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Techno-economic-assessment of the methanol synthesis from captured CO_2 and modular nuclear power-based electrolysis

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ABSTRACT

Recently, several technical and political efforts targeted the reduction of CO_2 levels in the at- mosphere, accompanied by a strong incentivization of carbon-neutral fuel production. In this context, a methanol synthesis plant using H_2 originated from electrolysis powered with nuclear energy from fourth-generation micro-modular reactors is proposed here. This latest generation of nuclear reactors aims to transform the energy sector by enhancing the scalability, efficiency, safety, and sustainability of nuclear power. Prefabricated plants can be easily transported and installed at lower costs and with more flexibility, enabling an easier integration with chemi- cal plants. The purpose of this work is to perform an eco-techno-economic assessment of the methanol production fueled by nuclear-power-driven electrolysis and captured CO_2. The re- search involves the assessment of the integration of the methanol plant with various technologies for capturing and utilizing CO_2 (Direct Air Capture, Carbon Capture of flue gases, or utilizing cheap CO_2 from companies). The analysis emphasizes the positive impact of the coupling of electricity production, chemical synthesis and carbon capture in reducing greenhouse gas emis- sions and improving energy efficiency. The findings indicate that the integration of methanol synthesis with carbon capture presents considerable environmental benefits in comparison to tra- ditional methanol plants. Significant reductions compared to state of the art in CO_2 emissions were observed, ranging from −0.94 to −1.06 $kgCO_2$-eq/kgMeOH of the proposed technologies, in contrast to the 0.5–4.3 $kgCO_2$-eq/kgMeOH range for traditional plants. The economic analysis showed that the levelized cost of methanol production is 1809$ per ton in the worst-case scenario with DAC, and 1381$ and 1283$ per ton with CCU and benchmark technologies, respectively. These values are expected to decrease with the technological advances. Reducing the CapEx (of the DAC unit and nuclear batteries) and incorporating additional energy optimizations are the main drivers of the further enhancement of the economic competitiveness of the process.

1. Introduction

Methanol (CH_3OH) plays a vital role in industry, serving as a solvent and raw material for the production of numerous essential chemicals [1]. It serves as the main ingredient for the production of various chemicals like formaldehyde, methyl tert-butyl ether, and acetic acid, as well as being a starting point for key components in making everyday goods [2]. Methanol is recognized as a key raw material in the petro- chemical sector, with a worldwide demand of 98 Mt/year in 2021 [3], projected to rise to 190 Mt/year by 2030 [4]. However, the increasing need for methanol must be weighed against the energy sector, where conventional sources like oil, natural gas, and coal still meet global energy demands [5]. It is crucial to emphasize that these traditional resources are not renewable and contribute to the imbalance of the carbon cycle in the atmosphere. In addition, concerns about global warming and climate change have recently in- creased political efforts to avoid the worst effects of excess anthropogenic CO_2 in the atmosphere. Signed in 2015 by 196 countries, the Paris Agreement [6] aims to keep the global temperature well below 2°C above the preindustrial average level, increasing the ability to adapt to the ad- verse impacts of climate change. To this end, carbon emissions into the atmosphere must peak as soon as possible so that they can decrease later until a neutral balance is achieved. To address these challenges and ensure the sustainability of our energy and chemical production, it is important to investigate alternative and sustainable solutions [7]. Improvements in the produc- tion efficiency of key chemicals, even by a small percentage, can lead to

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substantial gains in profits, energy conservation, and environmental protection. In addition, there is an increasing consideration of different pathways for the production of methanol in a more environmentally friendly manner, for example, using different raw materials such as biogas and carbon dioxide [8]. However, compared to their fossil counterparts, the overall reduction in greenhouse gas emissions from these pathways is effective only if both the supplied energy and the chemical reactants are characterized by a low carbon intensity.

1.1. Applications

Today, methanol is the starting material for the production of a large number of chemical products. Several intermediate materials used in making common household items come from methanol, such as paints, solvents, resins, silicones, adhesives, antifreeze, plastics, detergents, and more [9]. In addition to its role in chemical synthesis, methanol can be utilized as a vehicle fuel alone or mixed with gasoline to create a high-octane, high-efficiency fuel that has lower emissions than regular gasoline [10]. The use of methanol is expected to increase in this sec- tor because it also decreases emissions (NO_x, SO_x, and particulate matter) when utilized [11]. Methanol is also a highly effective carrier of hydrogen, storing a greater amount of hydrogen in a single alcohol molecule compared to a molecule of methane or ammonia [12]. Since methanol is liquid under normal conditions, it can be easily managed, stored, and moved [13]. Methanol can release hydrogen through various methods: by reacting with water in steam reforming, reacting with oxygen in partial oxidation, or through methanol thermolysis [14]. Steam reforming stands out because it is the only reaction among the three that results in the production of three moles of hydrogen per mole of methanol, rather than two [15].

