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Techno-economic barriers of an industrial-scale methanol CCU-plant



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ABSTRACT

Global anthropogenic CO₂ emissions are expected to peak to 40 Gt in 2020. If these emissions are not mitigated climate change and global warming will further aggregate. Meanwhile, demand for products and fuels produced from fossil raw materials are increasing. CO₂, however, can be considered as feedstock for certain materials and processes. If CO₂ is catalytically synthesised with H₂ it can form a variety of hydrocarbons, such as methane, methanol (MeOH), higher alcohols, and liquid fuels. In this paper, a simulation model of a MeOH plant using CO₂ and H₂ as feedstock was developed in Aspen Plus^M. This is the first plant studied at an industrial-scale comparable with fossil MeOH plant units. The plant produces 5 kt chemical-grade MeOH daily that can be used as raw material for the chemical industry or as a fuel. The kinetic model, considering both CO and CO₂ as the source of carbon, accomplished high overall CO₂ conversion rate and close to stoichiometric raw material utilisation. Under the current market conditions, the MeOH plant is not feasible even at this scale. The most significant cost parameter making the plant non-viable is attributed to the high cost of H₂ produced by water electrolysis. A series of sensitivity analyses revealed that co-selling of O₂ by-product from the electrolyser and lowering the H₂ cost price have a significant factor in achieving a more competitive levelised cost of MeOH. These economic results are analysed in-depth with previous studies to reveal the effect of different economic assumptions.

1. Introduction

Global CO₂ emissions associated with anthropogenic activities equalled more than 32 Gt in 2016 [1] and will reach 40 Gt by 2020 [2]. Multiple scenarios are discussing how to reach the goals of the Paris agreement of limiting the global average temperature rise below $1.5 \,^{\circ}$ C above pre-industrial levels. Carbon capture (CC), a process where the emitted CO₂ is instead captured, is amongst the several options that could lead to reduced CO₂ emissions [2]. The captured CO₂ can be handled in two means: either stored e.g. in deep geological formations called carbon capture and storage (CCS), or utilised as a raw material in the production of carbon-based fuels or chemicals called carbon capture and utilisation (CCU) [3]. Even though the processes are similar in their purpose, their impact is significantly different. CCU is a more complex mitigation tool and should be evaluated on the system level as it is affected by not only how CO₂ is captured but also how long it is stored in that certain product [4]. Therefore, it is recommended to consider CCS and CCU processes as complementary processes instead of competitive ones.

From the global anthropogenic CO_2 emissions less than 1% is currently utilised [5]. CO_2 utilisation routes can be mainly divided into four groups: direct utilisation, mineralisation, biological conversion, and chemical conversion [4]. CO_2 can be utilised directly in food and beverages, as a refrigerant or a solvent, and in enhanced oil recovery (EOR). Building materials, such as concrete and carbonate aggregates can be also produced from CO_2 in a process called mineralisation. Biological conversion processes include gas fermentation, algae cultivation and use in greenhouses. Products via chemical conversion include urea, polymers, fuels and chemicals. Production of urea corresponds to more than half of the consumed CO_2 , while the production of inorganic carbonates, food and beverages, and application in EOR cover the other half. The rest of the CCU processes are still emerging. It is

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Abbreviations: CAPEX, Capital expenses; CEPCI, Chemical Engineering Plant Cost Index; CC, Carbon capture; CCS, Carbon capture and storage; CCU, Carbon capture and utilisation; DME, Dimethyl ether; EBITDA, Earnings before interest, taxes, depreciation and amortization; EOR, Enhanced oil recovery; FCI, Fixed capital investment; FTS, Fischer-Tropsch synthesis; FG, Flue gas; HC, Hydrocarbon; HEN, Heat exchange network; LCOMeOH, Levelised cost of methanol; LHV, Lower heating value; MeOH, Methanol; MTA, Methanol-to-aromatics; MTG, Methanol-to-gasoline; MTO, Methanol-to-olefins; MTP, Methanol-to-propylene; OPEX, Operational expenses; PEC, Purchased equipment cost; PEM, Proton exchange membrane; RON, Research Octane Number; RWGS, Reverse water-gas shift; VB, Vanden Busche

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Fig. 1. Specific energy of several compounds based on higher heating value and the route from CO₂ to MeOH via H₂.

estimated that these technologies have the potential to mitigate at least 10% of the global CO₂ emissions both directly and indirectly by reducing the consumption of fossil fuels [5].

Amongst the CCU technologies, chemical conversion of CO_2 via catalytic hydrogenation into hydrocarbons (HCs) is gaining significant interest. CO_2 is an abundant molecule, however, a very stable one which requires large energy input, such as H_2 as a reagent, to be transformed (Fig. 1). Meanwhile, the increasing share of renewable energy in the electrical grid needs sustainable storage options in times of power overproduction [6]. H_2 can be easily produced via water electrolysis to balance the intermittency of renewable electricity system [7]. However, H_2 is not considered an optimal final storage medium due to its limitations in its physical properties, high reactivity, and its unfavourable storage, transportation, and utilisation conditions [8]. Yet, the combination of the two molecules, CO_2 and H_2 , produces a wide range of products that can offer a solution in the transition to a higher share of renewables in energy system [9].

Catalytic hydrogenation of CO_2 to HCs includes the synthesis of methane, methanol (MeOH, CH_3OH), higher alcohols, and liquid HCs [10], shown in Fig. 2. HCs, especially liquid HCs are still inevitable fuels for the nearby future due to their high energy density, and compatibility with the current fuel infrastructure [8]. Electrification of heavyweight road, sea and air transport and the energy-intensive industry is possible through these intermediaries at present [11]. Catalytic hydrogenation syntheses, as the name indicates, are carried out over different catalysts depending on the desired end-product. In most cases, there are multiple routes available to achieve the same product (Fig. 2). Methane can be produced either directly from CO_2 and H_2 , or via the reverse water-gas shift (RWGS) reaction first producing CO followed by hydrogenation. RWGS can be also the first step to produce different HCs such as kerosene or gasoline in the Fischer-Tropsch synthesis (FTS) process. HCs can be also produced through MeOH in methanol-to-olefins (MTO), methanol-to-propylene (MTP), methanolto-gasoline (MTG), and methanol-to-aromatics (MTA) processes, or directly over bi-functional catalysts [10].

Tremel et al. suggest [12] that out of the CO₂ hydrogenation pathways production of MeOH is the best option due to its technological maturity and compatibility with the current fuel infrastructure, production cost and public acceptance. MeOH is a versatile chemical compound that not only serves as a fuel, and hydrogen energy carrier, but it is also a base chemical for the chemical and petrochemical industry [8]. It has an energy density of 22.7 MJ/kg, approximately half of gasoline. It is a colourless, water-soluble liquid with a boiling point and freezing point at 64.6 °C and -97.6 °C respectively [13]. MeOH is highly toxic, but not carcinogenic as opposed to gasoline. MeOH is a favourable fuel in internal combustion engines [14]. It has Research Octane Number (RON) of 109 which means higher compression ratios and favourable combustion timings for high efficiency could be used [15]. The high heat of evaporation of MeOH, 1.17 MJ/kg [16] contributes to high RON too and also decreases charge temperatures. This increases charge densities and results in higher power output in the engine. The high heat of evaporation reduces combustion temperatures too. This is favourable for nitrogen oxides formation in combustion. Laminar flame speed of MeOH is higher than with gasoline [14]. The mass-based oxygen content of MeOH is 49.9% which contributes to soot-free combustion even with low air to fuel ratios [14].

MeOH is still mostly used in traditional processes in the chemical industry, such as the production of acetic acid and formaldehyde [17]. However, its global demand is increasing due to its role in the production of olefins, such as ethylene and propylene, the bases of the plastic industry. Through these processes, MeOH could play a significant role in the transformation of the plastic industry as well [18]. By 2020 the globally traded amount of MeOH is expected to reach 90 million tonnes [17]. Within the EU, MeOH is almost solely produced in Germany [19], but the overall production volumes are limited due to costly feedstock prices [20]. Therefore, EU countries are heavily dependent on imports [19].

Commercial MeOH is catalytically synthesised mostly from natural gas via an intermediary synthesis gas (syngas), a mixture of CO, H₂, and some CO₂ [8], [13]. MeOH synthesis from syngas follows Eqs. 13, where Eq. 2 is the endothermic RWGS reaction [21]. There is no consensus amongst researchers whether CO or CO₂ is the source of carbon in the synthesis, and the kinetics describing MeOH formation is still under discussion [22], [23]. MeOH production from CO₂ and H₂ occurs under similar process conditions and catalysts as its conventional synthesis [24]. However, as it can be seen from the stoichiometric balance Eqs. 1 and 3, MeOH synthesis from CO₂ has a much lower yield, as one-third of H₂ ends up as water [10].



Fig. 2. Pathways of catalytic conversion of CO₂ and H₂ to different hydrocarbons.



1 ossil-nee electricity

Fig. 3. Boundary conditions of the MeOH – CCU plant considered in this study, the blue part considered in process modelling, the yellow part considered in economic analysis.

$$CO + 2H_2 \leftrightarrow CH_3OH \qquad \Delta H_{300\,K} = -90.77 \frac{kJ}{mol}$$
 (1)

$$CO_2 + H_2 \leftrightarrow CO + H_2O \qquad \Delta H_{300\,K} = 41.21 \frac{kJ}{mol}$$
(2)

$$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O \qquad \Delta H_{300K} = -49.16 \frac{kJ}{mol}$$
(3)

Simulation of MeOH synthesis process from CO₂ and H₂ has been an emerging topic since the early 2000s following its experimental demonstration in Saito et al. [25]. Process simulations focus on technical feasibility often coupled with economic feasibility producing fuel-grade MeOH. Van-Dal and Bouallou [26] simulated a fuel-grade MeOH - CCU plant including the CC unit and water electrolyser. The utility impact of the CC unit on the coal power plant, where CO₂ originates, was reduced due to the steam supplied by the MeOH plant. Kiss [27] utilised wet H₂, a by-product from the chlor-alkali process, through a stripping unit. The stripping unit not only removed water from wet H₂ but led to complete recycling of CO2. The process eliminated the economic barrier of sourcing cheap H₂ for the MeOH synthesis while keeping the utility consumption minimal. Abdelaziz et al. [28] developed three processes of CO₂ hydrogenation to MeOH differing in flue gas (FG) treatment. The processes were compared in CO₂ emission levels, utility consumption and economic viability. Even though the highest conversion, MeOH production rate, and profit were of the CO₂ capture case, the water removal case was selected as the best performing case due to its significantly lower CO2 emission. The water removal process was improved with a heat integration design, which led to a significant reduction in utility consumption. Pérez-Fortes et al. [29] evaluated the environmental benefit and economic viability of a MeOH-CCU plant opposed to a conventional MeOH plant. They found that the CCU plant is not financially viable due to the expensive H₂; however, it can accomplish CO₂ emission reduction. Szima and Cormos [30] achieved a self-sufficient MeOH - CCU plant, excluding the water electrolyser unit, by the use of a gas turbine for purged streams and addition of organic Rankine cycles. The study found that the plant is still not profitable, as the production cost is double that of conventionally produced MeOH. Other studies [6,31-34] agree that while the process is technically feasible and contributes to CO2 emission reduction the financial unattractiveness withholds investments to such MeOH-CCU plants. Currently, there is only one commercial MeOH - CCU plant in operation located in Iceland, where the fossil-free electricity is cheaply available [13]. Majority of these studies focused on the whole plant setup with MeOH plant, CC and electrolyser unit or a mix of the possible setups, while not differentiating the economic scope from the technical one.

