Supplementary Material

1 LCO CALCULATION PROCEDURE

1.1 Total capital cost (TCC)

The contribution of an employed equipment i to the total capital cost C_i^{TCC} can be calculated by the direct (DCC) and indirect (ICC) capital cost, or by the grassroot capital cost C_i^{GR}, or by the bare module cost C_i^{BM} as below

$$C_i^{\text{TCC}} = C_i^{\text{DCC}} + C_i^{\text{ICC}} \tag{S1}$$

$$C_i^{\text{TCC}} = C_i^{\text{GR}} \left(1 + F_{\text{contingency}}\right) + C_i^{\text{GR}} F_{\text{engineering}} \tag{S2}$$

$$C_i^{\text{TCC}} = C_i^{\text{BM}} F^{\text{TM}} \left(1 + F^{\text{GR}}\right) \left(1 + F_{\text{contingency}}\right) + C_i^{\text{BM}} F^{\text{TM}} \left(1 + F^{\text{GR}}\right) F_{\text{engineering}} \tag{S3}$$

where the factors $F_{\text{contingency}}$, $F_{\text{engineering}}$ are employed to account for contingency and engineering cost, while the factors F^{TM} and F^{GR} are the total module factor and the grassroot factor. If not specially mentioned below for a specific equipment, these involved factors are specified by default as $F_{\text{contingency}} = 0.2$, $F_{\text{engineering}} = 0.3$, $F^{\text{TM}} = 1.18$ and $F^{\text{GR}} = 0.35$.

1.1.1 Solar power tower plant

As aforementioned, the design and optimization of CSP, particularly the heliostat field, is crucial for minimizing the final product cost. For each design of the whole system, the nominal capacity and heat requirement of SOE subsystem are obtained by simultaneous utility sizing and heat cascade calculation in OSMOSE. Then, given the design DNI, solar multiple, full-load storage hours and the cycle design thermal efficiency, the capacity of thermal storage is determined together with an updated cycle design thermal efficiency by taking into account the process heat supply for SOE subsystem. Then, for the given plant capacity, the cost data is updated and input to SAM platform based on DLR cost functions. Afterwards, with respect to the reduction of total cost, automatic generation of the heliostat layout and optimization of the solar field geometry is performed by SolarPILOT to obtain the optimal heliostat count and layout, receiver height and diameter, and tower height. Eventually, the cost breakdown and hourly performance of the optimal CSP design is obtained for calculating the LCO.The employed cost functions predicted for 2025 by DLR are summarized below(Choe et al., 2021):

1.1.1.1 Direct capital cost (DCC)

Total direct capital cost is calculated by

$$C_{\text{csp}}^{\text{DCC}} = \left(C_{\text{hs}}^{\text{GR}} + C_{\text{hf}}^{\text{GR}} + C_{\text{tow}}^{\text{GR}} + C_{\text{rec}}^{\text{GR}} + C_{\text{pb}}^{\text{GR}} + C_{\text{bop}}^{\text{GR}} + C_{\text{tes}}^{\text{GR}}\right) \left(1 + F_{\text{contingency}}\right) \tag{S4}$$

where the subscripts, hs, hf, tow, rec, pb, bop and tes, stand for heliostat site improvement, heliostat field, tower, receiver, power block, balance of plant and thermal energy storage, respectively. The contingency factor is 7%.

- Heliostat field
  - Site improvement cost: 5.24 \$/kWe
  - Heliostat field cost: 103 $\$/\text{m}^2$

- Tower

  The standard formulation of capital cost of the tower employed in SAM is in the following formulation:

$$C_{\text{tow}}^{\text{GR}} = C_{\text{fixed}}\, e^{\alpha\left(H_{\text{tow}} - \frac{H_{\text{rec}}}{2} + \frac{H_{\text{hs}}}{2}\right)} \tag{S5}$$

  where the C_{fixed}, α and H represent tower fixed cost, scaling exponential factor and the height of tower (tow), receiver (rec) and heliostat (hs). The values of C_{fixed} and α are regressed as 1277033.3 \$ and 0.01135 from DLR's cost data (Fig. S1).

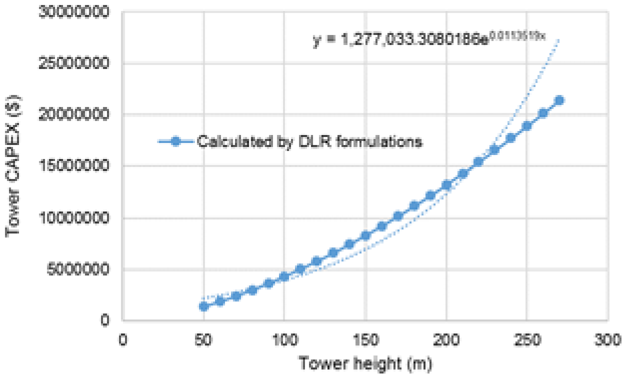

Figure S1. Regression of tower cost

- Receiver

  The receiver cost is formulated as

$$C_{\text{rec}}^{\text{GR}} = C_{\text{ref}} \left(\frac{A}{A_{\text{ref}}}\right)^{\alpha} \tag{S6}$$

  where the C_{ref}, A_{ref} and α represent the receiver reference cost, reference area and scaling exponential factor. As mentioned in (Dieckmann et al., 2016), a 20% reduction is expected up to 2025, thus the reference cost is reduced by 20% from the value reported in (Dieckmann et al., 2016) as 82400000 \$ for a reference area of 1571 m^2, while the scaling factor is taken the same as 0.7.

- Power block

  The specific cost of power block is needed by SAM. Thus, once the nominal power capacity of the CSP ($\dot{W}_{\text{cap}}$ in kWe) is known, the specific cost c_{pb} (\$/kWe) can be calculated by the following equation from DLR

$$c_{\text{pb}} = \frac{C_{\text{pb}}^{\text{GR}}}{\dot{W}_{\text{cap}}} = \frac{1100 \times 150000 \left(\frac{\dot{W}_{\text{cap}}}{150000}\right)^{0.8}}{\dot{W}_{\text{cap}}} \tag{S7}$$

- Balance of plant

  The specific cost of balance of plant is needed by SAM. Thus, once the nominal power capacity of the CSP ($\dot{W}_{\text{cap}}$ in kWe) is known, the specific cost c_{bop} (\$/kWe) can be calculated by the following equation from DLR

$$c_{\text{bop}} = \frac{C_{\text{bop}}^{\text{GR}}}{\dot{W}_{\text{cap}}} = \frac{319 \times 150000 \left(\frac{\dot{W}_{\text{cap}}}{150000}\right)^{0.8}}{\dot{W}_{\text{cap}}} \tag{S8}$$

- Thermal storage
  The specific cost of thermal storage is needed by SAM, which can be easily calculated by

$$c_{\text{tes}} = \frac{C_{\text{tes}}^{\text{GR}}}{C_{\text{cap,tes}}} = \frac{6.8\text{e}7 \left(\frac{C_{\text{cap,tes}}}{3154000}\right)^{0.8}}{C_{\text{cap,tes}}} \tag{S9}$$

  where the symbol $C_{\text{cap,tes}}$ stands for the thermal storage capacity in kWhth (kWh thermal energy). The variation of total and specific storage cost has been illustrated in Fig. S2.