1.2. Methanol production process

Methanol is commonly produced from syngas ($COx + H_2$), which can come from different sources. In particular, natural gas is the most commonly used feedstock for the production of methanol. However, in recent years, alternative approaches based on renewable sources (such as CO_2 and biomass) have been developed [16]. Currently, the mixture of H_2, CO and CO_2 (syngas) is produced mainly by reforming natural gas. It can also be synthesized by reforming or partial oxidation of different carbon-based materials (e.g. coal, petroleum, heavy oil, etc.). Methane is the preferred feedstock because syngas can be produced with a lower energy consumption, capital investment and operating cost. In addition, the resulting syngas shows low concentration in impurities [17]. The production and purification of syngas is crucial in the methanol production process because it represents more than half of the total investment when the feedstock is natural gas and up to 70–80 % [9] when the raw material is coal. Methanol production from synthesis gas involves the following reaction [18]:

CO hydrogenation:

$$CO + 2H_2 \leftrightarrow CH_3OH\ \Delta H^\circ_{298} = \text{-}90.8\ \text{kJ/mol} \quad (1)$$

CO_2 hydrogenation:

$$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O\ \Delta H^\circ_{298} = \text{-}49.5\ \text{kJ/mol} \quad (2)$$

Water Gas Shift:

$$CO + H_2O \leftrightarrow CO_2 + H_2\ \Delta H^\circ_{298} = \text{-}41.2\ \text{kJ/mol} \quad (3)$$

Both hydrogenation reactions are exothermic and present a decrease in the number of moles. As a consequence, the conversion is favored by low temperatures and high pressures. In recent years, synthesis procedures have increasingly reduced pressures (from 50 to 100 bar), preferably close to the pressure of steam reforming, to minimize the operating cost associated with gas compression. Despite thermodynamic limitations, methanol synthesis is conducted at approximately 200–300°C due to the catalyst's activity temperature range [19]. In 1923, BASF patented a methanol production process based on syngas at very high temperatures and pressures (300–400°C and 250–350 atm). A significant breakthrough came with the introduction of methane steam reforming, resulting in cleaner syngas and enabling the use of a more effective Cu/ZnO catalyst. This advancement, proposed by Imperial Chemical Industries (ICI) in 1996, reduced process temperature and pressure to around 300°C and 100 atm. In the following years, Lurgi developed a process with even lower pressure and temperature requirements (230–250°C and 40–50 atm). Currently, methanol selectivity exceeds 99.8 % with an energy efficiency of approximately 75 % [9].

Green chemistry aims at synthesizing methanol entirely from renewable resources. A possible way is through the catalytic or electrochemical hydrogenation of CO_2 [20]. Efficient $Cu/ZnO/Al_2O_3$ catalysts, similar to those used in syngas-based methanol production, are used [21]. The primary limitation of the widespread implementation of this process is the availability of CO_2 and H_2 [22]. While carbon dioxide is abundant in exhaust sources (such as the flue gases of power plants using fossil fuels and industrial plants) and in the atmosphere, hydrogen is mainly derived from fossil sources. The main technology to produce green hydrogen is water electrolysis, paired with renewable energy sources (wind, solar, etc.), which, being very energy-intensive, require large and invasive wind or solar farms [23]. Waste biomass holds promise as a potential feedstock for methanol production [24]. Most technologies for methanol production utilizing biomass as a feedstock closely resemble those used when exploiting fossil fuels as raw materials. During the gasification process, oxygen combusts a portion of the biomass to generate heat. The combustion gases (CO_2 and water) react with the remaining biomass, resulting in the production of CO and H_2 [25]. The production of e-methanol is incentivized by the Renewable Energy Directive III (RED III), which aims to promote the use of renewable energy and reduce greenhouse gas (GHG) emissions in the European Union by 2030. E-methanol is considered a Renewable Fuel of Non-Biological Origin (RFNBO) [26]. This term considers all gaseous and liquid renewable fuels that do not rely on biomass. The main technology to produce these RFNBOs is the use of electrolysis powered by renewable electricity to produce hydrogen. This hydrogen can be combined with nitrogen to produce ammonia or with carbon to produce various synthetic hydrocarbons like e-methanol. The Renewable Energy Directive sets a binding mandate for these RFNBOs. By 2030, green hydrogen and e-fuels need to account for 1 % of all fuels used in the transport sector. Considering the significant amount of additional renewable capacity required to produce RFNBOs, member states managed to reduce the level of ambition in two ways. To partially compensate for their higher cost compared to biofuels, each 1 MJ of RFNBOs can be double-counted as 2 MJ towards meeting the target [27].