Moreover, justification and comparison of the economic viability study is often lacking.

In this paper, a MeOH – CCU plant producing 5 kt/d chemical-grade MeOH was developed in Aspen Plus[™] V8.8. According to the knowledge of the authors, this is the first time that the economic results of an industrial-scale MeOH-CCU plant have been published. This production capacity is in line with the output of the fossil natural gas-based ones [17]. The plant is studied from clearly separated technical and economic viability point of view. In this work, the technical part focuses on the MeOH-CCU plant without the CC and electrolyser units where the applied kinetic model, considering also dimethyl ether (DME) byproduct formation, and the design parameters are presented thoroughly making it accessible for reproduction. The developed synthesis setup and applied process conditions were optimised to achieve a lower feedstock consumption than earlier reported. The economic study investigates the viability of the plant under current market conditions by systematically analysing a series of sensitivity analyses to understand the barriers of viability. Moreover, this work summarises the economic data from previous works in a new visual approach and discusses the effect of these different economic assumptions.

2. Materials and methods

In the present paper, a MeOH plant was considered producing 5000 t chemical-grade MeOH daily from CO_2 and H_2 . The size of this plant is compatible with the operating units of the largest producer of fossil-based MeOH [17]. Pure CO_2 is assumed to be originating from industrial FG, while pure H_2 is produced by a typical proton exchange membrane (PEM) water electrolyser. The MeOH plant is evaluated from both technical and economic performance point of view, as presented in Fig. 3. Technical performance evaluation is based on process simulation solely focusing on the MeOH synthesis and distillation plant with the gas furnace (blue part of Fig. 3). The assumed CC plant and water electrolyser plant are not included in the process simulation; therefore, they are not part of the technical evaluation scope either.

In the economic analysis first, the viability of the plant is examined under the current market conditions. In this part, marked with yellow in Fig. 3, the water electrolyser was considered to be owned by the MeOH plant owners. This consideration portrays a more realistic plant setup due to the reported challenges of H₂ storage and transport [33]. To account for this ownership, the price of H₂ was adopted at a levelised cost from an industrial-scale electrolyser. Moreover, the possibility of selling the by-product O₂ from the electrolysis process was examined.

In this section, first, the process simulation of the MeOH plant is



Fig. 4. Process flowsheet of MeOH-CCU plant developed in Aspen Plus™.

described in detail. Especially the kinetic model characterising the catalyst in the reactor bed is presented, followed by the parameters of the reactor, and distillation unit. Finally, the heat integration with the combustion of the off-gas streams is presented. After the process simulation, the evaluation parameters are presented, starting with the parameters selected for the technical performance evaluation followed by the economic ones.

2.1. Process simulation of methanol synthesis and distillation unit

In this research, a MeOH-CCU plant producing 5 kt/day chemicalgrade MeOH was simulated by Aspen Plus™ V8.8, the process flowsheet is presented in Fig. 4. Pure CO₂ is fed at 2 bar and 18 °C from the CC unit and compressed in a four-stage compressor system (COMPR1-4) with intercooling (HX1-3) to 50 bar. Pure H₂ is fed at 50 bar and 50 °C from the electrolyser and is mixed with CO2 and the recycled gases (MIXER1). The makeup gas stream is then heated (HX4) to 230 °C and fed to an isothermal plug-flow reactor (REACTOR). The gases leaving the reactor are cooled down to 30 °C (HX5) and then separated (SEP1) to liquid raw MeOH and non-reacted gases. After purging (SPLITTER) 0.1 wt% of the nonreacted gases to prevent the accumulation of byproducts and non-reacted gases in the reactor, the rest is recycled to minimise the feedstock losses. The amount of purge was selected in a way that the hot utility demand is satisfied within the plant. Raw MeOH is expanded to 1 bar (SEP2) to further remove the non-reacted gases, specifically CO_2 , to reduce the distillation demand. Before the two-step distillation, raw MeOH is heated (HX6) to 87 °C. In the first distillation column (DIST) water is separated from MeOH and leaves at the bottom. MeOH enters the second column (RECT), where by-products and nonreacted gases are removed from product MeOH. The bottom of the second column is recycled to the first one due to containing a significant amount of MeOH beside the water. Condensed product MeOH leaves from the top of the second column at 60 °C and is further cooled down (HX7) to 30 °C for storage. The off-gas streams (PURGE, CO2RICH, and VAPOUR) are mixed (MIXER2) and used for hot FG generation as they contain H₂ and MeOH.

2.1.1. Kinetic model of methanol synthesis and reactor

The isothermal fixed bed reactor is packed with Cu/Zn/Al/Zr catalyst, which was specifically designed for MeOH synthesis via CO_2 hydrogenation [35]. The kinetic model used in this paper was developed by Graaf et al. [36] instead of the widely applied kinetic model developed by Vanden Bussche (VB) [37]. Graaf's kinetic model considers both CO_2 and CO as the carbon source for MeOH as opposed to VB's model considering only CO_2 . Beside the MeOH formation, the Graaf model also accounts for the RWGS reaction (Eq. 5). Graaf's kinetic model was chosen over VB's model due to the uncertainty of the carbon source in the MeOH synthesis [22]. Moreover, Graaf's model also predicts higher MeOH yield as compared to VB's according to Asif et al. [38]. The rate equations (Eqs. 4–6) described below correspond to the earlier introduced equilibrium reactions (Eqs. 1–3) accordingly [36]:

$$r_{CH3OH, CO, A}^{\prime} = \frac{k_A K_{CO} [f_{CO} f_{H_2}^{1.5} - f_{CH_3OH} / (f_{H_2}^{0.5} K_{P,A})]}{(1 + K_{CO} f_{CO} + K_{CO_2} f_{CO_2}) [f_{H_2}^{0.5} + (K_{H_2O} / K_{H_2}^{0.5}) f_{H_2O}]}$$
(4)

$$\dot{r}_{H2O,B} = \frac{k_B K_{CO_2} [f_{CO_2} f_{H_2} - f_{H_2O} f_{CO} / K_{P,B}]}{(1 + K_{CO} f_{CO} + K_{CO_2} f_{CO_2}) [f_{H_2}^{0.5} + (K_{H_2O} / K_{H_2}^{0.5}) f_{H_2O}]}$$
(5)

$$r_{CH30H, C02, C}^{'} = \frac{k_C K_{C02} [f_{C02} f_{H_2}^{1.5} - f_{CH_30H} f_{H_2O} / (f_{H_2}^{1.5} K_{P,C})]}{(1 + K_{C0} f_{C0} + K_{C02} f_{C02}) [f_{H_2}^{0.5} + (K_{H_2O} / K_{H_2}^{0.5}) f_{H_2O}]}$$
(6)

where r'_i is reaction rate for compound i, k_i is the reaction rate constant for reaction i, K_i is the adsorption equilibrium constant for compound i, f_i is the fugacity for compound i, and $K_{P,i}$ is the equilibrium constant of reaction i.

Aside from the main reactions (Eqs. 1–3) applied in literature [27], this model also considered the synthesis of the most important by-product. Formation of DME (Eq. 7) happens simultaneously to MeOH formation over the catalyst [22] according to the following reaction rate equation (Eq. 8) [39]:

$$2CH_3OH \leftrightarrow CH_3OCH_3 + H_2O \tag{7}$$

$$\dot{r}_{DME} = \frac{k_D K^2 _{CH_3 OH} \left[C^2 _{CH_3 OH} - (C_{H_2 O, DME} C_{DME}) / K_{P, DME} \right]}{(1 + 2^* \sqrt{K_{CH_3 OH} C_{CH_3 OH} K_{CO} f_{CO}} + K_{H_2 O, DME} C_{H_2 O, DME})^4}$$
(8)

where r'_{DME} is reaction rate for DME, k_D is the reaction rate constant, K_i is the adsorption equilibrium constant for compound i, C_i is the molarity for compound i, and $K_{P,DME}$ is the equilibrium constant.

The original Graaf model [36] is adjusted with equilibrium constants ($K_{P,A}$, $K_{P,B}$, $K_{P,C}$) from Lim et al. [40], and experimental data

Table 1

Parameter values for the kinetic model of methanol synthesis used in this work.

Parameter	Value	Unit	Reference
k_A	$4.0638 \times 10^{-6} \exp\left(\frac{-11695}{RT}\right)$	kmol/kg _{cat} •s•Pa	[35]
k_B	$9.0421 \times 10^8 \exp\left(\frac{-112860}{RT}\right)$	$kmol/kg_{cat} \cdot s \cdot Pa^{0.5}$	[35]
k _C	$1.5188 \times 10^{-33} \exp\left(\frac{-266010}{RT}\right)$	$kmol/kg_{cat}$ •s•Pa	[35]
k_D	$8.54 \times 10^{6} \exp\left(\frac{-123779}{RT}\right)$	$kmol/kg_{cat}$ •s•Pa	[41]
K _{CO}	$8.3965 \times 10^{-11} \exp\left(\frac{118270}{RT}\right)$	Pa^{-1}	[35]
K_{CO_2}	$1.7214 \times 10^{-10} \exp\left(\frac{81287}{RT}\right)$	Pa^{-1}	[35]
$K_{H_{\rm 2}O}/K_{H_{\rm 2}}^{0.5}$	$4.3676 \times 10^{-12} \exp\left(\frac{115080}{RT}\right)$	$Pa^{-0.5}$	[35]
K _{CH3OH}	$7.9 \times 10^{-4} \exp\left(\frac{70500}{RT}\right)$	m ³ /kmol	[39]
$K_{H_2O,DME}$	$8.4 \times 10^{-2} \exp\left(\frac{41100}{RT}\right)$	m ³ /kmol	[39]
$K_{P,A}$	$2.31 \times 10^{-23} \exp\left(\frac{98438}{BT}\right)$	Pa^{-2}	[40]
$K_{P,B}$	$2.81 \times 10^{-2} \exp\left(\frac{43939}{RT}\right)$	-	[40]
$K_{P,C}$	$6.50 \times 10^{-21} \exp\left(\frac{54499}{\text{BT}}\right)$	Pa^{-2}	[40]
$K_{P,DME}$	$1.06 \times 10^{-1} \exp\left(\frac{21858}{RT}\right)$		[42]

fitted by An et al. [35] over a Cu/Zn/Al/Zr catalyst. The detailed validation and description of how to implement the kinetic model to Aspen Plus[™] has been reported by Kiss et al. [27]. Table 1 provides a summary of the parameter values for the kinetic model used in this paper.

Sizing of the isothermal fixed-bed reactor was based on the design from Kiss et al. [27]. Pressure drop in the reactor was considered with the Ergun equation [26]. The characteristics of the reactor and catalyst applied in this paper can be found in Table 2.