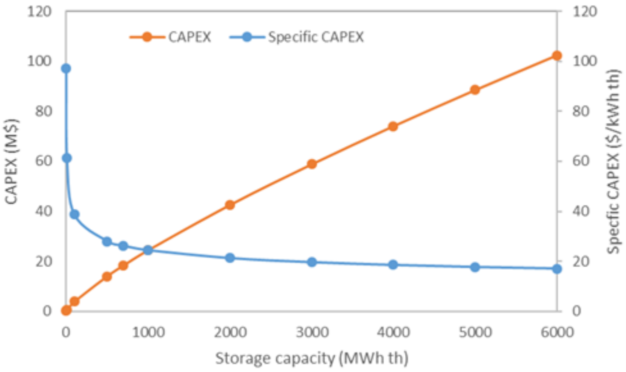

Figure S2. Cost of thermal storage

1.1.1.2 *Indirect capital cost (ICC)*

Total indirect capital cost considers the total land cost, EPC and owner cost, and tax:

$$C_{\text{csp}}^{\text{ICC}} = C_{\text{land}} + C_{\text{EPC\&owner}} + C_{\text{tax}} \tag{S10}$$

- Total land cost (C_{land})
  The land specific cost is specified as 2.47 $\$/\text{m}^2$ (10000 $\$/\text{acre}$). The total land use is estimated by the size of heliostat field.
- EPC (engineer-procure-construct) and owner cost ($C_{\text{EPC\&owner}}$)
  13% of total direct cost
- Sale tax (C_{tax}) (The sale tax is not considered when employing CSP to drive SOE, as most of the electricity generated by CSP is used by the electrolyzer.)
  Sales tax rate 5%, sale tax basis 80% of the total direct cost

1.1.2 PV

Specific investment cost of a commercial PV system (c_{pv}) is reported as 2.16 $/We in 2015 by NREL and 1.068 €/We for 2025. The total investment cost of a PV system (in $) is calculated by

$$C_{\text{pv}}^{\text{TCC}} = \left(\dot{W}_{\text{nom}} + \dot{Q}_{\text{nom}}\right) \gamma_{\text{pv}} c_{\text{pv}} \tag{S11}$$

where the $\dot{W}_{\text{nom}}$, $\dot{Q}_{\text{nom}}$ and γ_{pv} are the nominal power load of the electrolyzer subsystem, the nominal process heat required by the electrolyzer subsystem from the molten-salt storage, and the share of nominal PV capcity in the nominal power requirement of the electrolyzer subsystem.

1.1.3 SOE

The cost function for calculating the initial investment cost of SOE unit given by CEA is based on the CEA stack of 50 cells × 196 cm^2. The number of stacks (n_{stack}) is first calculated by the power consumption of the whole SOE unit:

$$n_{\text{stack}} = 1.32 \frac{\dot{W}_{\text{unit}}}{9800\, i_{\text{cell}} V_{\text{cell}}} = 1.32 \frac{\dot{W}_{\text{unit}}}{\dot{W}_{\text{stack}}} \tag{S12}$$

where the symbols $\dot{W}_{\text{unit}}$, $\dot{W}_{\text{stack}}$ are the power required (W) of the whole SOE unit and a stack, while i_{cell} and V_{cell} represents the operating current density (A/cm^2) and voltage (V) of a single cell.

Since the SOLIDPower (SP) stack of 64 cells × 80 cm^2 is employed for SOE simulation, the number of SOLIDPower stack should be converted to that of CEA stack based on the total cell area:

$$n_{\text{stack}} = 1.32 \left(\frac{\dot{W}^{\text{SP}}_{\text{unit}}}{\dot{W}^{\text{SP}}_{\text{stack}}} A^{\text{SP}}_{\text{cell}} n^{\text{SP}}_{\text{cell}} \right) / \left(A^{\text{CEA}}_{\text{cell}} n^{\text{CEA}}_{\text{cell}} \right) \tag{S13}$$

where the symbol A_{cell} and n_{cell} are the single-cell area and the cell number per stack.

For a small system with $n_{\text{stack}} < 350$, the cost of the whole SOE stack (in €) is calculated by

$$C^{\text{GR,ini}}_{\text{soe}} = -1.641\, n^2_{\text{stack}} + 5.660\text{e}3\, n_{\text{stack}} + 5.204\text{e}4 \tag{S14}$$

While for a large system with $n_{\text{stack}} > 350$, the cost of the whole SOE stack (in €) is calculated by

$$C^{\text{GR,ini}}_{\text{soe}} = -4.784\text{e}{-2}\, n^2_{\text{stack}} + 4.119\text{e}3\, n_{\text{stack}} + 4.962\text{e}5 \tag{S15}$$

Regular renewal of the stack is required due to stack degradation with an renewal frequency of average every 6 years of operation. For each stack replacement, additional 42% of initial CAPEX is expensed. Thus, considering 3 replacements for a plant life of 20 years, the total replacement cost can be estimated to an average 6%/year of replacement expenses ($3 \times 0.42/20 = 6.3\%$). Thus, the total cost (in €) of the SOE unit with stack replacement can be calculated

$$C^{\text{GR}}_{\text{soe}} = C^{\text{GR,ini}}_{\text{soe}} (1 + 0.42\, n_{\text{renew}}) = C^{\text{GR,ini}}_{\text{soe}} (1 + 0.063\, n) \tag{S16}$$

where the symbol n represents the plant life.

1.1.4 Heat exchanger network

The area and cost of heat exchanger network is estimated by a classical vertical heat transfer based on the composite curve. Detailed description of this estimation procedure can be found in elsewhere, e.g., chapter 15 of (Turton et al., 2008) and chapter 7 of (Mian, 2016). The estimation procedure works as follows:

- Identify the temperature intervals (v_i), the involved heat streams and the corresponding heat loads from the composite curve

- Estimate the average heat exchange coefficient ($\bar{U}_{v_i}$) of each vertical heat exchanger (v_i)
  - Average heat transfer coefficients of hot/cold composite flows ($\bar{U}_{\mathrm{h},v_i}$ and $\bar{U}_{\mathrm{c},v_i}$)

$$\bar{U}_{\mathrm{h},v_i} = \frac{\dot{Q}_{\mathrm{tot},v_i}}{\sum_{j\in\mathbb{H}_{v_i}} \frac{\dot{Q}_{j,v_i}}{U_j}} \qquad \bar{U}_{\mathrm{c},v_i} = \frac{\dot{Q}_{\mathrm{tot},v_i}}{\sum_{j\in\mathbb{C}_{v_i}} \frac{\dot{Q}_{j,v_i}}{U_j}} \tag{S17}$$

  where the $\dot{Q}_{\mathrm{tot},v_i}$ is the total heat transferred of the temperature interval v_i, the $\mathbb{H}_{v_i}$ ($\mathbb{C}_{v_i}$) represents a set of all hot (cold) streams involved in the temperature interval v_i, the $\dot{Q}_{j,v_i}$ stands for the amount of heat transferred by stream j in temperature interval v_i, and the U_j indicates the heat transfer coefficient of stream j.

  - Overall heat transfer coefficient

$$\bar{U}_{v_i} = \frac{1}{\frac{1}{\bar{U}_{\mathrm{h},v_i}} + \frac{1}{\bar{U}_{\mathrm{c},v_i}}} \tag{S18}$$

- Calculate the heat exchanger area of each temperature interval (A_{v_i}) and the total area (A_{tot})

$$A_{v_i} = \frac{\dot{Q}_{\mathrm{tot},v_i}}{\bar{U}_{v_i}\Delta T_{\mathrm{log}}} \qquad A_{\mathrm{tot}} = \sum A_{v_i} \tag{S19}$$

  where $\Delta T_{\mathrm{log}}$is the log temperature difference of the temperature interval v_i.