1.3. Nuclear energy

In the search for cheap electricity source for renewable H_2 production, nuclear energy could be a solution to provide a constant and reliable low-carbon supply. Among the nuclear energy production technologies, an increasing interest goes to small-scale applications such as the Micro-Modular Reactor (MMR). The MMR battery is made entirely of ceramic materials, with a melting temperature above 2000°C, and over 1000°C above the maximum temperature achievable if cooling is interrupted. These nuclear reactors are inherently stable since they shut down automatically if cooling is interrupted. Since energy production decreases with increasing temperature, the energy produced by the battery is controlled by adjusting the flow of the heat extraction medium. Cooling is commonly performed with Helium, which is completely inert and stable. The use of a different coolant than water makes hydrogen explosions impossible [28]. The batteries are used for electricity production, generating heat at 600°C, in the same operating temperature range as fossil fuel-powered generators, so they can be used

with existing plants and turbines by replacing coal, oil, or methane burners. These MMRs are designed to be used alone or in groups of 2–20 units to produce the energy required by the plant. MMR batteries can also be used to produce industrial heat, which is extracted from the nuclear citadel with a flow of molten salts, allowing convenient delivery of heat where needed in the plant [29].

1.4. Methanol synthesis from CO_2

Most of the current methanol production is based on syngas, obtained through the reforming of natural gas. Various studies in the literature [30] examine the use of CO_2 captured from fossil fuel power plants for methanol synthesis. For example, Bellotti et al. (2017) [31] conducted a feasibility study on a methanol synthesis plant that utilizes sequestered CO_2 and hydrogen produced through water electrolysis. Similarly, Van-Dal and Bouallou (2013) [32] designed a process that combines chemical capture of CO_2 from flue gases with electrolysis powered by low-carbon electricity, demonstrating significant energy savings and emission reductions.

Hao et al. [33] presented a technical, economic, and environmental analysis of methanol production through CO_2 capture, introducing structural optimizations in a combined cycle power plant. Cameli et al. (2024) [34] explored methanol synthesis routes based solely on renewable electricity, indicating that the cost of electrified methanol is expected to remain significantly higher than that of fossil fuel-based methanol by 2050, although the electrified process is carbon negative [35].

However, all these studies use renewable or fossil fuel energy and do not consider nuclear energy for methanol production. Some studies mention the application of nuclear energy in chemistry, such as the work by Schultz et al. (2009) [36], which explores the use of non-carbon-based energy sources to reduce CO_2 emissions and produce synthetic fuels. Additionally, Ramirez- Corredores et al. [37] analyzed the opportunities and challenges in developing integrated energy systems to transform CO_2 through chemical processes, but did not focus on specific simulations or a particular type of nuclear reactor.

This paper proposes a low-carbon emission methanol synthesis plant configuration that employs nuclear energy from fourth-generation micro-modular reactors. The objective is to reduce greenhouse gas emissions by producing e-methanol through the hydrogenation of CO_2 exploiting only renewable energy coming from the nuclear reactor.

The hydrogen source selected for this study is water electrolysis. The main reasons are the maturity and the scalability of this technology, which align well with the process scale of a nuclear reactor. On the other hand, the carbon sources considered for this study are as follows:

1. Direct air capture (DAC): extracting CO_2 directly from the atmosphere using DAC technology.
2. Flue gas capture: extracting CO_2 from industrial flue gases through Carbon Capture and Utilization (CCU) system.
3. Benchmark case - no CO_2 cost: acquiring CO_2 at no cost from companies seeking to dispose of it.

These carbon sources have different energy requirements, reflecting varying scenarios where CO_2 rich streams may or may not be available. The plant design and economic and environmental evaluation are performed for each case study. This paper illustrates the energy efficiencies of the innovative configurations compared to literature and industrial benchmarks. Moreover, it presents a study of the economic feasibility of the process, including a cash flow analysis. Following this, it assesses the environmental impacts and evaluates its advantages over currently used technologies.

2. Methods

In the following sections, the simulation of the plant using Aspen HYSYS V11 software will be discussed. The Peng-Robinson equation of state was selected to properly describe the fluid mixture.

