 0.003 & 0.098 & 0.003 & 3.053 \cdot 10^{-5} \\ 3.528 & 7.8 \cdot 10^{-4} & 2.986 & 0.028 \\ 0.245 & 0.004 & 0.143 & 0.005 \\ 0.165 & 3.25 \cdot 10^{-5} & 0.042 & 4.012 \cdot 10^{-4} \\ 0.016 & 0.221 & 0.017 & 0.001 \\ 0.228 & 4.55 \cdot 10^{-4} & 0.228 & 0.003 \end{bmatrix} \frac{10^3 \cdot \text{mol}}{\text{s}}$$

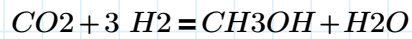
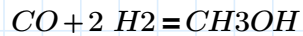
Represent in table form

$$Table = \begin{bmatrix} \text{"10^3 mol/s"} & \text{"S14"} & \text{"S15"} & \text{"S17"} & \text{"S18"} \\ \text{"H2O"} & 0.003 & 0.098 & 0.003 & 3.053 \cdot 10^{-5} \\ \text{"H2"} & 3.528 & 7.8 \cdot 10^{-4} & 2.986 & 0.028 \\ \text{"CO2"} & 0.245 & 0.004 & 0.143 & 0.005 \\ \text{"CO"} & 0.165 & 3.25 \cdot 10^{-5} & 0.042 & 4.012 \cdot 10^{-4} \\ \text{"methanol"} & 0.016 & 0.221 & 0.017 & 0.001 \\ \text{"methane"} & 0.228 & 4.55 \cdot 10^{-4} & 0.228 & 0.003 \end{bmatrix}$$

Calculate the net conversion

$$conversion := \phi_{comp}^{(S15)} + \phi_{comp}^{(S17)} - \phi_{comp}^{(S14)} = \begin{bmatrix} 98.246 \\ -540.992 \\ -97.917 \\ -122.893 \\ 221.33 \\ -0.118 \end{bmatrix} \frac{\text{mol}}{\text{s}}$$

Reactions taking place in the methanol synthesis reactor.



<i>Comp</i>	$Stoich^{(CO_to_methanol)}$	$Stoich^{(CO_2_to_methanol)}$
<i>H2O</i>	0	1
<i>H2</i>	-2	-3
<i>CO2</i>	0	-1
<i>CO</i>	-1	0
<i>methanol</i>	1	1
<i>methane</i>	0	0

Find the rates of the reactions by changing rates of the reactions:

$$r_{CO_to_methanol} := 123 \frac{mol}{s}$$

$$r_{CO_2_to_methanol} := 98 \cdot \frac{mol}{s}$$

$$Stoich \cdot r = \begin{bmatrix} 98 \\ -540 \\ -98 \\ -123 \\ 221 \\ 0 \end{bmatrix} \frac{mol}{s}$$

Good fit with conversion:

$$conversion = \begin{bmatrix} 98.246 \\ -540.992 \\ -97.917 \\ -122.893 \\ 221.33 \\ -0.118 \end{bmatrix} \frac{mol}{s}$$

$$\Phi_{methanol} := 7.02 \cdot \frac{kg}{s}$$

$$221 \cdot \frac{mol}{s} \cdot Mw(methanol) = 7.081 \frac{kg}{s}$$

Calculate the losses

$$\frac{\phi_{comp_{H_2, S18}}}{\phi_{comp_{H_2, S14}}} = 0.795\%$$

$$\frac{\phi_{comp_{CO, S18}}}{\phi_{comp_{CO, S14}}} = 0.243\%$$

$$\frac{\phi_{comp_{methanol, S18}}}{\phi_{comp_{methanol, S15}}} = 0.566\%$$

These losses are small enough to be neglected.

Syngas input

$$y_{methanol_H2} := \frac{1}{3} \cdot \frac{mol}{mol} \quad y_{methanol_CO} := 2 \cdot \frac{mol}{mol}$$

$$\Phi_{H_2} := \frac{\Phi_{methanol}}{y_{methanol_H2}} \cdot \frac{Mw(hydrogen)}{Mw(methanol)} = 1.325 \frac{kg}{s}$$

H2 may be added in the RWGS or in the methanol reactor, but always 3 mole per mole methanol

$$\Phi_{CO} := \frac{\Phi_{methanol}}{y_{methanol_CO}} \cdot \frac{Mw(CO)}{Mw(methanol)} = 3.068 \frac{kg}{s}$$

We have assumed that there are no losses, so the Internal Combustion Engine (ICE) has nothing to burn. Also, the article has significant input of methane going into the methanol synthesis and then into ICE. Our input gas has no methane. Therefore, the ICE is removed from the costs given in the article.

$$P_{el} := (11.67 + 0.92 + 1.92) \cdot MW = 14.51 \cdot 10^6 \cdot W$$

$$p_{el_methanol} := \frac{P_{el}}{\Phi_{methanol}} = 2.067 \frac{10^9 \cdot J}{ton} \quad p_{el_methanol} = 0.574 \frac{MW \cdot hr}{ton}$$

$$FCI := (50.73 + 20.21 + 1.19) \cdot 10^6 \cdot USD = 64.917 \cdot 10^6 \cdot \text{€}$$

$$CAPEX := FCI \cdot \frac{CEPCI(2024)}{CEPCI(2019)} \cdot CoC = 17.052 \frac{10^6 \cdot \text{€}}{yr}$$

$$CAPEX_{methanol} := \frac{CAPEX}{\Phi_{methanol} \cdot \tau} = 85.581 \frac{\text{€}}{\text{ton}}$$

$$\frac{CAPEX}{CoC \cdot \Phi_{methanol}} = 384.859 \frac{\text{€}}{\text{ton} \cdot \text{yr}}$$

$$\Phi_{H2_total} := \Phi_{H2} \cdot \tau = 37.608 \frac{10^3 \cdot \text{ton}}{\text{yr}}$$

Literature

Rajae et al., 2024 [18]