- Calculate minimum number of heat exchangers N_{min} and the average heat exchanger area ($\bar{A}$)

$$N_{\mathrm{min}} = (N_{\mathrm{str}} - 1) + (N_{\mathrm{pstr}} - 1) \qquad \bar{A} = \frac{A_{\mathrm{tot}}}{N_{\mathrm{min}}} \tag{S20}$$

  where the N_{str} is the total number of heat streams, and N_{pstr} is the number of pinch streams.

- Calculate the bare module cost of the heat exchange network (in $)

$$C^{\mathrm{BM}}_{\mathrm{hen}} = \left(1\mathrm{e}4 + 800\, N_{\mathrm{min}}\bar{A}^{0.8}\right) F_{\mathrm{p}}F_{\mathrm{m}} \tag{S21}$$

  where F_{p} and F_{m} are the pressure and material factors. It is assumed that the material used for all heat exchanger are stainless steel with $F_{\mathrm{m}} = 3$, while F_{p} is determined based on the actual operating pressure of the system by the formulation given in Fig. 5.37 of (Ulrich and Vasudevan, 2004). The values, $1\mathrm{e}4$, 800 and 0.8 in Eq. S21, have been employed in Aspen Energy Analyzer (a software from AspenTech to address heat exchanger network design) as well.

1.1.5 Electrical heater (fired heater)

The electrical heater (in $) is treated as a fired heater for costing (Fig. 5.27 of (Ulrich and Vasudevan, 2004)):

$$C^{\mathrm{BM}}_{\mathrm{eh}} = \left(284.37\,\dot{Q}_{\mathrm{eh}}^{0.8131}\right) F_{\mathrm{p}}F_{\mathrm{m}} \left(\frac{CEPCI_{2017}}{CEPCI_{2004}}\right) \tag{S22}$$

where F_{p} and F_{m} are the pressure and material factors. Stainless steel is assumed to be used with the material factor of 2.7. Similarly, the pressure factor can be determined by the Fig. 5.27 (Ulrich and Vasudevan, 2004).

1.1.6 Compressor/pump

All compressors for different gases involved, e.g., sweep air, H_2, syngas and methane, are modeled by multi-stage isentropic compression with inter-cooling. The maximum pressure ratio per stage (γ_{stage}) is specified as 3. The stage number is determined by an equal distribution of pressure ratio over total pressure ratio desired:

$$n_{\text{stage}} = \frac{\log\left(\gamma_{\text{tot}}\right)}{\log\left(\gamma_{\text{stage}}\right)} \tag{S23}$$

Then, the total power required and outlet temperature can be calculated by isentropic compression. The minimum number of compressors in operation ($n_{\text{comp}}^{\text{operation}}$) is then computed with respect to a maximum fluid power of for a single compressor ($\dot{W}_{\text{single}}^{\text{max}} = 8000\,\text{kW}$). The costing of centrifugal compressors is considered (Fig. 5.30 of (Ulrich and Vasudevan, 2004)):

$$C_{\text{comp}}^{\text{BM}} = n_{\text{comp}}^{\text{operation}} 10^{k_1 + k_2 \log\left(\dot{W}_{\text{single}}\right) + k_3\left(\log\left(\dot{W}_{\text{single}}\right)\right)^2 + k_4\left(\log\left(\dot{W}_{\text{single}}\right)\right)^3} F_{\text{m}} F_{\text{bkp}} \left(\frac{CEPCI_{2017}}{CEPCI_{2004}}\right) \tag{S24}$$

where the coefficient $\boldsymbol{k}$ equals to $\{3.808\,16,\ 6.497\,82\text{e}{-2},\ 3.252\,27\text{e}{-1},\ -3.916\,22\text{e}{-2}\}$. The material factor, F_{m}, is taken as 2.5 for carbon steel and 6.3 for stainless steel, while the backup factor, F_{bkp}, for considering spare compressors purchase is set as 2.5.

The costing of pumps is similar to that of the compressors, which is formulated as follows (Turton et al., 2008):

$$C_{\text{pump}}^{\text{BM}} = n_{\text{comp}}^{\text{operation}} 10^{k_1 + k_2 \log\left(\dot{W}_{\text{single}}\right) + k_3\left(\log\left(\dot{W}_{\text{single}}\right)\right)^2} F_{\text{bkp}} \left(a_1 + a_2 F_{\text{p}} F_{\text{m}}\right) \left(\frac{CEPCI_{2017}}{CEPCI_{1996}}\right) \tag{S25}$$

where the coefficient $\boldsymbol{k}$ equals to $\{3.5793,\ 0.3208,\ 0.02850\}$, while the coefficients a_1 and a_2 are 1.8 and 1.51, respectively. The backup factor, F_{bkp}, is specified as 3.21. The material factor F_{m} is 1.8 for carbon steel and 2.4 for stainless steel, while the pressure factor F_{p} is calculated as below:

$$F_{\text{p}} = \begin{cases} 1 & p \le 11\,\text{bar} \\ b_1 + b_2 \log\left(p-1\right) + b_3\left(\log\left(p-1\right)\right)^2 & p > 11\,\text{bar} \end{cases} \tag{S26}$$

where the coefficient $\boldsymbol{b}$ are $\{0.1682,\ 0.3477,\ 0.4841\}$, respectively.

1.1.7 Pressure vessel (Reactor/flash drum/column)

The drums, reactors and columns are basically pressure vessels, usually vertical pressure vessels. The vessel volume can be reasonably determined by the actual inlet volumetric flow $\dot{V}$ and the superficial speed $\bar{v}$ (or the residence time τ, or the gas hourly space velocity $GHSV$). The selection of superficial speed and residence time is usually based on the existing unit operation or experimental setup and may vary largely among the types of equipments.

- Vertical pressure vessel

The diameter (D) and height (H) of an industrial vertical vessel are usually within the range of [0.2, 5] and [1.2, 50] m. The cost of a vertical vessel can be computed as follows:

$$C_{\text{vv}}^{\text{BM}} = 10^{k_1 + k_2 \log(H) + k_3 (\log(H))^2} \left(a_1 + a_2 F_{\text{m}} F_{\text{p}}\right) \left(\frac{CEPCI_{2017}}{CEPCI_{1996}}\right) \tag{S27}$$

The values of the coefficients $\boldsymbol{k}$ are related to the vessel diameter:

$$\boldsymbol{k} = \begin{cases} \{3.3392,\, 0.5538,\, 0.2851\} & D \leq 0.3\,\mathrm{m} \\ \{3.4746,\, 0.5893,\, 0.2053\} & D \leq 0.5\,\mathrm{m} \\ \{3.6237,\, 0.5262,\, 0.2146\} & D \leq 1.0\,\mathrm{m} \\ \{3.7559,\, 0.6361,\, 0.1069\} & D \leq 1.5\,\mathrm{m} \\ \{3.9484,\, 0.4623,\, 0.1717\} & D \leq 2.0\,\mathrm{m} \\ \{4.0547,\, 0.4620,\, 0.1558\} & D \leq 2.5\,\mathrm{m} \\ \{4.1110,\, 0.6094,\, 0.0490\} & D \leq 3.0\,\mathrm{m} \\ \{4.3919,\, 0.2859,\, 0.1842\} & D \leq 5.0\,\mathrm{m} \end{cases} \tag{S28}$$