2.1. Technology identification and energy balance for plant's feed section

Technological and economic limits restrict the utilization of DAC technology at the industrial scale. Indeed, only a few processes for large-scale capture of atmospheric CO_2 are available at relevant scales. For this study, the reference simulated is obtained from Carbon Engineering [38]. The authors have designed an industrial plant that captures approximately $1Mt_{CO2}$ /year through a continuous process using an aqueous KOH sorbent coupled with a calcium caustic recovery loop. Regarding CCU and water electrolysis technologies, the Technology Readiness Level (TRL) is higher and numerous solutions can be found in industrial environments [39]. Several technologies with different characteristics, operating modes, costs, and energy consumption are available. Since these last two variables significantly influence the scale of the process and the economic analysis of this work, it is crucial to choose the most suitable and cost-effective technology. For the CC, among the various existing technologies, the choice was primarily based on energy requirements. Among those available in the literature, this study identified the Carbon Capture technology option with a solution of methyl diethanolamine (MDEA) with piperazine (PZ) as a promoter as the most suited. This carbon capture unit requires 2.24 GJ per ton of captured CO_2 of thermal energy [40]. For the H_2 production, an alkaline electrolyzer is chosen because it is more cost-effective and has a longer lifetime [41].

Each nuclear battery produces 3 million megawatt-hours of high-temperature thermal energy [29]. The power released by the nuclear battery is modular and has a maximum of 45 MW of thermal energy. For the plant under consideration, it was decided to adopt 3 reactors in parallel, each of them with a charge lasting 10 years. Consequently, the nominal available power is 112.5 MW_{th}. The electricity production is performed with a Brayton turbine with an efficiency of 38 % [42]. As illustrated in Table 1, the alkaline electrolyzer, the technologies for the CO_2 capture and the primary compressor are the most energy-intensive units of the plants. Therefore, an energy balance on the feed section (Eq. 4) ensures that the overall energy required by these units corresponds to the production of the nuclear batteries. This constraint has been coupled with an equation that relates the flow of H_2 and CO_2, ensuring the molar ratio between the two reactants is respectively equal to 1:3. The energy consumption per unit of carbon dioxide and hydrogen is listed in Table 1.

$$^{E}\text{battery} = {}^{e}\text{CO}_2\text{source} \cdot {}^{F}\text{CO}_2 + {}^{e}\text{el.} \cdot {}^{F}\text{H}_2 + {}^{W}\text{compressor} \quad (4)$$

2.1.1. Flowsheet description

The following section describes the methanol synthesis plant layout. Fig. 1 illustrates the Block Flow Diagram of the process from carbon dioxide and water to the product.

CO_2 is extracted from flue gas or atmospheric air at atmospheric conditions and it is fed into a multi-stage compressor to raise the pressure up to the electrolyzer discharge pressure, equal to 31 bar. Subsequently, the CO_2 and H_2 streams are further compressed, reaching the reactor pressure (70 bara). The unreacted gases after the reactive section are recycled back to the inlet of the first reactor, with a 5 % purge to

Table 1
Intensive energy demands.

	Value	Reference
Alkaline Electrolyzer [kWh/kgH_2]	53.39	[43]
DAC Thermal Energy [GJ/tCO_2]	5.25	[38]
DAC Electrical Energy [GJ/tCO_2]	0.28	[38]
CCU DMEA/PZ Thermal Energy [GJ/tCO_2]	2.74	[40]

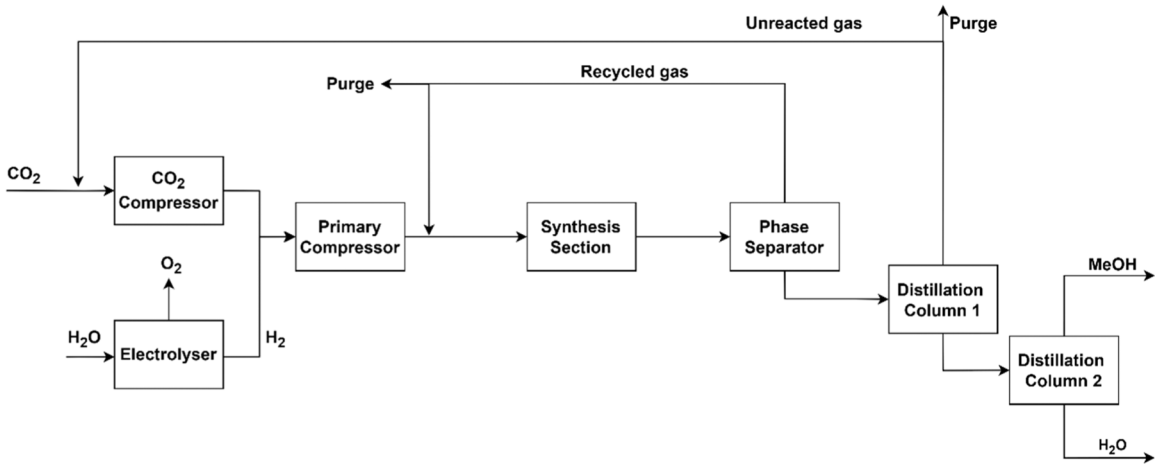


Fig. 1. Block Flow Diagram of the methanol synthesis plant.

remove inert components and avoid a snowball effect, as in industrial standards. The raw methanol is sent to the purification section, where methanol is recovered at the desired specification. The unreacted gases are partially recycled back into the feed section to enhance overall carbon conversion. The second purge is set equal to 5 % of the inlet stream.