2.1.2. Distillation unit of the methanol plant

The role of the distillation unit is to remove all the impurities, water and by-products from the raw MeOH stream up to the required purity. Here, by-products, except for DME, or impurities were not considered due to their low amount in the raw MeOH [24]. The distillation columns were designed to remove water and the unreacted gases leaving MeOH with at least 99.85 wt% purity. The design objectives for the distillation units were to 1) achieve chemical-grade MeOH, 2) minimise the losses of MeOH in the VAPOUR stream, and 3) keep the overall hot utility consumption of the unit under a certain limit. The distillation unit the design parameters, i.e. reflux ratio, boilup ratio, and distillate vapour fraction were tediously examined in a series of sensitivity analyses. The first column (DISTL) is responsible to remove the majority, more than 90 wt% of the water from raw MeOH, while in the second column (RECT) the non-reacted gases are removed. The detailed design parameters used in this paper can be found in Table 3.

2.1.3. Heat exchange network integration

Design and integration of the heat exchange network (HEN) was carried out with Aspen Energy Analyzer[™] V8.8. The software uses Pinch

Table 2

Design parameters of the Plug-flow reactor and the catalvst.

Parameter	Value
Number of tubes	4000
Length [m]	12
Diameter [m]	0.1
Catalyst density [kg/m ³]	1500
Bed voidage	0.68
Catalyst diameter [m]	0.006

 Table 3

 Design parameters of the two-step distillation columns.

Parameter	Column 1 (DISTL)	Column 2 (RECT)
Number of stages Feed stage Recycle stage Condenser type Reboiler type Reflux ratio (mole based) Boilup ratio (mole based) Pressure [bar] Distillate vapour fraction (mass	30 15 1 Partial-Vapor Kettle 1.1 0.6 1	30 15 - Partial-Vapor-Liquid Kettle 1.1 0.8 1 0.01
based)		

analysis [43] to minimise the energy utilisation of the plant. Cooling water at 18 °C was chosen as the cold utility, and the minimum temperature difference in all the heat exchangers was set to 10 °C. Hot FG was generated by the combustion of the off-gas streams (PURGE, CO2RICH, and VAPOUR on Fig. 4) to supply hot utility. The airflow was set with a design specification to result in FG O₂ content of 6 wt% on a dry basis. Finally, the FG is cooled down to 120 °C and is discarded.

2.2. Technical evaluation

The technical feasibility of the process is evaluated by the mass and energy balance of the MeOH plant after the implementation of HEN integration. Eq. 9 describes the energy efficiency of the MeOH-CCU plant:

$$\eta_{th} = \left(\frac{LHV_{MeOH} \times m_{MeOH}}{LHV_{H_2} \times m_{H_2} + W_{elec} + Q_{hol}}\right)$$
(9)

where η_{th} is the energy efficiency of the MeOH–CCU plant after heat integration, LHV_{MeOH} is lower heating value of MeOH, m_{MeOH} is mass of MeOH, LHV_{H2} is lower heating value of H₂, m_{H2} is mass of H₂, W_{elec} is electricity consumption, and Q_{hot} is hot utility consumption.

Conversion efficiencies of the feedstock are assessed by Eqs. 10–13. The overall conversion efficiencies are given for both CO₂ and H₂ in Eqs. 10 and 11 respectively. These conversions include the conversion of feedstock to any kind of compound, such as H₂ to water. Therefore, the actual conversion efficiencies of product recovery for both feedstocks are assessed by Eqs. 12 and 13:

$$CO_{2\,conv} = \left(\frac{CO_{2\,in} - CO_{2\,out}}{CO_{2\,in}}\right) \tag{10}$$

where $CO_{2 \text{ conv}}$ is the conversion of CO_{2} in the whole process, $CO_{2 \text{ in}}$ is the mass of CO_{2} entering the plant, and $CO_{2 \text{ out}}$ is the mass of CO_{2} exiting the plant in streams S17, METHANOL, BOTTOM on Fig. 4.

$$H_{2\,conv} = \left(\frac{H_{2\,in} - H_{2\,out}}{H_{2\,in}}\right) \tag{11}$$

where $H_{2 \text{ conv}}$ is the conversion of H_2 in the whole process, $H_{2 \text{ in}}$ is the mass of H_2 entering the plant, and $H_{2 \text{ out}}$ is the mass of H_2 exiting the plant in streams S17, METHANOL, BOTTOM on Fig. 4.

$$CO_{2 convMeOH} = \left(\frac{CO_{2 in} - CO_{2 out} - CO_{2 CO} - CO_{2 MeOHloss}}{CO_{2 in}}\right)$$
(12)

where $CO_{2convMeOH}$ is the conversion of CO_2 to the final MeOH product in the whole process, CO_{2CO} is the mass of CO_2 converted to CO in streams S17, METHANOL, BOTTOM on Fig. 4., and $CO_{2MeOHloss}$ is the mass of CO_2 converted to MeOH in streams S17 and BOTTOM on Fig. 4.

$$H_{2 convMeOH} = \left(\frac{H_{2 in} - H_{2 out} - H_{2 water} - H_{2 MeOHloss}}{H_{2 in}}\right)$$
(13)

where H_{2convMeOH} is the conversion rate of H₂ to product MeOH in

Table 4

Economic parameters.

Parameter	Value	Notes
Design and construction time	3 years	CAPEX is equally divided
Operational time	25 years	Only annual OPEX occurs
Yearly operating time	8760 hours	
Discount rate	7%	
Reference year	2018	All equipment price was calculated to this year
O ₂ production	7.95 kg/kg H ₂	Typical PEM electrolyser
Selling price of O ₂	100 €/t	[6]
Selling price of MeOH	320.5 €/t	10-year average [45]
Cost of CO ₂	25 €/t	[47]
Cost of H ₂	4100 €/t	[46]

the whole process, H_{2water} is the mass of H_2 converted to water in streams S17, METHANOL, BOTTOM on Fig. 4, and $H_{2MeOHloss}$ is the mass of H_2 converted to MeOH in streams S17 and BOTTOM on Fig. 4.

2.3. Economic evaluation

Economic feasibility of the MeOH - CCU plant is evaluated based on the EBITDA (Earnings before interest, taxes, depreciation and amortization) approach through calculating zero net present value (NPV) by the end of the lifetime. EBITDA is a useful metric for the evaluation of large investments as it neglects the financial items that can be country or company-specific [44]. If the calculated NPV at the end of the lifetime is below zero, it means that the plant is economically not feasible. The economic parameters and their values considered for the base case are presented in Table 4. Cost parameters were selected to best represent the current economic environment. Selling price of MeOH is the 10-year average of the posted European price provided by Methanex [45]. Cost of CO₂ was chosen as the cost of CO₂ emission allowance in the EU. This would mean that the CO₂ consumer pays to the emitter the same amount as the emitter pays for the emission. This is not an ideal solution, but as there is currently no market for such CO₂ emissions between emitter and consumer, we assumed this as the base case. The technologies and the costs associated with CC is outside of the scope of this study. As for the cost of H₂ the chosen value represents a typical industrial-scale PEM electrolyser operating full time [46].

Break-even values were calculated by linear programming in Excel. In the sensitivity analyses, the break-even values were determined when only one cost parameter was changed at a time. The option of O_2 by-product sales was regarded in each case to study its effect on the economic results. This was followed by estimating an optimum break-even case, for both O_2 selling options, where all three parameters were changed simultaneously. Finally, the results are compared to earlier findings based on the changes in the price of H₂.

2.3.1. Capital expenses of the methanol plant

CAPEX was estimated from the purchased-equipment cost (PEC), either directly from Aspen $Plus^{M}$ or based on reported literature. Neither the CC unit nor the water electrolyser unit was not considered in CAPEX calculations.

CAPEX was estimated based on a simplified relation between PEC and CAPEX given in Eq. 14:

$$CAPEX = 6.32 \times PEC \tag{14}$$

where PEC is the purchased-equipment cost. PEC only covers the equipment cost, while CAPEX includes costs for its installation, all construction work including piping, land, civil and architectural work, and costs for start-up, working capital, and research and development [48]. Most of the PEC was readily available from Aspen Plus[™]. PEC of separation vessels, compressors and distillation columns were provided by the in-built Aspen Process Economic Analyzer[™] V8.8, while PEC of the HEN was directly adopted from Aspen Energy Analyzer[™] V8.8 after

integration. The PEC provided by the different Aspen software was first adjusted from the original currency to euro, and then to the year 2018. However, the cost of the reactor and the gas furnace used for the combustion were based on the literature sources [49]. The equipment scaling followed Eq. 15 [48]:

$$EC_{model} = PEC_{lit} \left(\frac{X_{model}}{X_{lit}}\right)^{\alpha}$$
(15)

where PEC_{model} is the resized PEC used in this paper, PEC_{lit} is the original PEC found from literature, X_{model} is the capacity obtained from the process model used in this paper, X_{lit} is the design capacity in the literature, and α is the scaling exponent. The design variable for the reactor was the annual MeOH output, while for the gas furnace the heat duty. The scaling factor for both equipment was 0.6 based on Bejan [48].

All PECs were calculated for 2018. PECs from earlier than 2018 were adjusted by the annual Chemical Engineering Plant Cost Index (CEPCI) according to Eq. 16:

$$PEC_{2018} = PEC_0 \left(\frac{I_{2018}}{I_0}\right)$$
(16)

where PEC_{2018} is the PEC in 2018, PEC_0 is the original PEC, I_0 is the CEPCI for the original year and I_{2018} is the CEPCI in 2018 [50].

2.3.2. Operational expenses of the methanol plant

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OPEX took into account annual expenses occurring from salaries, insurance and taxes, and cost of raw materials and utilities. Annual OPEX is separated into fixed and variable OPEX that differ whether they are independent or dependent on the annual output of the plant. Some of the fixed OPEX is dependent on the fixed-capital investment (FCI) that can be calculated from CAPEX given in Eq. 17:

$$FCI = CAPEX/1.47 \tag{17}$$

where FCI is the fixed capital investment [48].

Fixed OPEX cover costs that are independent on the annual production of the plant, and would occur even if the plant is temporarily shut down, given in Eq. 18:

$$C_{fixed} = C_{DLC} \times n_w + C_{overhead} \times n_w + C_{AOM} + C_{insurance} + C_{local}$$
(18)

where $C_{\rm fixed}$ is the annual fixed O&M costs, $C_{\rm DLC}$ is the annual direct labour cost, $n_{\rm w}$ is the number of workers in the MeOH plant, $C_{\rm overhead}$ is the annual cost of overhead, $C_{\rm AOM}$ is the annual O&M costs, $C_{\rm insurance}$ is the annual insurance cost, and $C_{\rm local}$ is the annual local property taxes and fees.

The electrolyser unit is considered under variable OPEX for this study. Ideally, an electrolyser plant would be in very close proximity to the MeOH plant [33] or even belong to the same owner. Co-owning the MeOH plant and the electrolyser plant enables the possibility of co-selling the produced O_2 , which can be utilised in a nearby power plant for oxy-combustion, or sold to the chemical, or food industry [26], [51]. Variable OPEX include costs that depend on the annual production of the plant such as utility costs and feedstock costs according to Eq. 19:

$$C_{variable} = C_{CO_2} \times m_{CO_2} + C_{H_2} \times m_{H_2} + C_{elec} \times W_{elec} + C_{CW} + \frac{C_{cat} \times m_{cat}}{3}$$
(19)

where $C_{variable}$ is the annual variable O&M costs, C_{CO2} is the cost of CO₂, m_{CO2} is the mass of CO₂, C_{H2} is the cost of H₂, m_{H2} is mass of H₂, C_{elec} is the cost of electricity, W_{elec} is electricity consumption, C_{CW} is the cost of cooling water, C_{cat} is the cost of the catalyst, and m_{cat} is the mass of catalyst.