The constants a_1 and a_2 are 2.50 and 1.72, respectively. The material factor F_m is given as 1.0 for carbon steel, 4.0 for stainless steel, 9.8 for nickel alloy and 10.6 for titanium. The factors for more materials can be found in (Turton et al., 2008; Ulrich and Vasudevan, 2004). The pressure factor is decided by the rated pressure, 1.5 times of the nominal operating pressure (p):

$$F_\mathrm{p} = \begin{cases} 1.25 & 1.5\,p \leq 0.5 \text{ bar} \\ 1.00 & 1.5\,p \leq 4.7 \text{ bar} \\ b_1 + b_2 \mathrm{log}\,(p-1) + b_3\,(\mathrm{log}\,(p-1))^2 + b_4\,(\mathrm{log}\,(p-1))^6 + b_5\,(\mathrm{log}\,(p-1))^8 & 1.5\,p > 4.7 \text{ bar} \end{cases} \tag{S29}$$

where the coefficient $\boldsymbol{b}$ equals to $\{0.5146, 0.6838, 0.2970, 0.0235, 0.0020\}$.

- Flash drum, the gas-liquid separator

For a flash drum, the residence time is usually selected as 300 s. The volumetric flows (m^3/s) of gas and liquid in the drum are assumed to be equal to each other. Thus, the number of the drums required can be first determined as follows

$$n_\text{drum} = \text{ceil}\left(\left(\frac{\left(2\,\dot{V}_\text{tot}\tau/\pi\right)^{\frac{1}{3}}}{D_\text{max}}\right)^3\right) \tag{S30}$$

where the maximum diameter allowed D_max is 4 m. The volumetric flowrate of a single vessel is expressed

$$\dot{V}_\text{single} = \frac{\dot{V}_\text{tot}}{n_\text{vv}} \tag{S31}$$

Then, the dimension of a single vessel (D_single and H_single) is determined:

$$D_\text{single} = \left(\frac{2\,\dot{V}_\text{single}\tau}{\pi}\right)^{\frac{1}{3}} \tag{S32}$$

$$H_{\text{single}} = \begin{cases} 3\,D_{\text{single}} & p-1 \leq 19 \text{ bar} \\ 4\,D_{\text{single}} & p-1 \leq 34 \text{ bar} \\ 5\,D_{\text{single}} & p-1 > 34 \text{ bar} \end{cases} \tag{S33}$$

With the dimension and bare module cost of a single vessel obtained by Eq. S27, the total bare module cost of all drums equipped is given as

$$C_{\text{drum}}^{\text{BM}} = n_{\text{drum}} C_{\text{single}}^{\text{BM}} \tag{S34}$$

- Reactor

The cost of a reactor depends on the reactor type, pressure level, material type and actual inlet volumetric flowrate. The number and size of the reactors are defined by the total volumetric flow, the superficial gas velocity and the gas hourly space velocity.

The reactor diameter is determined similarly to Eq. S30 but by the superficial gas velocity:

$$n_{\text{reactor}} = \text{ceil}\left(\left(\frac{2\sqrt{\frac{\dot{V}_{\text{tot}}}{\pi \bar{v}}}}{D_{\text{max}}}\right)^2\right) \tag{S35}$$

$$\dot{V}_{\text{single}} = \frac{\dot{V}_{\text{tot}}}{n_{\text{reactor}}} \tag{S36}$$

$$D_{\text{single}} = \begin{cases} 2\sqrt{\frac{\dot{V}_{\text{single}}}{\pi \bar{v}}} & \text{Fixed-bed catalytic methanation reactor and MeOH-to-DME reactor} \\ 2\sqrt{\frac{\dot{V}_{\text{single}}}{\alpha \pi \bar{v}}} & \text{MeOH and DME-to-gasoline reactor; } \alpha\text{=0.92 (fixed bed), 0.49 (slurry bed)} \end{cases} \tag{S37}$$

The reactor volume is calculated by the gas hourly space velocity (in h^{-1}) based on the volumetric flowrate at standard conditions (15 °C and 1 bar):

$$V_{\text{tot}} = \frac{3600\,\dot{V}_{\text{tot}} \frac{p}{p_{\text{std}}} \frac{T_{\text{std}}}{T}}{GHSV} \tag{S38}$$

$$V_{\text{single}} = V_{\text{tot}}/n_{\text{reactor}} \tag{S39}$$

The determination of the reactor diameter differs from the reactor type:

$$H_{\text{single}} = \begin{cases} \frac{4\,V_{\text{single}}}{\pi D_{\text{single}}^2} + 0.914 & \text{Fixed-bed catalytic methanation reactor} \\ \beta D_{\text{single}} & \text{MeOH and DME-to-gasoline reactor; } \beta\text{=1.62 (fixed bed), 3.15 (slurry bed)} \\ 1.62\,D_{\text{single}} & \text{MeOH-to-DME reactor} \end{cases} \tag{S40}$$

With the updated diameter, the volume of a single reactor is corrected as

$$V_{\text{single}} = H_{\text{single}} \frac{\pi D_{\text{single}}^2}{4} \tag{S41}$$

With the calculated n_{reactor}, D_{single}, H_{single} and V_{single}, the reactor cost without catalyst fill is

$$C_{\text{reactor}}^{\text{BM}} = \begin{cases} n_{\text{reactor}} C_{\text{vv}}^{\text{BM}} & \text{Adiabatic reactor; } C_{\text{vv}}^{\text{BM}} \text{ determined by Eq. S27} \\ n_{\text{reactor}} C_{\text{jr}}^{\text{BM}} & \text{Isothermal reactor; } C_{\text{jr}}^{\text{BM}} \text{ given below} \end{cases} \tag{S42}$$

The isothermal reactor is treated as a jacketed reactor for costing:

$$C_{\text{jr}}^{\text{BM}} = 10^{k_1 + k_2 \log(V) + k_3 (\log(V))^2} F_{\text{p}} F_{\text{m}} \left(\frac{CEPCI_{2017}}{CEPCI_{2004}} \right) \tag{S43}$$

where the reactor volume is calculated as mentioned above, while the coefficient $\boldsymbol{k}$ equals to $\{3.765965, 0.230014, 0.118244\}$. The material factor F_{m} is 3.0 for carbon steel and 7.6 for stainless steel, while the pressure factor F_{p} is 1.0 ($p \leq 6$), 1.4 ($p \leq 11$), 1.6 ($p \leq 16$), 2.0 ($p \leq 21$), 3.0 ($p \leq 4.1$), 4.3 ($p \leq 81$), 6.5 ($p \leq 161$), 13 ($p \leq 321$).

For the reactors involved, the superficial gas velocity is collected and validated: 0.5 m/s for fixed-bed methanation reactor, 0.317 m/s for fixed-bed MeOH reactor, 0.135 m/s for slurry-bed MeOH reactor, 0.2 m/s for MeOH-to-DME reactor, 0.2136 m/s for DME-to-gasoline reactor. The gas hourly space velocity for the isothermal methanation reactor is set as 2400 h^{-1}.