2.1.2. *Synthesis and purification sections*

Fig. 2 shows in detail the synthesis and purification sections of the process. The syngas mixture (Stream 5) is first pre-heated exploiting the heat of the product stream from the synthesis reactor. The minimum temperature approach is equal to 20 °C to ensure enough driving force for the heat exchange. A heater brings the mixture to the synthesis temperature, equal to 250 °C. Afterward, the reactive mixture is sent to a first reactor. The dimensions of the reactor are estimated by ensuring a Gas Hourly Space Velocity (GHSV) equal to 5000 h^{-1} to enhance carbon conversion [44]. Due to limited conversion, the product stream is cooled down to 40°C to separate methanol and water from the unreacted gases. The gaseous mixture is then sent to a second reactive subsection. The specifications do not change between the two reactive subsections. The recycle stream is equipped with a recycle compressor to compensate for the pressure drop of the synthesis section. The two liquid products are combined and the mixture enters into the purification section. A first distillation column, working at a pressure of 2 bara, separates the more volatile products (CO_2, CO, and H_2) from water and methanol. The overhead products are recycled back and mixed with the pure carbon dioxide feed stream. The percentage of the purge is assumed to be equal to 5 % of the inlet stream. The raw methanol from the top of the column is fed to a second distillation column where methanol is recovered with a commercial purity of 99.85 w/w %. The second specification of the column is the methanol recovering from the top, fixed to be equal to 99 %. The reflux ratio of the second column and the feed tray have been optimized to reduce the required power at the reboiler. The reactors are packed beds containing a $Cu/ZnO/Al_2O_3$ commercial catalyst. The kinetic model proposed by Vanden Bussche and Froment [45] is implemented to describe the mixture reactive behavior. The model assumes that CO_2 is the main carbon source for the synthesis of methanol and considers the inhibitory effect of water formed by the RWGS reaction. The reactors are modeled as isothermal because this simplification has a low impact on the economic estimation while reducing significantly the computational time [46]. The Ergun equation is applied to estimate the pressure drop. Since the reactor is assumed to be isothermal, the void fraction is the only parameter needed to describe the reactivity and pressure drop inside the tube bundle system. The value of the void fraction is assumed to be equal to 0.387, retrieved from industrial standard [47].

Eqs. 5 and 6 describe the kinetic scheme proposed by Vanden Bussche and Froment, where pressures and temperatures are respectively

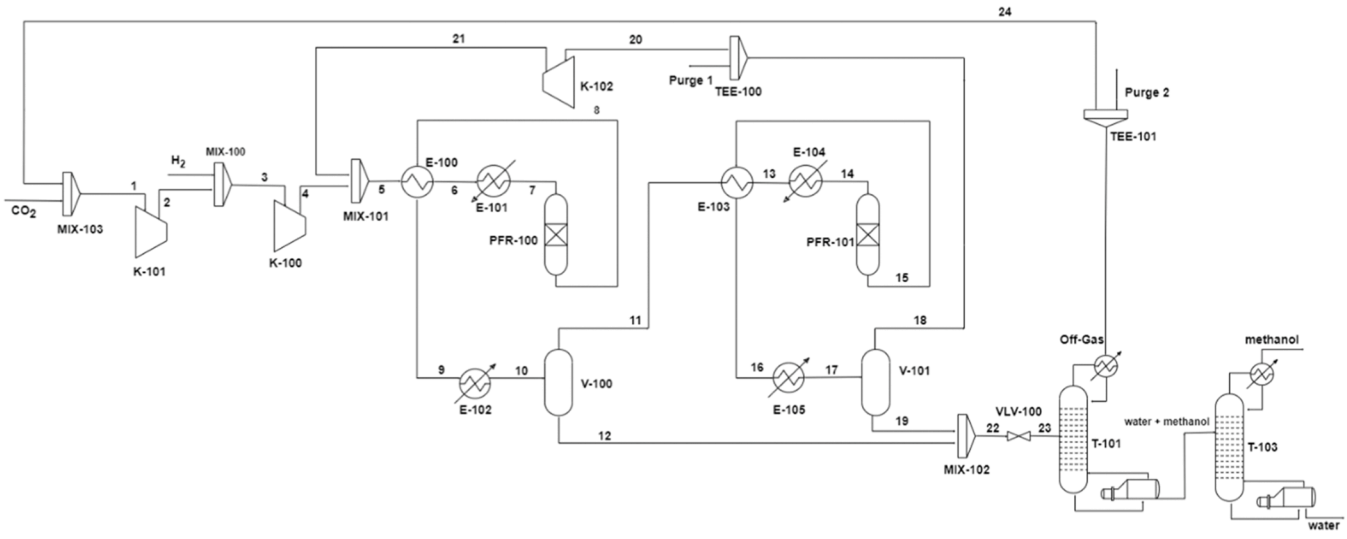


Fig. 2. Process Flow Diagram of synthesis and purification section.