The detailed list of fixed and variable OPEX considered and their values are given in Table 5.

Table 5

Components and assumptions of OPEX.

FIXED OPEX	Value	Comment
Direct labour cost	60000 €/a/person	[52]
Admin and general overhead	18000 €/a/person	30% of direct labour cost
cost		[52]
Number of workers	56	[52]
Annual O&M	1.5% of FCI	[52]
Insurance	0.5% of FCI	[52]
Local property taxes and fees	0.5% of FCI	[52]
VARIABLE OPEX		
CO ₂	25 €/t	[47]
H ₂	4100 €/t	[46]
Electricity	30 €/MWh	[53]
Cooling water	1131214 €/year	Aspen Energy Analyzer™
		V8.8
Methanol synthesis catalyst	8.8 €/kg	Changed every 3 years [32]

3. Results and discussion

In this section, the results of the process simulation, technical performance and economic feasibility including sensitivity analyses are presented. The results are compared to similar simulations, followed by an in-depth discussion of the arising differences.

3.1. Technical results

The MeOH – CCU plant produces 5 kt chemical-grade MeOH daily. Fig. 5 shows the mass balance of the plant. The plant uses a stoichiometric mix of fresh CO₂ and H₂. The final products of the plant are mainly, 98.7 wt%, water in the BOTTOM stream (see Fig. 4 and Fig. 5) and MeOH in the METHANOL stream (see Fig. 4 and 5). Only a minor amount of unreacted feedstock can be found in the off-gas streams (stream S16 on Fig. 4) and some CO₂ in the METHANOL stream. As expected from Eq. 3, the formation of MeOH from CO₂, one-third of the H₂ is used for the formation of water. In the combustion of the off-gas streams, all the valuable H₂ and MeOH are utilised to produce only water vapour and CO₂. The formation of DME is negligible in the process, and less than 0.02 wt% can be found in the final product. The detailed summary of the mass balance for selected streams is shown in Table A1 in the Appendix.

Table 6 shows the main technical parameters of the MeOH–CCU plant. The results are compared to earlier presented works by Szima and Cormos [30] and Pérez-Fortes et al. [29] due to their analogy both in the developed process model and in its evaluation. All three plants operate with a stoichiometric mix of CO₂ and H₂. The plant developed in this paper uses the lowest amount of feedstock out of the three designs. This can be explained by the different kinetic models, kinetic parameter values, and operating conditions used in the reactor. Differences in the CO₂ conversion rate are also attributed to the earlier listed alterations. The complete conversion of H₂ both in this paper and in the work of Szima and Cormos [30] was accomplished by the combustion of H₂ in the energy recovery unit. For the present study, the

Table 6

Comparison with previously reported performance data of MeOH – CCU plants [29,30], *calculated based on LHV of H_2 .

	This paper	[30]	[29]	Unit
CO ₂ usage H ₂ usage Overall CO ₂ conversion Overall H ₂ conversion Methanol purity Hot utility Cooling utility Electricity usage CO ₂ emission	1.397 0.192 98.37 100 99.9 0 0.81 0.175 0.023	1.41 0.194 97.25 100 99.9 0 2.83 -0.06 0.04	1.46 0.199 93.85 n.a 99.9 0.436 0.862 0.169	kg/kg MeOH kg/kg MeOH % wt% kWh/kg MeOH kWh/kg MeOH kWh/kg MeOH kg/kg MeOH
Energy efficiency	84.38	53.93 (84.37)*	n.a	%

conversion efficiency of H_2 to MeOH product was found to be 65.8%, which is slightly lower than the expected conversion rate (66.67%) based on the equilibrium reactions (Eqs. 1–3). In the case of CO₂ conversion to MeOH product is the same rate as presented in Table 6 under overall CO₂ conversion as no CO is leaving the plant. The MeOH plant developed by Szima and Cormos [30] also generates supplementary electricity, the reason behind the negative electricity usage. This option was not considered for the plant presented in the current paper. The reported net energy efficiency of Szima and Cormos [30] are lower as it was based on the electricity needed for H_2 production, while this work is based on LHV of H_2 . If their results are calculated the same way the energy efficiency of their model is the same than the efficiency of the plant presented in this work, reaching 84.37%.

The overall CO₂ conversion was 98.4% which is in good comparison with other simulations presented in Table 7. This paper is based on the work of Kiss et al. [27] and shows an improvement of the reported conversion rate for the dry hydrogen process without the stripper unit. The other presented studies are also connected, the more recent designs showing an improvement. The process models of Pérez-Fortes et al. [29] and Abdelaziz et al. [28] were based on the VB kinetic model [37] and process flowsheet developed by Van-Dal and Bouallou [26]. Meanwhile, the process model of Szima and Cormos [30] is also based on the work of Van-Dal and Bouallou [26], however, the kinetic model was based on Graaf's model [36]. The improvements within the models were achieved by process flowsheet and condition optimisation.

3.1.1. Integration of the heat exchange network of the methanol plant

The Aspen Plus model showed that the MeOH−CCU plant required 671 MW cooling load and 502 MW heating load. This includes the cooling demand for both the hot FG stream (FLUEGAS) through HX8 and the reactor. The hot and cold streams of the MeOH plant and their characteristics are shown in Table A2. Pinch analysis was carried out in Aspen Energy Analyzer[™] V8.8, as described earlier, for the integration of the HEN. Fig. 6 shows the Grand Composite Curve which illustrates the availability of heat integration within the plant. The Pinch point is located at 70.7 °C, as shown in Fig. 6, above which hot utility is needed, while below cooling water is consumed. It is visible that heat integration within the plant is possible, as there are enough hot streams within



Fig. 5. Mass balance of the MeOH plant including combustion of off-gas streams (FG = flue gas).

Table 7

Comparison of c	overall CO_2 co	nversion of sil	milar MeOH plan	t simulations.
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Fig. 6. Grand Composite Curve of the MeOH plant (temperature including the 10 °C temperature difference used in the integration).

the plant to supply the needed hot utility for the cold streams. This means that all hot utility could be covered from within the plant. However, there is still a significant amount of cold utility needed to be supplied from outside of the plant.

After the integration of the HEN, only cooling water needs to be supplied from outside of the plant. The minimum cold utility of the plant is 168.8 MW. The detailed parameters of the integrated HEN can be found in Table A3 in the Appendix.

3.1.2. Availability of feedstock and resources

Production of 5000 t methanol from CO2 and H2 via water electrolysis requires an exceptional amount of these resources. The plant consumes 6984 t CO2 and 960 t H2 daily. In this paper, the H2 generation was assumed via electrolysis from renewable electricity, and CO₂ originating from industrial FG. To produce the needed amount of H₂ feed it needs 48 GW h from renewable electricity [54]. On an annual level, this would account for 1.7% of the renewable electricity produced in the EU in 2017 [55]. Currently, there is no single wind farm, offshore or onshore [56], that would reach the required installed capacity of 3.7 GW [57]. Similarly, the same is true for solar photovoltaic farms located in the EU [58]. However, it is projected that by 2030 installed capacity of wind power and photovoltaic will reach 327 GW and 270 GW respectively [59]. By 2040 offshore wind energy will provide the largest share of electricity production [57]. Moreover, it is proposed that several of the offshore wind farms will be solely dedicated to producing green H₂ as this would lead to significant cost advantages as opposed to direct grid-connected generation [57].

 CO_2 can be found abundantly in the air, however, due to its low concentration, in this paper industrial sources were considered for feedstock. Supplying the necessary annual amount is feasible with CC in industrial zones in million tonnes range annually [60]. Large-scale, high concentration point sources include emissions from the steel and iron industry, cement production plants, refineries, and above all fossilfuelled power plants [61]. Captured CO_2 from the different source points can be connected through pipelines creating so-called CO_2 hubs [62], [63]. Therefore, the location selection of a MeOH – CCU plant is highly influenced by the nearby availability of both feedstocks.



Fig. 7. Breakdown of purchased equipment cost of 5 kt/d MeOH plant.

3.2. Economic results

The economic viability of the designed MeOH – CCU plant is evaluated by NPV calculation for the considered lifetime of the plant. CAPEX was estimated from PEC and was divided equally for the 3 years of construction time. Fig. 7 shows the distribution of the PEC for the main equipment considered in the plant. The costliest equipment in the MeOH plant is the HEN accounting to more than one-third of the PEC closely followed by the compressors. Total PEC equals to 60.5 million ϵ , while total CAPEX is slightly above 382 million ϵ . Detailed results of PEC can be found in Table A4 in the Appendix (Fig. 8).

The economic feasibility of the designed MeOH plant was investigated under the current market conditions. From the annual OPEX, the most significant cost parameters are the feedstock costs corresponding to more than 98%. Out of the two feedstocks, H₂ contributes considerably more to the annual OPEX even though its much lower consumption. The annual cost for H₂ covers more than 94% of the OPEX, while annual cost for CO₂ equals to 4%. The total annual OPEX is above 1500 million \in , while the annual income from MeOH sales is below 600 million \in . If the selling of O₂ is considered, it generates additional income in the amount of 278 million \in ; however, this would still not be enough to break even. Therefore, under these market conditions, the developed plant is not feasible and would never reach a break-even point.

3.2.1. Sensitivity analysis

Economic variables affecting the viability most dominantly were investigated in a series of sensitivity analyses to reach the break-even point. Effect of changes in the cost of H₂, cost of CO₂, selling price of MeOH were the studied parameters either when the co-selling option of O₂ by-product from the electrolyser was considered or omitted. Table 8 shows the break-even values for the evaluated parameters. MeOH selling price must be more than twice the average market price for both assessed options. This price is only 3% lower than the one reported by Pérez-Fortes et al. [29] for the option of O₂ selling. However, the feedstock costs in this paper are substantially higher, for H₂ 4100 €/t vs. $3090 \notin/t$, and $CO_2 25 \notin/t$ vs. $0 \notin/t$. As H_2 contributes the most to the OPEX a large drop in its cost is necessary to reach the break-even point. As shown in Table 8 it has to be almost 50% lower than the current market price to break even. For the cost of CO₂, negative break-even values were allowed meaning that the owner of the MeOH-CCU plant would receive payment to utilise the emission.

Comparing the options of O2 co-sale, when O2 is sold the feedstock costs become higher as compared to the option when O2 is not sold. This happens since the plant owner can afford higher expenses due to the additional income from O2 sales. This is more visible from Fig. 8.



Fig. 8. Sensitivity analysis of MeOH price and H₂ cost on the NPV as incremental changes in the base values, a) when O₂ is not sold, b) when O₂ is sold.

 Table 8
 Base case and break-even values of the studied economic parameters.

	Base case values [€/t]	Break-even value [€/t]		
O ₂ selling	No	No	Yes	
Selling price of MeOH	320.5	852.4	699.9	
Cost of H ₂	4100	1326.7	2121.7	
Cost of CO ₂	25	-356.1	-246.8	

Fig. 8 shows in more detail how the NPV is affected when the selling price of MeOH and the cost of H2 changes. Comparing the break-even values depending on whether O2 is not sold (Fig. 8a) to when it is sold (Fig. 8b) it is evident that the income for the sale of O2 by-product would create a substantial advantage.