- Distillation column

The investment cost of a distillation column includes two parts: 1) the cost of vertical vessel and 2) the cost of tower packing. The sizing of the pressure vessel is based on a superficial mass flow (G) of $1\ \text{kg}\,\text{s}^{-1}\text{m}^{-2}$ to determine the column diameter of a single column (D_{single}):

$$D_{\text{single}} = 2\sqrt{\frac{\dot{m}_{\text{single}}}{\pi G}} \tag{S44}$$

$$n_{\text{column}} = \frac{\dot{m}_{\text{tot}}}{\dot{m}_{\text{single}}} \tag{S45}$$

A loop determining the column number is introduced to ensure that the column diameter is below 5 m. Then, the height equivalent to theoretical plate (HETP) is calculated heuristically:

$$HETP = \begin{cases} 0.5 & D_{\text{single}} < 0.5 \text{ m} \\ 0.5\, D_{\text{single}}^{0.3} & D_{\text{single}} \geq 0.5 \text{ m} \end{cases} \tag{S46}$$

Then, the height of the vertical vessel can be calculated simply by the number of trays obtained from a rigorous calculation of the column (e.g., Radfrac column model in Aspen Plus):

$$H_{\text{single}} = n_{\text{trays}} HETP \tag{S47}$$

With the column dimension known, the cost of the vertical vessel used can be obtained by Eq. S27.

The cost of tower packing is formulated as

$$C_{\text{tp}}^{\text{BM}} = 10^{k_1 + k_2 \log(H)} F_{\text{m}} \left(\frac{CEPCI_{2017}}{CEPCI_{1996}} \right) \tag{S48}$$

where the coefficients $\boldsymbol{k}$ considers the impact of column diameter:

$$\boldsymbol{k} = \begin{cases} \{2.1630,\ 0.9656\} & D_\text{single} \leq 0.3\,\text{m} \\ \{2.5210,\ 0.9764\} & D_\text{single} \leq 0.5\,\text{m} \\ \{3.0169,\ 1.0000\} & D_\text{single} \leq 1.0\,\text{m} \\ \{3.2160,\ 0.9847\} & D_\text{single} \leq 1.5\,\text{m} \\ \{3.3848,\ 0.9808\} & D_\text{single} \leq 2.0\,\text{m} \\ \{3.6023,\ 0.9682\} & D_\text{single} \leq 2.5\,\text{m} \\ \{3.7921,\ 0.9697\} & D_\text{single} \leq 3.0\,\text{m} \\ \{3.9986,\ 0.9833\} & D_\text{single} > 3.0\,\text{m} \end{cases} \tag{S49}$$

The material factor F_m is 1.2 for carbon steel, 2.2 for 304SS and 4.2 for 316SS.

Eventually, the total bare module cost of the distillation column is calculated by

$$C_\text{column}^\text{BM} = n_\text{column}\left(C_\text{vv}^\text{BM} + C_\text{tp}^\text{BM}\right) \tag{S50}$$

1.2 Operation and maintenance cost (O&M)

The O&M cost are contributed by each separate equipment, and the resource use and waste/pollutant mission of the whole system. For most equipment, the fixed O&M cost per year can be treated to be simply proportional (F^OMC) to its total capital cost:

$$C_i^\text{OMC} = F^\text{OMC} C_i^\text{TCC} \tag{S51}$$

where the OM factor is set as 0.04 for compressor/pump, 0.04 for reactor, 0.04 for drum, 0.01 for CSP, 0.01 for PV, 0.02 for SOE. However, for reactors, additional O&M cost is introduced due to catalyst replacement. The catalyst cost can be readily calculated by catalyst productivity by volume θ_V (kg product per hour per liter catalyst) or by mass θ_M (kg product per hour per kg catalyst) and the product mass flow $\dot{m}_\text{product}$ or bed void fraction ϵ_bed:

$$C_\text{cat}^\text{ini} = f c_\text{cat}\rho_\text{cat}V_\text{cat} = f c_\text{cat}\rho_\text{cat}\frac{3.6\,\dot{m}_\text{product}}{\theta_\text{V}} = f c_\text{cat}\frac{3600\,\dot{m}_\text{product}}{\theta_\text{M}} = f c_\text{cat}\rho_\text{cat}\left(1 - \epsilon_\text{bed}\right)V_\text{tot} \tag{S52}$$

$$C_\text{cat}^\text{tot} = \text{ceil}\left(\frac{n}{n_\text{renewal}}\right)C_\text{cat}^\text{ini} \tag{S53}$$

where C_cat^ini and C_cat^tot are the cost of initial catalyst fill and the total catalyst cost over the plant lifetime. The multiple factor f depends on the type of reactor system: For example, for a three-reactor DME-to-gasoline system, two reactors operate normally to process all feed flows while the remaining is under catalyst regeneration, typically for zeolite catalyst; for such a system, the multiple factor f equals to 1.5. The symbol c_cat, ρ_cat and n_renewal represent the specific cost (\$/kg), density (kg/m^3) and the renewal time of the catalyst.

For methanation reactor, nickel catalyst (50 wt% Ni) is employed with a density of 3120 kg/m^3, a bed void fraction of 0.5, a price of 55 $\$/\text{kg}$ and a renewal time of 4 years. For MeOH reactor, Cu-based catalyst (Cu/Zn/Al/O) is utilized with a productivity of 0.9 kg/h/L, a density of 1775 kg/m^3, a price of 21.4 \$/kg and a renewal time of 4 years. For DME reactor, Al_2O_3 catalyst (52.9 Al/47.1 O wt%) is used with a productivity of 0.96 kg/h/L-cat, a density of 3950 $\mathrm{kg/m^3}$, a price of 22.7 \$/kg and a renewal time of 3 years. For gasoline reactor, zeolite catalyst (ZSM-5) is applied with a productivity of 0.25 kg/h/L-cat, a density of 740 $\mathrm{kg/m^3}$, a price of 132 \$/kg, a multiple factor of 1.5 (three reactor system) and a renewal time of 2 years.

The annual resources (res), emissions (emm) and by-products (byp) i is calculated by scaling the nominal rate ($\dot{P}_{\text{s},i}$ in kg/s) with the ratio of annual product ($\dot{P}_{\text{y,prod}}$) and nominal product rate ($\dot{P}_{\text{s,prod}}$ in kg/s):

$$C_{\text{res/emm/byp},i} = c_{\text{res/emm/byp},i}\dot{P}_{\text{s},i}\left(\frac{\dot{P}_{\text{y,prod}}}{\dot{P}_{\text{s,prod}}}\right) \tag{S54}$$

The major resources used include water (0.01 €/kg, 10 €/ton), CO_2 (0.04 €/kg), grid electricity (0.04365 €/kWh, 43.65 €/MWh).

1.3 LCO formulation

1.3.1 Levelized capital cost/CAPEX

The levelized capital cost ($C_{\text{L}}^{\text{TCC}}$) is calculated by multiply the total capital cost (C^{TCC}) with the capital recovery factor (CRF)

$$C_{\text{L}}^{\text{TCC}} = C^{\text{TCC}}CRF = \sum C_i^{\text{TCC}}\frac{r\left(1+r\right)^n}{\left(1+r\right)^n-1} \tag{S55}$$

where the symbols r and n are the discount rate and the plant life.