expressed in bar and Kelvin. The kinetic constants follow the Arrhenius law (Eq. 7) and its parameters are shown in Table 2. The thermodynamic equilibrium constants (Eqs. 8 and 9) are given by Graaf et al. (1986) [48]. Appendix A elucidates the procedure to rearrange the kinetic model, allowing the simulation of the reactor in Aspen HYSYS V11, and also its new parameters.

Methanol synthesis:

$$r_{CH_3OH} = \frac{k_1 P_{CO_2} P_{H_2} \left(1 - \frac{1}{K_{eq1}} \frac{P_{H_2O} P_{CH_3OH}}{P_{H_2}^3 P_{CO_2}}\right)}{\left(1 + k_2 \frac{P_{H_2O}}{P_{H_2}} + k_3 P_{H_2}^{0.5} + k_4 P_{H_2O}\right)^3} \left[\frac{\text{mol}}{\text{kg}_{\text{cat}} \cdot \text{s}}\right] \quad (5)$$

Reverse water gas shift reaction:

$$r_{RWGS} = \frac{k_5 P_{CO_2} \left(1 - K_{eq2} \frac{P_{H_2O} P_{CO}}{P_{CO_2} P_{H_2}}\right)}{\left(1 + k_2 \frac{P_{H_2O}}{P_{H_2}} + k_3 P_{H_2}^{0.5} + k_4 P_{H_2O}\right)} \left[\frac{\text{mol}}{\text{kg}_{\text{cat}} \cdot \text{s}}\right] \quad (6)$$

$$k_i = A_i \exp\left(\frac{B_i}{RT}\right) \quad (7)$$

$$\log_{10} K_{eq1} = \frac{3066}{T} - 10.592 \quad (8)$$

$$\log_{10} \frac{1}{K_{eq2}} = \frac{2073}{T} + 2.029 \quad (9)$$

2.2. Economic analysis

An economic analysis of the plant is necessary to assess its feasibility from a financial perspective. Both an estimation of capital and manufacturing costs have been performed. The costs of the equipment are calculated using the Module Costing Technique introduced by Guthrie in the 1970s [49]. Most of the units must be made of stainless steel because the mixtures contain hydrogen, which may cause embrittlement. The CEPCI index is exploited to actualize the bare module cost of the different units and it equals 800.8 [50]. It is assumed that the steam required by the reboilers of both columns is partially produced by cooling the reactor. The parameters assumed for the economic analysis are reported in Table 3.

2.2.1. DAC, carbon capture system, alkaline electrolyzer and nuclear battery cost

Regarding the MMR battery, the empty nuclear plant, including the molten salt heat ex- changer, costs 50 million dollars, while each nuclear fuel load of 3 million thermal MWh costs approximately 35 million dollars. The reactor vessel is expected to have a lifespan of at least three refueling [29]; therefore, it is not necessary to replace it in the lifespan of the methanol plant. The CapEx of the alkaline electrolyzer is calculated considering their modular price of 800 $/kW [51]. CapEx of the entire DAC unit are obtained by applying the six-tenth rule (Eq. 10) to the estimation provided by Carbon Engineering [38]

$$\frac{\text{cost B } (\$)}{\text{cost A } (\$)} = \left(\frac{\text{capacity B}}{\text{capacity A}}\right)^{0.6} \quad (10)$$

Table 2
Parameters values for the kinetic model.

k_i	A_i	B_i [J/mol]
k_1	1.07	40,000
k_2	3453.38	–
k_3	0.499	17,197
k_4	$6.62 \cdot 10^{-11}$	124,119
k_5	$1.22 \cdot 10^{10}$	−98,084

Table 3
Metric used for economic analysis.