Reaching the break-even values for either of the O_2 selling options is not possible in the near future; however, a combination of less radical changes in all three parameters at the same time would be possible. When break-even points are optimised so that all the parameters are varied together, the results show more realistic values, see Table 9. The selling price of MeOH for both options is below the 10-year maximum selling price from Methanex which is 450 ϵ /t [45], while the cost of CO₂ only needs to decrease by a maximum of 2.4% of the base case. The most significant change would be still necessary for the cost of H₂; however, it is less drastic compared to single parameter variation, requiring a reduction by at least 42%.

3.2.2. Economic discussion

In this section, the economic results from this study are compared to previous studies based on H_2 cost and scale as presented in Figs. 9 and 10 respectively. Fig. 9 confirms that the cost of H_2 has a substantial impact on the LCOMeOH; however, it is also clear that it is not the only influencing factor. Beyond the inevitable differences in the economic assumptions such as discount rate, feedstock prices other than H_2 , and operating hours, several significant parameters result in a considerable shift in the LCOMeOH. One of them is the annual output of the plant. In Fig. 9, when compared to other economic feasibility studies, the result of this paper is slightly outside of the boundaries of earlier published works [12,29–31,33,38]. Compared to the other studies this paper considered the highest H_2 cost; however, the final LCOMeOH is still

 Table 9

 Break-even values when the studied economic parameters are varied together.

	Break-even value [€/t]		
O ₂ selling	No	Yes	
Selling price of MeOH	396	374.5	
Cost of H ₂	1726	2407	
Cost of CO ₂	24.4	24.5	

significantly below the earlier reported ones. This can be seen especially when compared to the break-even points from Pérez-Fortes et al. [29]. This result is due to the lower feedstock usage, but mostly to the significantly larger annual output capacity of the developed MeOH plant. Regarding the results of Kourkoumpas et al. [31], their reported LCOMeOH is lower due to the low H₂ cost. In their report, H₂ was produced only in times when the electricity cost was low, which resulted in a significantly lower H₂ cost than in the other literature.

There can be even further differences between two seemingly similar studies such as in the findings of Pérez-Fortes et al. [29] versus Szima and Cormos [30]. As Fig. 10 shows, the annual output is more than fourfold in the earlier one, while the break-even value for the selling price of MeOH is quite close to each other. This is due to how the boundary of the plants was defined. While Pérez-Fortes et al. [29] defined the economic boundaries solely for the synthesis and distillation unit, Szima and Cormos [30] also included cost calculations for the water electrolyser plant.

Minor influences can be attributed to the applied kinetic model and process conditions in the plant, which affects the consumption of raw materials. Moreover, the design of an integrated HEN would lead to decreased consumption of utilities also diminishing the final LCOMeOH.

Based on Fig. 9 and 10 it is apparent that comparing economic feasibility studies based on a single parameter is not justified. Therefore, it is usually not straightforward to interpret and compare economic studies. Not only economic parameters should be reported correctly, but also system boundaries and technical parameters. However, this becomes difficult when some of the main parameters are not reported in the studies.

4. Conclusion

Carbon capture and utilisation processes will play an important part in CO₂ mitigation by capturing the emitted CO₂ and storing it in products that otherwise would be made from fossil fuels. CO₂ can be catalytically converted in the presence of H₂ to methane and liquid hydrocarbons. However, these processes can only be beneficial in CO₂ mitigation if H₂ arrives from non-fossil sources. Amongst the several chemical compounds that can be synthesised from CO₂ and H₂, methanol seems to be an attractive option due to its versatile application, and exceptional physical and chemical characteristics. MeOH is not only a fuel, but a base chemical for the chemical industry, and nowadays for the petrochemical industry as well.

In this paper, a MeOH – CCU plant, comparable in size to fossil natural gas-based MeOH plant units was developed in Aspen Plus[™] to investigate its technical and economic viability. The plant produces from pure CO_2 and $H_2 5$ kt chemical-grade MeOH daily that can be used either as fuel or as raw material for the chemical industry. With the integration of the heat exchange network, the developed plant operates without external hot utility, and the final cold utility consumption was



Fig. 9. The impact of hydrogen cost on the LCOMeOH compared to the 5 kt/d MeOH plant of this study with co-selling of O₂ [12,29,31,33,38].



Fig. 10. The impact of annual MeOH output on the LCOMeOH compared to the 5 kt/d MeOH plant of this study with co-selling of O₂ [12,29,31,33,38,64].

also reduced. The MeOH-CCU plant is technically feasible and can operate under similar operating conditions and equipment than the currently existing natural gas-based MeOH plants. The applied process conditions achieved close to stoichiometric feedstock consumption at 1397 kg CO₂ and 192 kg H₂ to produce 1 t of MeOH. Despite the reduced raw material use, producing CO2-based MeOH under the current market conditions is non-viable. The feasibility of the MeOH-CCU plant is highly dependent on the cost of feedstock and the price of final products. Considering the co-selling possibility of O2 by-product could significantly decrease the final levelised cost of MeOH. Break-even of the plant is possible if the H₂ production costs are halved to 2100 \in /t, or CO_2 price becomes negative, meaning that the CO_2 consumer is rewarded to utilise the captured CO₂. The developed industrial-scale MeOH-CCU consumes 7000 t of CO2 and 960 t H2 daily. If H2 is produced via water electrolysis electricity cost and availability play an important role in achieving competitiveness. Therefore, MeOH-CCU plants with water electrolyser unit should not only be in industrial regions with high penetration of fossil-free electricity but also where this electricity is cheaply available. An industrial-scale MeOH-CCU plant situated in an industrial harbour, where electricity from offshore wind and CO₂ from the industrial emissions are available, could compete with the current fossil MeOH market prices in the future.

Several research groups have proposed different approaches to estimate LCOMeOH, all of them agree that the cost of H_2 is the bottleneck of this process. The question is how this high H_2 cost could be offset by incentives for the utilisation, or by penalisation for the emission of fossil CO₂ to support power-to-X technologies. Moreover, a distinct separation from fossil-based MeOH, and the creation of a market for bio- and renewable MeOH and its derivates could increase the competitiveness of the CO_2 hydrogenation process.

CRediT authorship contribution statement

Judit Nyári: Conceptualization, Methodology, Software, Validation, Visualization, Writing - original draft. Mohamed Magdeldin: Conceptualization, Supervision, Writing - original draft. Martti Larmi: Writing - review & editing, Supervision. Mika Järvinen: Supervision, Writing - review & editing. Annukka Santasalo-Aarnio: Conceptualization, Writing - review & editing, Funding acquisition.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A

Table A1

Detailed mass balance of selected streams of the developed MeOH plant.