1.3.2 Annual operation and maintenance cost/OPEX

The annual OM cost (C_{L}^{OM}) is a summation of a fixed OM cost, catalyst cost and resource/emission/by-product cost, as described in section 1.2:

$$C_{\text{L}}^{\text{OMC}} = \sum_{i\in\boldsymbol{D}} C_i^{\text{OMC}} + \sum_{j\in\boldsymbol{C}} C_{\text{cat},j} + \sum_{k\in\boldsymbol{R}} C_{\text{res},k} + \sum_{m\in\boldsymbol{E}} C_{\text{emm},m} + \sum_{n\in\boldsymbol{B}} C_{\text{byp},n} \tag{S56}$$

where the sets $\boldsymbol{D}$, $\boldsymbol{C}$, $\boldsymbol{R}$, $\boldsymbol{E}$ and $\boldsymbol{B}$ are the collection of involved devices, catalysts, resources, emissions and by-products. All the costs are on an annual basis.

1.3.3 LCO

With the annualized capital and OM costs calculated, the levelized product cost (€/kg) can be obtained simply by

$$LCO = \frac{C_{\text{L}}^{\text{TCC}} + C_{\text{L}}^{\text{OMC}}}{\dot{P}_{\text{y,prod}}} \tag{S57}$$

where the $\dot{P}_{\text{y,prod}}$ stands for the annual/yearly production of the main product (kg/year).

2 PROCESS DESCRIPTION AND SCREENING

2.1 Methane synthesis

There are many technology options available for methane synthesis (**?**). The fixed-bed reactor is chosen in consideration of commercialization level. Methanation from H_2/, CO_2 mixture or from syngas are highly exothermic, therefore the chemical equilibrium and catalysts favor a lower reaction temperature. To control the reacting temperature with the range 200–550 °C, as is desired by the catalysts, several techniques are usually employed: gas recirculation from reactor outlet to reactor inlet, jacked-cooling, staged-feed of one reactants or water injection. As the high reacting temperature of fixed-bed methanation compared with fluidized-bed or three-phase reactors resulting low conversion rate in one bed, a series 2–4 beds are usually needed to ensure the desired conversion rate. Additionally, another strategy to increase the conversion rate is to cool down the gases and remove water from the gas mixture. Therefore, the fixed-bed methanation concept with a maximum of 3 serial reactors with gas recirculation, jacked-cooling or staged-feed of CO_2 are investigated under the pressurized condition of the electrolyzer as shown in Fig. S3. The flowsheet can be adapted for the following several cases for both steam- and co-electrolysis.

- Option 1: Adiabatic reactors with gas recirculation
- Option 2: Adiabatic reactors with gas recirculation and staged CO_2 feed
- Option 3: Jacked reactors without gas recirculation and staged CO_2 feed

The reaction has been modeled by the equilibrium reactors and the approach temperature to the equilibrium has been estimated from a demonstration project. All reactors can be flexibly switched between adiabatic reactor and isothermal (jacked-cooling) reactor for specific necessity. The first and second reactors are equipped with gas recirculation due to the large conversion and heat released. The third one, if employed, is to ensure a high purity of methane produced. Each reactor is followed by a gas cooler and a flash drum to separate water from the gas mixture, thus preparing for the next reactor. Depending on the working pressure, not all reactors will be employed: For each given working condition, the purity out of each flash drum is checked, and if the checked purity meets the requirement, the flowsheet above will not be considered in thermo-economic evaluation and lifecycle assessment.

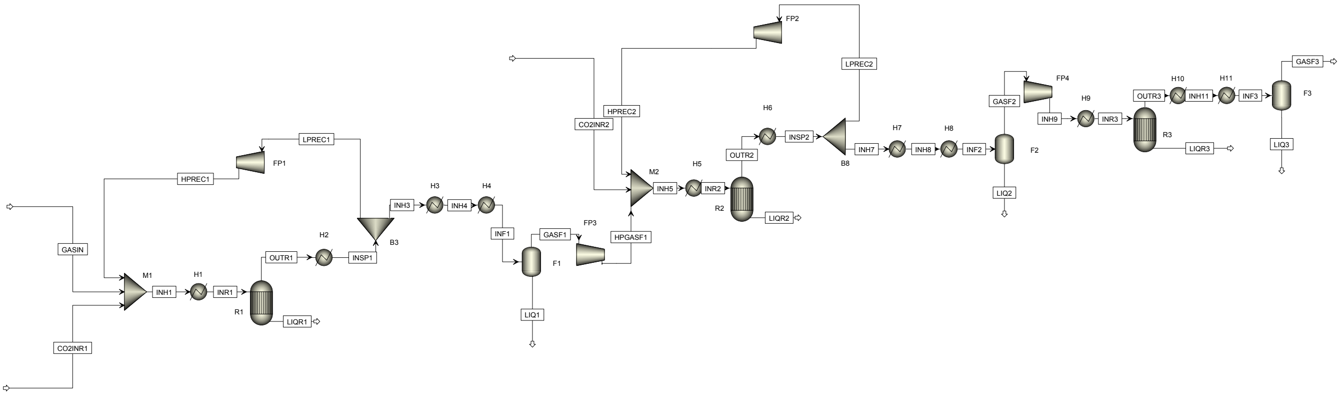

Figure S3. General flowsheet for fixed-bed methanation. (The GASIN stream could be H_2/H_2O mixture or syngas mixture. If syngas is fed, then the mass flowrates of CO_2 feed streams, CO2INR1 and CO2INR2, are forced to be 0. In this way, this flowsheet is applicable to both H_2/CO_2 and syngas conversion.)

From design viewpoint, the adiabatic methanation is much easier while resulting in either large reactor size (investment cost) or a lower conversion rate, while the jacked/isothermal methanation with specific heat transfer design could reduce the reactor size substantially, thus is more economically viable. Thermodynamically, isothermal methanation realizes very high conversion rate. The steam cooling with wet syngas feed may be important to help control the outlet temperature of the 1st reactor. With dry syngas feed, the adiabatic methanation option 1 can hardly control the R1 outlet temperature under 290 °C, even with a very large recirculation ratio of 95%.

For methanation from syngas, there is almost no difference in the amount of the final methane produced and the methane purity of over 98% between adiabatic methanation with gas recirculation and Jacked methanation. However, the adiabatic concept cannot realize a high single-pass conversion rate, thus requires a high gas recirculation rate. The high recirculation rate largely increases the volumetric feed flowrates of the reactor. There is a significant difference in the reactor size (capital investment) of the two concepts. The advantage of wet-syngas feed should be highlighted for controlling the outlet temperature of reactors. However, it is also clear that the presence of water also largely increases the volumetric flows into the 1st reactor. If with dry-syngas feed, it is found that even with a large recirculation ratio of 95%, the outlet temperature of the 1st reactor of the adiabatic methanation (option 1) is still as high as 320 °C. Another point to be highlighted is that, when fixing the amount of H_2 fed, the methane production from syngas is more than that from H_2, since 1 mole CO methanation needs only 3 mole H_2 while 1 mole CO_2 requires 4 mole H_2.

The water injection option for the temperature control is not studied as a separate case, as the high-temperature steam electrolyzer mostly works with a fuel utilization factor around 50% (in this deliverable) to 80%. This means that there is naturally some steam contented in the H_2 feed, which in fact helps to control the reactor temperature. More importantly, for pressurized operation of electrolyzer, the methanation reactors operate under the same pressure, thus basically no compressor is needed to compress electrolysis product for methanation. From these aspects, when coupling high-temperature steam electrolyzer with methanation, there is no need to configure a flash drum to produce dry H_2 before entering methanator. It is also worth noting that for all the flowsheets for the synthesis of carbon fuels, methane, methanol and gasoline, the specific heat exchanger network is not designed, since the network varies largely depending on the process integration level.