Metric	Value
HP steam price (46 bar) [$/kg]	0.0155
Cooling water price [$/t]	0.0595
Operation time [h/y]	8000
Plant life [t]	30
$ value [year]	2023
Discount rate (%)	7
Methanol price [$/t]	1300
Oxygen price [$/Nm^3]	0.124

Finally, the Carbon Capture System capital cost is estimated with Eq. (11) which is based on the plant capacity of 2808 ton/h, in terms of gas entering the separator [52]. To consider the size effect on investment costs, a standard factor of 0.65 is used [31].

$$C = 75.45 \cdot 10^6 \cdot \left(\frac{M_{\text{in}}}{2.808 \cdot 10^6}\right)^{0.65} \quad (11)$$

2.3. Cash flow analysis

The cash flow analysis is conducted to estimate financial and economic KPIs, such as the internal rate of return (IRR), the payback time, the levelized cost of production (LCOP) and the net present value (NPV). The analysis considers scenarios with and without an annual interest rate and includes the potential sale of carbon credits. The assumptions employed to carry out the cash flow analysis are listed in Table 4.

Cash flow analysis has been conducted in all three cases, both with and without the selling of carbon credits. The annualization factor is 7 %. The grass-roots cost has been considered as the capital investment. An annual inflation rate of 2 % was assumed increasing the methanol prize over time. The complete cash flow analysis for all cases is provided in the Supplementary material.

2.4. Efficiency and environmental assessment

A set of key performance indicators (KPIs) is used to assess the economic viability of the process and the relative emissions. Energy efficiency (Eq. 12) is the first KPI and is defined as the ratio between the energy attainable from the produced MeOH and the energy provided to the system

$$\text{Energy efficiency} = \frac{\dot{F}_{\text{MeOH}} \cdot \text{LHV}_{\text{MeOH}}}{E_{\text{in}}} \quad (12)$$

Where F_{MeOH} is the mass flow rate of the produced methanol, LHV_{MeOH} is the lower heating value, which represents the amount of heat released during combustion (for methanol it is equal to 19.9 MJ/kg) and E_{in} is the energy provided by nuclear batteries [53].

In this study, only direct CO_2 emissions associated with the core process steps (CO_2 capture, hydrogen production via electrolysis, and methanol synthesis) were considered in the life cycle assessment. Regarding indirect emissions, only those related to electricity generation from the nuclear power plant were included. Other indirect CO_2

Table 4
Summary of assumptions and parameters.

Parameter	Value/Description
Annual interest rate (*i*)	7 %
Periodic investment	Initial at year 0 Every 10 years (3 new batteries and 1 new electrolyzer)
Plant capacity	The plant runs immediately at full capacity
Plant lifetime (*t*)	30 years
Straight line depreciation	10 years for nuclear batteries and alkaline electrolyzer. 30 years for process equipment.

emissions, such as those related to plant construction or auxiliary processes, were not taken into account.

Greenhouse gas (GHG) emission is the second KPI and accounts for the entire carbon footprint of the plant. Apart from the supply of electricity, the total carbon footprint of the electrolyzer ranges between 43 and 287 gCO_2, eq/kgH2. The lower end of the range relates to installations for which no electrode replacement is accounted for, while higher numbers have multiple replacements over the 20-year lifetime. Given that the average lifespan of an alkaline electrolyzer is 10 years, no electrode replacement was planned, and consequently, a value of 90 gCO_2,eq/kgH2 was considered in this study [54]. For the DAC technology, a conservative emission value of 50 $gCO_2/tonCO_2$ was considered [55]. For the MMR battery, the specified emission value is 11.5 gCO_2/kWh as provided by the manufacturer [29]. Comparing these values with the carbon footprints of various energy sources (Table 5), it can be observed that this battery has much lower impacts compared to other sources.

Direct GHG emissions into the atmosphere are caused by the purge streams from the MeOH synthesis reactor. The carbon footprint of the conventional MeOH production process is highly influenced by the geographical location of the production site, resulting in significant variability. Reported values in the literature range from 0.5 $kgCO_2$-eq $kgMeOH^{-1}$ [56] to 1.8 $kgCO_2$- eq $kgMeOH^{-1}$, even reaching 4.3 $kgCO_2$-eq $kgMeOH^{-1}$. Therefore, a conservative value of 0.7 $kgCO_2$-eq $kgMeOH^{-1}$ has been considered.