	BOTTOM	CO2FEED	FEED	FLUEGAS	H2FEED	METHANOL	PRODUCT
Temperature [°C]	102.539	18	230	1624.077	50	30	230
Pressure [bar]	1	2	50	1	50	1	49.66581
Vapor fraction	0	1	1	1	1	0	1
Total flow [kmol/hr]	6568.28	6610.977	1.64E + 05	1280.478	19832.93	6507.575	1.51E + 05
Total flow [kg/hr]	1.18E + 05	2.91E + 05	9.17E+05	35191.58	39980.81	2.09E + 05	9.17E + 05
Total flow [l/min]	2153.957	1.32E + 06	2.33E + 06	3.37E+06	1.83E + 05	4416.829	2.15E + 06
Mass flow [kg/hr]							
WATER	1.18E + 05	0	1240.172	4651.949	0	0.0204476	1.20E + 05
MEOH	8.98E-07	0	12009.57	0	0	2.08E + 05	2.22E + 05
H ₂	2.99E-97	0	3.01E + 05	0	39980.81	1.26E-04	2.61E + 05
CO ₂	2.70E-64	2.91E + 05	5.72E + 05	4512.037	0	216.2665	2.83E + 05
CO	3.89E-100	0	27019.01	0	0	1.17E-04	27047.39
O ₂	0	0	0	2109.181	0	0	0
N ₂	0	0	0	23918.41	0	0	0
DME	1.43E-66	0	4313.497	0	0	39.82348	4398.256
Mass fraction	1	0	1 055 00	0 1001000	0	0.005.00	0 10000 4
WEOL	1 7 FOE 10	0	1.35E-03	0.1321893	0	9.80E-08	0.130394
меон	7.39E-12 2.52E 102	0	0.0130932	0	1	0.9987722 6.05E.10	0.242362
11 ₂ CO-	2.33E-102 2.28E-69	1	0.5279958	0 1282135	0	1.04F-03	0.2040917
CO2	3.28E-105	0	0.0203530	0.1202133	0	5 59F-10	0.000244
0.	0	0	0	0 0599342	0	0	0
N ₂	0	0	0	0.679663	0	0	0
DME	1.21E-71	0	4.70E-03	0	0	1.91E-04	4.80E-03
Mole fraction							
WATER	1	0	4.21E-04	0.2016609	0	1.74E-07	0.0440834
MEOH	4.27E-12	0	2.29E-03	0	0	0.9991119	0.046072
H ₂	2.26E-101	0	0.9114741	0	1	9.62E-09	0.8601393
CO_2	9.34E-70	1	0.0793517	0.0800665	0	7.55E-04	0.0426583
CO	2.11E-105	0	5.89E-03	0	0	6.40E-10	6.41E-03
0 ₂	0	0	0	0.0514763	0	0	0
N ₂	0	0	0	0.6667962	0	0	0
DME	4.73E-72	0	5.72E-04	0	0	1.33E-04	6.34E-04
	RAWMEOH	RECYCLE	S10	S11	S13	S14	S16
Temperature [°C]	RAWMEOH 29.85033	RECYCLE 29.85033	S10 42.63616	S11 30.84703	S13 66.37457	S14 66.29512	S16 40.95338
Temperature [°C] Pressure [bar]	RAWMEOH 29.85033 45	RECYCLE 29.85033 45	\$10 42.63616 50	S11 30.84703 1	S13 66.37457 1	S14 66.29512 1	S16 40.95338 1
Temperature [°C] Pressure [bar] Vapor fraction	RAWMEOH 29.85033 45 0	RECYCLE 29.85033 45 1	\$10 42.63616 50 1	\$11 30.84703 1 0	\$13 66.37457 1 1	\$14 66.29512 1 0	S16 40.95338 1 1
Temperature [°C] Pressure [bar] Vapor fraction Total flow [kmol/hr]	RAWMEOH 29.85033 45 0 13,173.87	RECYCLE 29.85033 45 1 1.37E + 05	S10 42.63616 50 1 1.37E+05	\$11 30.84703 1 0 13141.6	\$13 66.37457 1 1 10586.63	\$14 66.29512 1 0 4013.304	S16 40.95338 1 1 235.4029
Temperature [°C] Pressure [bar] Vapor fraction Total flow [kmol/hr] Total flow [kg/hr]	RAWMEOH 29.85033 45 0 13,173.87 3.30E + 05	RECYCLE 29.85033 45 1 1.37E + 05 5.87E + 05	S10 42.63616 50 1 1.37E + 05 5.86E + 05	S11 30.84703 1 0 13141.6 3.29E + 05	\$13 66.37457 1 1 10586.63 3.33E+05	\$14 66.29512 1 0 4013.304 1.22E+05	S16 40.95338 1 1 235.4029 4010.582
Temperature [°C] Pressure [bar] Vapor fraction Total flow [kmol/hr] Total flow [kg/hr] Total flow [l/min] Mass flow [kg/hr]	RAWMEOH 29.85033 45 0 13,173.87 3.30E + 05 6523.999	RECYCLE 29.85033 45 1 1.37E + 05 5.87E + 05 1.31E + 06	S10 42.63616 50 1 1.37E + 05 5.86E + 05 1.23E + 06	S11 30.84703 1 0 13141.6 3.29E+05 6510.464	S13 66.37457 1 1 10586.63 3.33E+05 4.90E+06	S14 66.29512 1 0 4013.304 1.22E+05 2713.799	S16 40.95338 1 1 235.4029 4010.582 1.02E+05
Temperature [°C] Pressure [bar] Vapor fraction Total flow [kmol/hr] Total flow [kg/hr] Total flow [l/min] Mass flow [kg/hr] WATER	RAWMEOH 29.85033 45 0 13,173.87 3.30E + 05 6523.999 1.18E + 05	RECYCLE 29.85033 45 1 1.37E + 05 5.87E + 05 1.31E + 06 1241.415	S10 42.63616 50 1 1.37E+05 5.86E+05 1.23E+06 1240.172	S11 30.84703 1 0 13141.6 3.29E + 05 6510.464 1.18E + 05	S13 66.37457 1 1 10586.63 3.33E+05 4.90E+06 8070.958	\$14 66.29512 1 0 4013.304 1.22E + 05 2713.799 8070.936	S16 40.95338 1 235.4029 4010.582 1.02E+05 14.12141
Temperature [°C] Pressure [bar] Vapor fraction Total flow [kmol/hr] Total flow [kg/hr] Total flow [kg/hr] Mass flow [kg/hr] WATER MEOH	RAWMEOH 29.85033 45 0 13,173.87 3.30E + 05 6523.999 1.18E + 05 2.10E + 05	RECYCLE 29.85033 45 1 1.37E + 05 5.87E + 05 1.31E + 06 1241.415 12021.61	S10 42.63616 50 1 1.37E+05 5.86E+05 1.23E+06 1240.172 12009.57	S11 30.84703 1 0 13141.6 3.29E + 05 6510.464 1.18E + 05 2.10E + 05	\$13 66.37457 1 1 10586.63 3.33E+05 4.90E+06 8070.958 3.24E+05	\$14 66.29512 1 0 4013.304 1.22E+05 2713.799 8070.936 1.14E+05	S16 40.95338 1 1 235.4029 4010.582 1.02E+05 14.12141 1945.665
Temperature [°C] Pressure [bar] Vapor fraction Total flow [kmol/hr] Total flow [kg/hr] Total flow [l/min] Mass flow [kg/hr] WATER MEOH H ₂	RAWMEOH 29.85033 45 0 13,173.87 3.30E + 05 6523.999 1.18E + 05 2.10E + 05 7.171677	RECYCLE 29.85033 45 1 1.37E + 05 5.87E + 05 1.31E + 06 1241.415 12021.61 2.61E + 05	S10 42.63616 50 1 1.37E + 05 5.86E + 05 1.23E + 06 1240.172 12009.57 2.61E + 05	S11 30.84703 1 0 13141.6 3.29E + 05 6510.464 1.18E + 05 2.10E + 05 0.0192521	\$13 66.37457 1 1 10586.63 3.33E+05 4.90E+06 8070.958 3.24E+05 0.0192521	\$14 66.29512 1 0 4013.304 1.22E+05 2713.799 8070.936 1.14E+05 3.98E-11	S16 40.95338 1 1 235.4029 4010.582 1.02E+05 14.12141 1945.665 268.2537
Temperature [°C] Pressure [bar] Vapor fraction Total flow [kmol/hr] Total flow [kg/hr] Total flow [l/min] Mass flow [kg/hr] WATER MEOH H ₂ CO ₂	RAWMEOH 29.85033 45 0 13,173.87 3.30E + 05 6523.999 1.18E + 05 2.10E + 05 7.171677 1644.426	RECYCLE 29.85033 45 1 1.37E + 05 5.87E + 05 1.31E + 06 1241.415 12021.61 2.61E + 05 2.81E + 05	S10 42.63616 50 1 1.37E+05 5.86E+05 1.23E+06 1240.172 12009.57 2.61E+05 2.81E+05	S11 30.84703 1 0 13141.6 3.29E + 05 6510.464 1.18E + 05 2.10E + 05 0.0192521 607.066	\$13 66.37457 1 1 10586.63 3.33E+05 4.90E+06 8070.958 3.24E+05 0.0192521 607.0734	\$14 66.29512 1 0 4013.304 1.22E+05 2713.799 8070.936 1.14E+05 3.98E-11 7.39E-03	S16 40.95338 1 1 235.4029 4010.582 1.02E+05 14.12141 1945.665 268.2537 1709.204
Temperature [°C] Pressure [bar] Vapor fraction Total flow [kmol/hr] Total flow [kg/hr] Total flow [l/min] Mass flow [kg/hr] WATER MEOH H ₂ CO ₂ CO	RAWMEOH 29.85033 45 0 13,173.87 3.30E + 05 6523.999 1.18E + 05 2.10E + 05 7.171677 1644.426 1.386823	RECYCLE 29.85033 45 1 1.37E+05 5.87E+05 1.31E+06 1241.415 12021.61 2.61E+05 2.81E+05 2.7046	S10 42.63616 50 1 1.37E + 05 5.86E + 05 1.23E + 06 1240.172 12009.57 2.61E + 05 2.81E + 05 2.81E + 05 27019.01	S11 30.84703 1 0 13141.6 3.29E + 05 6510.464 1.18E + 05 2.10E + 05 0.0192521 607.066 7.02E-03	S13 66.37457 1 1 10586.63 3.33E+05 4.90E+06 8070.958 3.24E+05 0.0192521 607.0734 7.02E-03	S14 66.29512 1 0 4013.304 1.22E+05 2713.799 8070.936 1.14E+05 3.98E-11 7.39E-03 8.35E-11	\$16 40.95338 1 235.4029 4010.582 1.02E+05 14.12141 1945.665 268.2537 1709.204 28.43271
Temperature [°C] Pressure [bar] Vapor fraction Total flow [kmol/hr] Total flow [kg/hr] Mass flow [kg/hr] WATER MEOH H ₂ CO ₂ CO O ₂	RAWMEOH 29.85033 45 0 13,173.87 3.30E + 05 6523.999 1.18E + 05 2.10E + 05 7.171677 1644.426 1.386823 0	RECYCLE 29.85033 45 1 1.37E+05 5.87E+05 1.31E+06 1241.415 12021.61 2.61E+05 2.81E+05 2.7046 0	S10 42.63616 50 1 1.37E + 05 5.86E + 05 1.23E + 06 1240.172 12009.57 2.61E + 05 2.81E + 05 2.7019.01 0	S11 30.84703 1 0 13141.6 3.29E + 05 6510.464 1.18E + 05 2.10E + 05 0.0192521 607.066 7.02E-03 0	S13 66.37457 1 10586.63 3.33E+05 4.90E+06 8070.958 3.24E+05 0.0192521 607.0734 7.02E-03 0	S14 66.29512 1 0 4013.304 1.22E + 05 2713.799 8070.936 1.14E + 05 3.98E-11 7.39E-03 8.35E-11 0	S16 40.95338 1 235.4029 4010.582 1.02E+05 14.12141 1945.665 268.2537 1709.204 28.43271 0
Temperature [°C] Pressure [bar] Vapor fraction Total flow [kmol/hr] Total flow [kg/hr] Total flow [l/min] Mass flow [kg/hr] WATER MEOH H ₂ CO ₂ CO O ₂ N ₂	RAWMEOH 29.85033 45 0 13,173.87 3.30E + 05 6523.999 1.18E + 05 2.10E + 05 7.171677 1644.426 1.386823 0 0	RECYCLE 29.85033 45 1 1.37E + 05 5.87E + 05 1.31E + 06 1241.415 12021.61 2.61E + 05 2.81E + 05 2.81E + 05 2.7046 0 0	S10 42.63616 50 1 1.37E + 05 5.86E + 05 1.23E + 06 1240.172 12009.57 2.61E + 05 2.81E + 05 2.7019.01 0 0	S11 30.84703 1 0 13141.6 3.29E + 05 6510.464 1.18E + 05 2.10E + 05 0.0192521 607.066 7.02E-03 0 0	S13 66.37457 1 10586.63 3.33E + 05 4.90E + 06 8070.958 3.24E + 05 0.0192521 607.0734 7.02E-03 0	S14 66.29512 1 0 4013.304 1.22E + 05 2713.799 8070.936 1.14E + 05 3.98E-11 7.39E-03 8.35E-11 0 0	S16 40.95338 1 235.4029 4010.582 1.02E+05 14.12141 1945.665 268.2537 1709.204 28.43271 0
Temperature [°C] Pressure [bar] Vapor fraction Total flow [kmol/hr] Total flow [kg/hr] Total flow [l/min] Mass flow [kg/hr] WATER MEOH H ₂ CO ₂ CO O ₂ N ₂ DME	RAWMEOH 29.85033 45 0 13,173.87 3.30E+05 6523.999 1.18E+05 2.10E+05 7.171677 1644.426 1.386823 0 0 80.41048	RECYCLE 29.85033 45 1 1.37E + 05 5.87E + 05 1.31E + 06 1241.415 12021.61 2.61E + 05 2.81E + 05 2.81E + 05 2.7046 0 0 4317.845	S10 42.63616 50 1 1.37E+05 5.86E+05 1.23E+06 1240.172 12009.57 2.61E+05 2.81E+05 27019.01 0 0 4313.497	S11 30.84703 1 0 13141.6 3.29E+05 6510.464 1.18E+05 2.10E+05 0.0192521 607.066 7.02E-03 0 52.71877	S13 66.37457 1 10586.63 3.33E + 05 4.90E + 06 8070.958 3.24E + 05 0.0192521 607.0734 7.02E-03 0 52.73549	S14 66.29512 1 0 4013.304 1.22E + 05 2713.799 8070.936 1.14E + 05 3.98E-11 7.39E-03 8.35E-11 0 0 0.0167132	S16 40.95338 1 235.4029 4010.582 1.02E+05 14.12141 1945.665 268.2537 1709.204 28.43271 0 44.90484
Temperature [°C] Pressure [bar] Vapor fraction Total flow [kmol/hr] Total flow [kg/hr] Total flow [kg/hr] Mass flow [kg/hr] WATER MEOH H ₂ CO ₂ CO O ₂ N ₂ DME Mass fraction	RAWMEOH 29.85033 45 0 13,173.87 3.30E+05 6523.999 1.18E+05 2.10E+05 7.171677 1644.426 1.386823 0 0 80.41048	RECYCLE 29.85033 45 1 1.37E + 05 5.87E + 05 1.31E + 06 1241.415 12021.61 2.61E + 05 2.81E + 05 27046 0 0 4317.845	S10 42.63616 50 1 1.37E + 05 5.86E + 05 1.23E + 06 1240.172 12009.57 2.61E + 05 2.81E + 05 2.81E + 05 27019.01 0 0 4313.497	S11 30.84703 1 0 13141.6 3.29E+05 6510.464 1.18E+05 2.10E+05 0.0192521 607.066 7.02E-03 0 0 52.71877	S13 66.37457 1 10586.63 3.33E + 05 4.90E + 06 8070.958 3.24E + 05 0.0192521 607.0734 7.02E-03 0 52.73549	S14 66.29512 1 0 4013.304 1.22E+05 2713.799 8070.936 1.14E+05 3.98E-11 7.39E-03 8.35E-11 0 0.0167132	S16 40.95338 1 1 235.4029 4010.582 1.02E+05 14.12141 1945.665 268.2537 1709.204 28.43271 0 0 44.90484