It can be concluded that the concept of adiabatic methanation with wet syngas feed and gas recirculation and the concept of jacked methanation with dry/wet gas feeds are more worthy to compare from thermo-economic viewpoint than other concepts.

2.2 Methanol synthesis

Methanolization reactor is generally less exothermic than the methanation reactor. The typical operating temperature ranges from 220 to 280 °C, while the operating pressure is between 50 to 100 bar. Beyond 280–300 °C, the catalyst would be subjected to sintering and fusion, resulting in permanent damage of the catalyst. Higher pressures favor methanol synthesis from the equilibrium standpoint; however, the increase above 80 bar does not exerts very significant impact on the conversion rate. In this deliverable, the temperature and pressure is first set at 260 °C and 70 bar. Since the operating pressure of methanolization reactor is much higher than that of the electrolyzer, gas compression for feeding to the reactor is required. This means that the products of high-temperature electrolyzer should be cooled down to 40 °C and the water drainage should be separated for gas compression. The flowsheet of methanol synthesis and upgrade is illustrated in Fig. S4, which works for both H_2 feed or syngas feed. The gas mixture out of the reactor is first cooled down to 40 °C to separate methanol/liquid water for methanol distillation. The gas mixture out of the flash drum is split to two parts: 99% is recirculated back the reactor for increasing the conversion rate, while 1% is burned to purge the system by removing continuously certain amount of inert gases. The methanol/water liquid is throttled down to 1.2 bar and then heated up to 80 °C to distillation column. High purity of methanol up to 99.5% can be obtained. The distillation column is rigorously modeled and tuned automatically based on the column feed: The feed-to-distillate ratio, the number of stage and the reflux ratio. A short-cut column model, DSTWU, is configured to provide heuristics for choosing reasonable reflux ratio, the number of stages and the feed stage. The mass purity of methanol product reaches 99%, with an adapted design of distillation column: 16 stages, 0.901 reflux ratio and 0.506 distillate-to-feed ratio.

For methanolization, there is no degree of freedom for the design of system layout. Large gas recirculation is generally required as per-pass conversion rate is rather low. However, the operating pressure would be investigated to find the trade-off between conversion rate and investment cost in the thermo-economic evaluation.

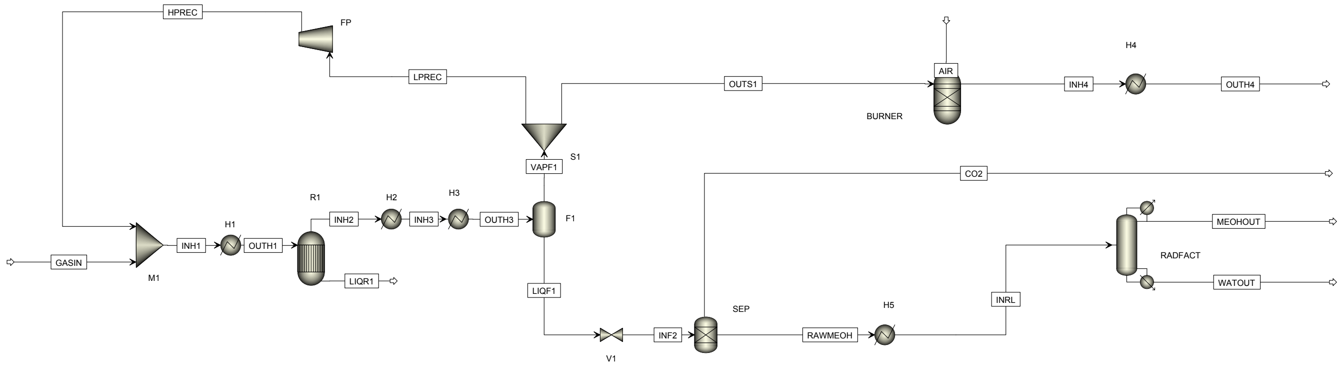

Figure S4. Methanolization flowsheet for both H_2 and syngas feed.

2.3 Methanol-to-Gasoline synthesis and purification

Methanol-to-Gasoline process is employed for producing gasoline from H_2/CO_2 mixture or syngas. The whole process converting raw gases to gasoline, assumed to be represented by n-heptane (C_7H_{16}), involves methanol synthesis reactor, methanol separation, methanol-to-DME reactor via methanol dehydration, gasoline reactor and a complex separation process to extract gasoline and valuable byproducts. The performance of methanol synthesis reactor for both feeds, H_2/CO_2 or syngas, has been discussed above, thus only the sub-processes after methanol separation are considered in this section. Essentially, for both cases, the MtG flowsheet is the same, as shown in Fig. S5.

As illustrated in Fig. S5, methanol is first synthesized via the process described in Fig. S4, purified and stored for continuous feed to MtG process. The methanol is then pumped up to 23 bar, vaporized and superheated to 297 °C, and then fed to an adiabatic fixed-bed DME reactor, in which methanol is converted to an equilibrium mixture of methanol, DME and water. The mixture of a temperature of 407 °C and 22 bar then enters the gasoline reactor for gasoline production. Due to limited data published on the MtG reactor, thus a simplified RYield reactor is used to simulate the product yield structure (the product molar distribution given per kg of pure methanol input to a DME reactor) of the MtG reactor.

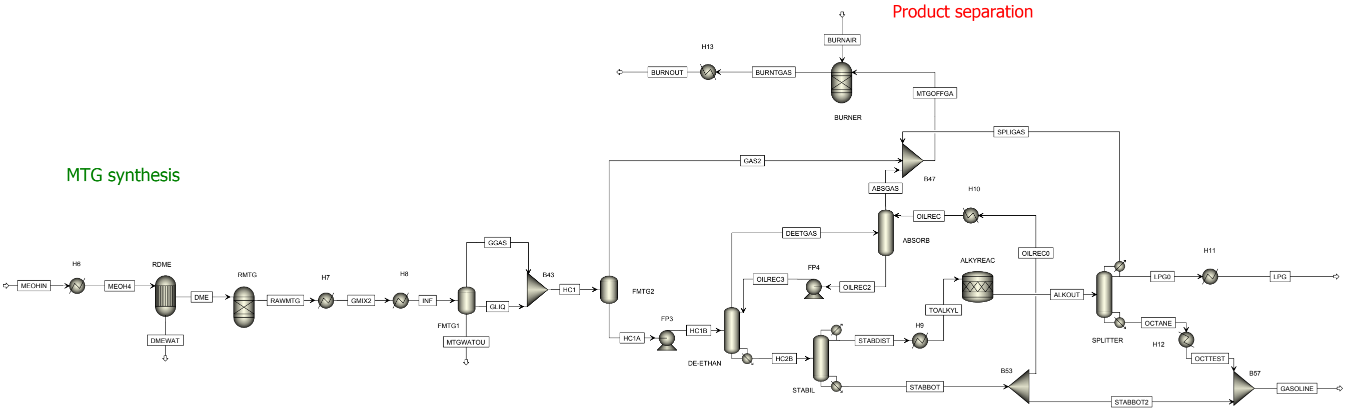

Figure S5. Methanol-to-Gasoline synthesis and product purification. (RDME: Methanol-to-DME reactor via methanol dehydration; RMTG: Gasoline reactor, modelled by yield reactor)

