Change log (hidden)

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: Rajaee 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

$Comp$	$f^{\langle S14 \rangle}$ (1%)	$f^{\langle S15 \rangle}$ (1%)	$f^{\langle S17 \rangle}$ (1%)	$f^{\langle S18 \rangle}$ (1%)
$H2O$	0.07	30.27	0.08	0.07
$H2$	73.05	0.24	73.52	64.35
$CO2$	5.07	1.22	3.52	12.04
CO	3.42	0.01	1.04	0.92
$methanol$	0.34	68.03	0.41	2.87
$methane$	4.73	0.14	5.61	5.77

$StreamNr$	ϕ $\left(\frac{kmol}{hr}\right)$
$S14$	17386
$S15$	1170
$S17$	14622
$S18$	157

Calculate molar flows

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

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

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

Reactions taking place in the methanol synthesis reactor.

$$CO + 2\ H2 = CH3OH$$

$$CO2 + 3\ H2 = CH3OH + H2O$$

$Comp$	$Stoich^{\langle CO\_to\_methanol \rangle}$	$Stoich^{\langle CO2\_to\_methanol \rangle}$
$H2O$	0	1
$H2$	−2	−3
$CO2$	0	−1
CO	−1	0
$methanol$	1	1
$methane$	0	0

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

$$r_{CO\_to\_methanol} := 123\ \frac{mol}{s} \qquad r_{CO2\_to\_methanol} := 98 \cdot \frac{mol}{s}$$

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

Good fit with conversion:

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

$$\Phi_{methanol} := 7.02 \cdot \frac{kg}{s} \qquad 221 \cdot \frac{mol}{s} \cdot Mw(methanol) = 7.081\ \frac{kg}{s}$$

Calculate the losses

$$\frac{\phi_{comp_{H2,S18}}}{\phi_{comp_{H2,S14}}} = 0.795\%$$

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

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

These losses are small enough to be neglected.

Syngas input

$$y\_methanol\_H2 := \frac{1}{3} \cdot \frac{mol}{mol} \qquad y\_methanol\_CO := 2 \cdot \frac{mol}{mol}$$

$$\Phi_{H2} := \frac{\Phi_{methanol}}{y\_methanol\_H2} \cdot \frac{Mw(hydrogen)}{Mw(methanol)} = 1.325 \ \frac{kg}{s}$$

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.

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

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

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

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

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

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

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

Literature

Rajaee et al., 2024 [18]