Temperature [°C] Pressure [bar] Vapor fraction Total flow [kmol/hr] Total flow [kg/hr] Total flow [l/min] Mass flow [kg/hr] WATER MEOH H ₂ CO ₂ CO O ₂ N ₂ DME Mass fraction WATER	RAWMEOH 29.85033 45 0 13,173.87 3.30E+05 6523.999 1.18E+05 2.10E+05 7.171677 1644.426 1.386823 0 0 80.41048 0.3582424	RECYCLE 29.85033 45 1 1.37E + 05 5.87E + 05 1.31E + 06 1241.415 12021.61 2.61E + 05 2.81E + 05 2.7046 0 0 4317.845 2.12E-03 2.020 000	S10 42.63616 50 1 1.37E + 05 5.86E + 05 1.23E + 06 1240.172 12009.57 2.61E + 05 2.81E + 05 2.81E + 05 2.81E + 05 27019.01 0 0 4313.497 2.12E-03	S11 30.84703 1 0 13141.6 3.29E+05 6510.464 1.18E+05 2.10E+05 0.0192521 607.066 7.02E-03 0 0 52.71877 0.3595178 2.6004777	S13 66.37457 1 10586.63 3.33E + 05 4.90E + 06 8070.958 3.24E + 05 0.0192521 607.0734 7.02E-03 0 52.73549 0.0242287	S14 66.29512 1 0 4013.304 1.22E+05 2713.799 8070.936 1.14E+05 3.98E-11 7.39E-03 8.35E-11 0 0 0.0167132 0.0659871 0.0659871	S16 40.95338 1 1 235.4029 4010.582 1.02E+05 14.12141 1945.665 268.2537 1709.204 28.43271 0 0 44.90484 3.52E-03 0.4011000
Temperature [°C] Pressure [bar] Vapor fraction Total flow [kmol/hr] Total flow [kg/hr] Total flow [l/min] Mass flow [kg/hr] WATER MEOH H ₂ CO ₂ CO O ₂ N ₂ DME Mass fraction WATER MEOH	RAWMEOH 29.85033 45 0 13,173.87 3.30E + 05 6523.999 1.18E + 05 2.10E + 05 7.171677 1644.426 1.386823 0 0 80.41048 0.3582424 0.6365103	RECYCLE 29.85033 45 1 1.37E + 05 5.87E + 05 1.31E + 06 1241.415 12021.61 2.61E + 05 2.7046 0 4317.845 2.12E-03 0.0204883 2.412E-03	S10 42.63616 50 1 1.37E+05 5.86E+05 1.23E+06 1240.172 12009.57 2.61E+05 2.81E+05 27019.01 0 4313.497 2.12E-03 0.0204883	S11 30.84703 1 0 13141.6 3.29E + 05 6510.464 1.18E + 05 2.10E + 05 0.0192521 607.066 7.02E-03 0 52.71877 0.3595178 0.6384775 5.0395178	S13 66.37457 1 10586.63 3.33E + 05 4.90E + 06 8070.958 3.24E + 05 0.0192521 607.0734 7.02E-03 0 52.73549 0.0242287 0.9737905	S14 66.29512 1 0 4013.304 1.22E+05 2713.799 8070.936 1.14E+05 3.98E-11 7.39E-03 8.35E-11 0 0.0167132 0.0659871 0.9340127	S16 40.95338 1 1 235.4029 4010.582 1.02E+05 14.12141 1945.665 268.2537 1709.204 28.43271 0 0 44.90484 3.52E-03 0.4851329
Temperature [°C] Pressure [bar] Vapor fraction Total flow [km/hr] Total flow [kg/hr] Total flow [l/min] Mass flow [kg/hr] WATER MEOH H ₂ CO ₂ CO O ₂ N ₂ DME Mass fraction WATER MEOH H ₂ CO	RAWMEOH 29.85033 45 0 13,173.87 3.30E + 05 6523.999 1.18E + 05 2.10E + 05 7.171677 1644.426 1.386823 0 0 80.41048 0.3582424 0.6365103 2.17E-05 2.17E-05	RECYCLE 29.85033 45 1 1.37E + 05 5.87E + 05 1.31E + 06 1241.415 12021.61 2.61E + 05 2.7046 0 0 4317.845 2.12E-03 0.0204883 0.4449605 2.4720202	\$10 42.63616 50 1 1.37E + 05 5.86E + 05 1.23E + 06 1240.172 12009.57 2.61E + 05 2.7019.01 0 4313.497 2.12E-03 0.0204883 0.4449601 4.702006	S11 30.84703 1 0 13141.6 3.29E + 05 6510.464 1.18E + 05 2.10E + 05 0.0192521 607.066 7.02E-03 0 52.71877 0.3595178 0.6384775 5.85E-08 1.04E 02	S13 66.37457 1 10586.63 3.33E+05 4.90E+06 8070.958 3.24E+05 0.0192521 607.0734 7.02E-03 0 52.73549 0.0242287 0.9737905 5.78E-08 1.021 0.021	S14 66.29512 1 0 4013.304 1.22E+05 2713.799 8070.936 1.14E+05 3.98E-11 7.39E-03 8.35E-11 0 0.0167132 0.0659871 0.9340127 3.26E-16 6.045.00	\$16 40.95338 1 235.4029 4010.582 1.02E+05 14.12141 1945.665 268.2537 1709.204 28.43271 0 44.90484 3.52E-03 0.4851329 0.0668864 0.405756
Temperature [°C] Pressure [bar] Vapor fraction Total flow [kmol/hr] Total flow [kg/hr] Total flow [l/min] Mass flow [kg/hr] WATER MEOH H ₂ CO ₂ CO O ₂ N ₂ DME Mass fraction WATER MEOH H ₂ CO ₂ CO	RAWMEOH 29.85033 45 0 13,173.87 3.30E + 05 6523.999 1.18E + 05 2.10E + 05 7.171677 1644.426 1.386823 0 0 80.41048 0.3582424 0.6365103 2.17E-05 4.98E-03 4.90E of	RECYCLE 29.85033 45 1 1.37E + 05 5.87E + 05 1.31E + 06 1241.415 12021.61 2.61E + 05 2.81E + 05 2.7046 0 0 4317.845 2.12E-03 0.0204883 0.4449605 0.4789823 0.04789823	\$10 42.63616 50 1 1.37E + 05 5.86E + 05 1.23E + 06 1240.172 12009.57 2.61E + 05 2.7019.01 0 4313.497 2.12E-03 0.0204883 0.4449601 0.4789826 0.20420044	S11 30.84703 1 0 13141.6 3.29E + 05 6510.464 1.18E + 05 2.10E + 05 0.0192521 607.066 7.02E-03 0 52.71877 0.3595178 0.6384775 5.85E-08 1.84E-03 2.15 00	S13 66.37457 1 10586.63 3.33E+05 4.90E+06 8070.958 3.24E+05 0.0192521 607.0734 7.02E-03 0 52.73549 0.0242287 0.9737905 5.78E-08 1.82E-03 2.11E.00	S14 66.29512 1 0 4013.304 1.22E+05 2713.799 8070.936 1.14E+05 3.98E-11 7.39E-03 8.35E-11 0 0.0167132 0.0659871 0.9340127 3.26E-16 6.04E-08 6.92E-16	S16 40.95338 1 235.4029 4010.582 1.02E+05 14.12141 1945.665 268.2537 1709.204 28.43271 0 44.90484 3.52E-03 0.4851329 0.0668864 0.4261736
Temperature [°C] Pressure [bar] Vapor fraction Total flow [kmol/hr] Total flow [kg/hr] Mass flow [kg/hr] WATER MEOH H ₂ CO ₂ CO O ₂ N ₂ DME Mass fraction WATER MEOH H ₂ CO ₂ CO O ₂ N ₂ DME Mass fraction WATER MEOH H ₂ CO ₂ CO O ₂ N ₂ DME	RAWMEOH 29.85033 45 0 13,173.87 3.30E + 05 6523.999 1.18E + 05 2.10E + 05 7.171677 1644.426 1.386823 0 0 80.41048 0.3582424 0.6365103 2.17E-05 4.98E-03 4.20E-06 0	RECYCLE 29.85033 45 1 1.37E + 05 5.87E + 05 1.31E + 06 1241.415 12021.61 2.61E + 05 2.7046 0 4317.845 2.12E-03 0.4449605 0.4789823 0.0460943	\$10 42.63616 50 1 1.37E + 05 5.86E + 05 1.23E + 06 1240.172 12009.57 2.61E + 05 2.81E + 05 2.7019.01 0 4313.497 2.12E-03 0.0204883 0.4449601 0.4789826 0.0460944	S11 30.84703 1 0 13141.6 3.29E + 05 6510.464 1.18E + 05 2.10E + 05 0.0192521 607.066 7.02E-03 0 52.71877 0.3595178 0.6384775 5.85E-08 1.84E-03 2.13E-08	S13 66.37457 1 10586.63 3.33E+05 4.90E+06 8070.958 3.24E+05 0.0192521 607.0734 7.02E-03 0 52.73549 0.0242287 0.9737905 5.78E-08 1.82E-03 2.11E-08 0	S14 66.29512 1 0 4013.304 1.22E + 05 2713.799 8070.936 1.14E + 05 3.98E-11 7.39E-03 8.35E-11 0 0.0167132 0.0659871 0.9340127 3.26E-16 6.04E-08 6.82E-16	S16 40.95338 1 235.4029 4010.582 1.02E+05 14.12141 1945.665 268.2537 1709.204 28.43271 0 44.90484 3.52E-03 0.4851329 0.0668864 0.4261736 7.09E-03 0
Temperature [°C] Pressure [bar] Vapor fraction Total flow [kmol/hr] Total flow [kg/hr] Mass flow [kg/hr] WATER MEOH H ₂ CO ₂ CO O ₂ N ₂ DME Mass fraction WATER MEOH H ₂ CO ₂ CO O ₂ N ₂ DME Mass fraction WATER MEOH H ₂ CO ₂ CO 0 2 No	RAWMEOH 29.85033 45 0 13,173.87 3.30E + 05 6523.999 1.18E + 05 2.10E + 05 2.10E + 05 7.171677 1644.426 1.386823 0 0 80.41048 0.3582424 0.6365103 2.17E-05 4.98E-03 4.20E-06 0	RECYCLE 29.85033 45 1 1.37E + 05 5.87E + 05 1.31E + 06 1241.415 12021.61 2.61E + 05 2.81E + 05 2.7046 0 0 4317.845 2.12E-03 0.0204883 0.4449605 0.4789823 0.0460943 0 0	\$10 42.63616 50 1 1.37E + 05 5.86E + 05 1.23E + 06 1240.172 12009.57 2.61E + 05 2.7019.01 0 4313.497 2.12E-03 0.0204883 0.4449601 0.4789826 0.0460944 0	S11 30.84703 1 0 13141.6 3.29E + 05 6510.464 1.18E + 05 2.10E + 05 0.0192521 607.066 7.02E-03 0 52.71877 0.3595178 0.6384775 5.85E-08 1.84E-03 2.13E-08 0 0	S13 66.37457 1 10586.63 3.33E+05 4.90E+06 8070.958 3.24E+05 0.0192521 607.0734 7.02E-03 0 52.73549 0.0242287 0.9737905 5.78E-08 1.82E-03 2.11E-08 0	S14 66.29512 1 0 4013.304 1.22E+05 2713.799 8070.936 1.14E+05 3.98E-11 7.39E-03 8.35E-11 0 0.0167132 0.0659871 0.9340127 3.26E-16 6.04E-08 6.82E-16 0 0	S16 40.95338 1 235.4029 4010.582 1.02E+05 14.12141 1945.665 268.2537 1709.204 28.43271 0 44.90484 3.52E-03 0.4851329 0.0668864 0.4261736 7.09E-03 0
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Temperature [°C] Pressure [bar] Vapor fraction Total flow [kmol/hr] Total flow [kg/hr] Total flow [l/min] Mass flow [kg/hr] WATER MEOH H ₂ CO ₂ CO O ₂ N ₂ DME Mass fraction WATER MEOH H ₂ CO ₂ CO O ₂ N ₂ DME Mass fraction WATER MEOH H ₂ CO ₂ CO DME MEOH H ₂ CO ₂ CO DME MO ME MO ME MO MO ME MO MO MO ME MO MO MO ME MO MO MO ME MO MO MO ME MO MO ME MO MO ME MO MO ME MO MO ME MO MO ME MO MO ME MO ME MO MO ME MO ME MO ME MO ME MO ME MO ME MO ME MO ME MO ME MO ME MO ME MO ME MO ME MO ME MO ME MO ME MO ME MEO ME MO ME MO ME MO ME MO ME MO ME MO ME ME MEO ME MO ME MO ME ME ME ME ME MO ME ME ME ME ME ME ME ME ME ME	RAWMEOH 29.85033 45 0 13,173.87 3.30E + 05 6523.999 1.18E + 05 2.10E + 05 7.171677 1644.426 1.386823 0 0 80.41048 0.3582424 0.6365103 2.17E-05 4.98E-03 4.20E-06 0 2.43E-04	RECYCLE 29.85033 45 1 1.37E + 05 5.87E + 05 1.31E + 06 1241.415 12021.61 2.61E + 05 2.81E + 05 2.7046 0 0 4317.845 2.12E-03 0.0204883 0.4449605 0.4789823 0.0460943 0 0 7.36E-03	S10 42.63616 50 1 1.37E + 05 5.86E + 05 1.23E + 06 1240.172 12009.57 2.61E + 05 2.7019.01 0 4313.497 2.12E-03 0.0204883 0.4789826 0.0460944 0 7.36E-03	S11 30.84703 1 0 13141.6 3.29E + 05 6510.464 1.18E + 05 2.10E + 05 0.0192521 607.066 7.02E-03 0 52.71877 0.3595178 0.6384775 5.85E-08 1.84E-03 2.13E-08 0 0 1.60E-04	S13 66.37457 1 10586.63 3.33E + 05 4.90E + 06 8070.958 3.24E + 05 0.0192521 607.0734 7.02E-03 0 52.73549 0.0242287 0.9737905 5.78E-08 1.82E-03 2.11E-08 0 1.58E-04	S14 66.29512 1 0 4013.304 1.22E+05 2713.799 8070.936 1.14E+05 3.98E-11 7.39E-03 8.35E-11 0 0.0167132 0.0659871 0.9340127 3.26E-16 6.04E-08 6.82E-16 0 1.37E-07	S16 40.95338 1 235.4029 4010.582 1.02E+05 14.12141 1945.665 268.2537 1709.204 28.43271 0 44.90484 3.52E-03 0.4851329 0.0668864 0.4261736 7.09E-03 0 0.0111965
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Temperature [°C] Pressure [bar] Vapor fraction Total flow [kmol/hr] Total flow [kg/hr] Total flow [l/min] Mass flow [kg/hr] WATER MEOH H ₂ CO ₂ CO O ₂ N ₂ DME Mass fraction WATER MEOH H ₂ CO ₂ CO Q ₂ N ₂ DME MEOH H ₂ CO ₂ CO Q ₂ N ₂ DME MEOH H ₂ CO ₂ CO CO CO CO CO CO CO CO CO CO CO CO CO	RAWMEOH 29.85033 45 0 13,173.87 3.30E + 05 6523.999 1.18E + 05 2.10E + 05 7.171677 1644.426 1.386823 0 0 80.41048 0.3582424 0.6365103 2.17E-05 4.98E-03 4.20E-06 0 0 2.43E-04 0.4986383 0.4981191	RECYCLE 29.85033 45 1 1.37E + 05 5.87E + 05 1.31E + 06 1241.415 12021.61 2.61E + 05 2.81E + 05 2.7046 0 0 4317.845 2.12E-03 0.0204883 0.4449605 0.4789823 0.0460943 0 0 7.36E-03 5.02E-04 2.73E-03	S10 42.63616 50 1 1.37E + 05 5.86E + 05 1.23E + 06 1240.172 12009.57 2.61E + 05 27019.01 0 4313.497 2.12E-03 0.0204883 0.4449601 0.4789826 0.0460944 0 7.36E-03 5.02E-04 2.73E-03	S11 30.84703 1 0 13141.6 3.29E + 05 6510.464 1.18E + 05 2.10E + 05 0.0192521 607.066 7.02E-03 0 52.71877 0.3595178 0.6384775 5.85E-08 1.84E-03 2.13E-08 0 0.1.60E-04 0.4998082 0.4990543	S13 66.37457 1 10586.63 3.33E + 05 4.90E + 06 8070.958 3.24E + 05 0.0192521 607.0734 7.02E-03 0 52.73549 0.0242287 0.9737905 5.78E-08 1.82E-03 2.11E-08 0 0.58E-04 0.0423181 0.9562698	S14 66.29512 1 0 4013.304 1.22E + 05 2713.799 8070.936 1.14E + 05 3.98E-11 7.39E-03 8.35E-11 0 0.0167132 0.0659871 0.9340127 3.26E-16 6.04E-08 6.82E-16 0 1.37E-07 0.11163 0.8883699	S16 40.95338 1 235.4029 4010.582 1.02E + 05 14.12141 1945.665 268.2537 1709.204 28.43271 0 44.90484 3.52E-03 0.4851329 0.0668864 0.4261736 7.09E-03 0 0.0111965 3.33E-03 0.2579494
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Table A2