The MtG effluent then enters the complex product recovery and upgrade process. The mixture is first condensed in FMTG1 and FMTG2 to separate the mixture to water, raw gasoline, purge and recycle gas streams. The condensed raw gasoline then enters the product recovery section, in which the raw gasoline is fractionated first by a de-ethanizer, DE-ETHAN. In this column, the C_2^- is separated overheat as DEETGAS and the bottoms HC2B enters a stabilizer, STABIL, where a stream of LPG is produced overhead, STABDIST. The stabilized gasoline, STABBOT, is then introduced to a gasoline splitter for recycling part of the gasoline OLIREC0, while the remaining becomes heavy gasoline, STABBOT2. The LPG stream produced by STABIL passes through an Alkylation reactor and then a column, SPLITTER, to obtain the final liquefied petroleum gas (LPG). The recovered light gasoline is mixed with the heavy gasoline STABBO2 to be the final gasoline product, GASOLINE.

Note that the flowsheet in Fig. S5 is semi-empirical model, which gives very less degrees of freedom to change the component design and operating conditions. Besides, the separation performance is quite sensitive to the feed composition. Thus, in this paper, the MtG process is evaluated with fixed design and specifications. Key components, descriptions and specification of the flowsheet are listed below:

- Fluidized bed reactor
- p=13.8 bar
- ZSM-5 zeolite catalyst
- Single-step in the fluidized-bed reactor from methanol to gasoline compounds
- Regeneration of the catalyst required
- In the gasoline boiling range above C_5 hydrocarbons, compounds were lumped together because they will all be included in the final product and will stay together through the fractionation steps
- Butanes were included because they are on the edge of acceptability for the gasoline product: Too much C_4 hydrocarbons, especially isobutene, can cause the reid vapor pressure to exceed allowable limits.
- Hydrocarbons with carbon numbers less than 4 were removed from the gasoline in the absorber column and sent to the fuel combustor for process heat.

Assumptions in the gasoline separation are:

- De-euthanizer (50% recoverable C_4^+ hydrocarbons to distillate, 90% butanes to bottoms)
- Absorber (overhead from absorber contains 33% C_4^+ hydrocarbons, lean oil and recovered hydrocarbons are fed back to de-euthanizer)
- Stabilizer (95% of C_4 hydrocarbons are recovered in the overhead of the stabilizer column)
- Splitter (Alkylation reactor: HF acid alkylation unit)
- LPG/Alkylate splitter

The simulation results show that the inlet molar composition of methanol is 0.982. The final gasoline product is with a molar composition of 0.638 C_7H_{16}-1, 0.217 C_5H_n, 0.091 C_4H_n, and 0.035 H_2O. The production rate of by-product liquefied petroleum gas is with a molar composition of 0.88 C_4H_{10}, 0.058 C_5H_n, 0.0458 C_3H_8 and 0.0144 H_2O. The production rates from methanol are 0.389 kg gasoline/kg methanol and 0.014 kg LPG/kg methanol.

For gasoline synthesis, since the gasoline reactor is rather empirical and the product upgrade process is sensitive to the feed composition, there is no degree of freedom in changing neither the system layout nor the operating conditions. Thus, in the thermo-economic evaluation, gasoline synthesis and product purification will be considered as completely fixed design.

2.4 End-product methane

2.4.1 Option 1: Adiabatic reactors with gas recirculation

As described above, the design specifications and assumptions for the adiabatic reactors with gas recirculation include: 1) All feed streams to all reactors are heated to 230 C. 2) Gas recirculation ratios for 1st and 2nd reactors are adapted between 0 to 0.95 to make sure the outlet temperature of the reactors could be reduced to around 290 C, which agrees with the industrial application. This temperature would reduce the risks of too high temperature peak in the reactor. 3) All CO2 is fed into the 1st reactor. 4) The flash drum works around 40 C to remove water drainage. 5) The feed H2 is from the electrolyzer working at 15 bar and 750 C, with a steam utilization factor of 50%. The feed H2/H2O mixture is cooled down to 230 C before entering the methanation. 6) The methanation system works under a pressure of 15 bar. It is clear with such a system configuration and working condition, only 2 reactors are necessary: The molar fraction of methane out of the second flash drum has reached already 98%. With the help of gas recirculation, the reactor outlet temperature can be controlled down to around 290 C. However, even with the remaining steam from electrolyzer, the gas recirculation ratio of the first reactor is still very large, 91%. The gas recirculation ratio of 2nd reaction is around 43%. It is remarkable that the size of the first reactor would be around 40 times larger than that of the second. The conversion rates in both reactors are 71% and 85 %, respectively.

2.4.2 Option 2: Adiabatic reactors with gas recirculation and staged CO2 feed

The specifications and assumptions for this configuration include: 1) All feed streams to all reactors are heated to 230 C. 2) Gas recirculation ratios for 1st and 2nd reactors are adapted between 0 to 0.95 to make sure the outlet temperature of the reactors could be reduced to around 290 C. 3) Half CO2 is fed into the 1st reactor, while the remaining is fed to the second. 4) The flash drum works around 40 C to remove water drainage. 5) The feed H2 is from the electrolyzer working at 15 bar and 750 C, with a steam utilization factor of 50%. The feed H2/H2O mixture is cooled down to 230 C before entering the methanation. 6) The methanation system works under a pressure of 15 bar.

As mentioned above, the benefit of such a system is to provide a more flexible control on the reactor temperature. The reactor outlet temperatures are all successfully controlled at around 290 C. More importantly, with staged feed, the total reaction heat released is distributed to two reactors, thus reducing the gas recirculation rate of the 1st reactor substantially. The final gas recirculation ratios are 85% and 93% for the 1st and 2nd reactors. The purity of methane out of the first reactor is rather low due to staged feed, but increase dramatically to 94% after the second reactor. This indicates that a third reactor is mostly needed to reach a methane purity over 98%. The conversion rates of hydrogen in all three reactors are 13%, 73% and 87%, respectively. Another observation is that the feed flowrates to the 1st and 2nd reactors are still over 30 times larger than the 3rd reactor.

2.4.3 Option 3: Jacked reactors without gas recirculation or staged CO2 feed

With jacked cooling, it is assumed that the reactor itself is particularly designed to fulfill effective heat transfer removing methanation heat. The specifications and assumptions include: 1) All feed streams to all reactors are heated to 230 C. 2) The reactor temperature is kept around 250 C, which has been reported as the optimal temperature for high catalyst activity, thus a high conversion rate. 3) All CO2 is fed into the 1st reactor. 4) The flash drum works around 40 C to remove water drainage. 5) The feed H2 is from the electrolyzer working at 15 bar and 750 C, with a steam utilization factor of 50%. The feed H2/H2O mixture is cooled down to 230 C before entering the methanation. 6) The methanation system works under a pressure of 15 bar.

Two jacked reactors can ensure a product methane purity of 98%, while a third reactor does not help too much for gaining large improvement in methane purity. No gas recirculation is needed, given the specific design for the isothermal operation of the reactor. The conversion rates of two reactors are 96% and 91%, respectively. More importantly, the size of the jacked reactor is much small compared with the adiabatic options. However, still the size difference between the 1st and 2nd is quite large.

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