Stream data of the MeOH plant extracted from Aspen Energy Analyser, cold streams require hot utility, hot streams require cooling.

Name of heat exchanger	Stream		Туре	Temperature [°C]		C _p [kW∕°C]	Duty [MW]
	From	То		Inlet	Outlet		
HX1	S1	S2	Hot	93	38	73.32	4.03
HX2	S3	S4	Hot	120	38	76.03	6.21
HX3	S5	S6	Hot	118	38	80.65	6.47
HX4	MIX	FEED	Cold	47	230	1387.90	254.56
HX5	PRODUCT	S8	Hot	230	30	11506.25	418.17
HX6	S11	S12	Cold	31	87	14180.61	166.21
HX7	S15	METHANOL	Hot	61	30	218.57	6.74
HX8	FLUEGAS	S17	Hot	1623	120	38.60	19.33
Reboiler of RECT	RECT	S14	Cold	66	66	175839.83	34.37
Condenser of DISTL	DISTL	S13	Hot	68	66	238293.73	86.35
Condenser of RECT	RECT	S15	Hot	64	61	4540.33	16.19
Reboiler of DISTL	DISTL	BOTTOM	Cold	103.5	103	94096.03	47.05
Heat of reactor	-	-	Hot	230.00	229.50	215049.81	107.52

Table A3

List of heat exchangers in the integrated HEN design.

HX name	Load [MW]	Hot side			Cold side		
		Stream	Temperature in [°C]	Temperature out [°C]	Stream	Temperature in [°C]	Temperature out [°C]
E-101	13.51	FLUEGAS to S17	1622.53	620.84	MIX to FEED	220.27	230.00
E-102	34.37	PRODUCT to S8	230.00	204.20	Reboiler of RECT to S14	65.71	66.27
E-103	69.86	Condenser of DISTL to S13	67.88	66.55	Cooling water	20.93	23.00
E-104	47.05	PRODUCT to S8	204.20	168.84	Reboiler of DISTL to	102.54	103.04
					BOTTOM		
E-105	107.52	Heat of REACTOR	230.00	229.50	MIX to FEED	142.80	220.27
E-106	100.94	PRODUCT to S8	168.84	115.38	MIX to FEED	70.07	142.80
E-107	2.81	S3 to S4	119.66	82.67	MIX to FEED	68.04	70.07
E-108	154.48	PRODUCT to S8	115.38	68.95	S11 to S12	60.31	86.80
E-109	5.83	FLUEGAS to S17	620.84	120.00	MIX to FEED	63.84	68.04
E-110	19.19	PRODUCT to S8	68.95	60.23	MIX to FEED	50.02	63.84
E-111	11.73	Condenser of DISTL to S13	66.55	66.41	S11 to S12	30.85	60.31
E-112	6.74	S15 to METHANOL	60.84	30.00	Cooling water	19.94	20.93
E-113	6.47	S5 to S6	118.20	38.00	Cooling water	19.94	20.93
E-114	4.03	S1 toS2	93.01	38.00	Cooling water	19.94	20.93
E-115	16.19	Condenser of RECT to S15	64.40	60.84	Cooling water	19.94	20.93
E-116	4.75	Condenser of DISTL to S13	66.41	66.35	MIX to FEED	46.59	50.02
E-117	62.15	PRODUCT to S8	60.23	30.00	Cooling water	18.00	19.94
E-118	3.40	S3 to S4	82.67	38.00	Cooling water	18.00	19.94

Table A4

Purchased equipment cost (PEC) of 5 kt/d MeOH plant.

Name of equipment	Source of PEC	Source value [million \$]	Year	Scaling factor	Design variable	Calculated PEC in 2018 [million €]
HEN Distillation columns Compressors Flash separators Reactor Gas furnace	Aspen Energy Analyzer [™] V8.8 Aspen Process Economic Analyzer [™] V8.8 Aspen Process Economic Analyzer [™] V8.8 Aspen Process Economic Analyzer [™] V8.8 [50]	24.52 5.93 22.76 0.54 16.39 4.64	2014 2014 2014 2014 2006 2006	n.a n.a n.a 0.6 0.6	n.a n.a n.a n.a MeOH output Heat duty	19.34 4.68 17.95 0.42 16.43 1.67

Appendix B. Supplementary data

Supplementary material related to this article can be found, in the online version, at doi:https://doi.org/10.1016/j.jcou.2020.101166.

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