The Cost of Avoided CO_2 (CCA) is the last indicator and represents the cost of one ton of CO_2 needed to balance the difference in methanol cost between electrified ($LCOP_{e\text{-}MeOH}$) and conventional ($LCOP_{ref}$) processes, based on the difference in emissions between the two processes (GHG_{ref} - $GHG_{e\text{-}MeOH}$). However, this indicator does not account for emissions resulting from the final use of methanol (e.g., combustion if used as a fuel), which would have the same impact on the GHG emissions of the two competitive processes. The CCA can effectively be considered a carbon penalty for the fossil-based process that economically equalizes the electrified alternative process [34]. For the calculation of this parameter, the LCOP values calculated bringing to zero the Discounted Net Profit Value and taking into account the sale of carbon credits has been used.

$$CCA = \frac{LCOP_{e-MeOH} - LCOP_{ref}}{GHG_{ref} - GHG_{e-MeOH}} \quad (13)$$

3. Results and discussion

In this section, the analysis of the simulation results for the methanol synthesis process is presented. Fig. 3 shows the material flows Sankey diagram of the entire process (DAC case). It can be observed that 93 % of the raw CO_2 is converted into products. The remaining 7 % of CO_2 leaves the process system as unconverted gas. The diagram also highlights the importance of the valorization of oxygen as a by-product of the electrolyzer, which represents an additional economic opportunity.

The energy Sankey Diagram in Fig. 4 illustrates the energy flow from the nuclear reactor to the main process units. 93 % of the initial 112.5 MW of nuclear thermal power is transferred to the Brayton turbine for electrical energy production. 62 % of the power at the turbine is lost due to the power loss of the turbine during the conversion process.

Table 5
CO_2 emissions per kWh for different energy sources [29].

Energy Source	gCO_2/kWh
Conventional nuclear	2
MMR battery	11.5
Eolic	17
Solar	34
Methane	500
Carbon	1000

To adopt a conservative approach, it has been assumed that no valorization of the process losses is possible. The power loss of the turbine is the main factor limiting the overall energy efficiency of the process. The electrolyzer uses the most significant portion of the electrical energy, which is the most energy-intensive unit of the process.

Besides the power required to obtain H_2 and CO_2 for the compression to the synthesis pressure, the ancillary power required (in the synthesis and purification section of the process) was calculated and reported in Table 6. This power, in the DAC case, represents 2.7 % of the nuclear batteries' power; therefore, these contributions are almost negligible. The heat released in the synthesis reactor is exploited as a hot utility at the reboilers of both columns, decreasing the OpEx. The use of the reaction heat reduces the additional power demand to 1 % of nuclear power production. This assumption is also confirmed for the CCU and Benchmark cases.

3.1. CapEx and OpEx estimation

Table 7 illustrates the capital expenditure for the three cases, divided into the main contributions. The DAC case requires higher investment as it is more expensive compared to CCU. The cost of the equipment and electrolyzer is similar for each of the cases, respectively equal to 30 M$ and 10 M$. The three empty nuclear reactors and the three refills represent the most significant contribution (255 M$) to the total grassroots cost.

Given the high grass root costs, in addition to the scenario with a plant lifetime of 10 years, scenarios with a plant lifetime of 20 and 30 years were also considered. Since each battery lasts 10 years, a new set of batteries will need to be purchased every 10 years, resulting in an expense of 105 M$. Furthermore, every 10 years it will be necessary to replace also the alkaline electrolyzer, as its lifetime is approximately 80,000 h [57]. For subsequent calculations

and the cash flow analysis, it was assumed that the price of the electrolyzer remains constant. However, as this is an up-and-coming and still-developing technology, it is expected that its CapEx will decrease over time. Tables 8 and 9 illustrate respectively the utility consumptions and OpEx costs.

A sensitivity analysis was performed on the main cost centers for the DAC and CCU case studies. Fig. 6 illustrates the dependence of the grassroots cost on the cost of the electrolyzer, the nuclear empty reactors, the nuclear charges and the DAC and CCU equipment.

3.2. Revenues

In addition to methanol, the studied plant also produces a significant amount of oxygen, which is a valuable compound. As a result, we have two sources of profit. Since the product is e-methanol, produced using renewable raw materials and a renewable energy source, a price of 1300 $/tMeOH is chosen. Furthermore, an additional benefit to consider, which partly justifies the high cost of e-methanol, is the availability of incentives for advanced biofuels, amounting to 375 euros/CIC. One CIC corresponds to one Ton of Oil Equivalent (TOE), equal to 11,700 thermal kWh. In the case of e-methanol, these incentives translate into a gain of 177 euros per ton of methanol [58]. Table 10 illustrates productions and revenues for all considered cases.

Since the early 2000s, carbon credits have been introduced. These represent the reduction of one ton of CO_2 or its equivalent and can be purchased from certified projects that reduce or avoid greenhouse gas emissions, facilitating emission offsetting and promoting environmental sustainability. A scenario was then considered where these credits were sold, leading to increased profits. These carbon credits lead to an annual gain of approximately 3 million, considering the 2023 price of 105 euros/ton of CO_2 [59]. Finally, a comparison was made between the cost of nuclear energy and electricity generated from other sources. Nuclear energy contributes 25.5 M$ per year to the operative expenditure. On the other hand, if traditional electricity generated from fossil fuels is

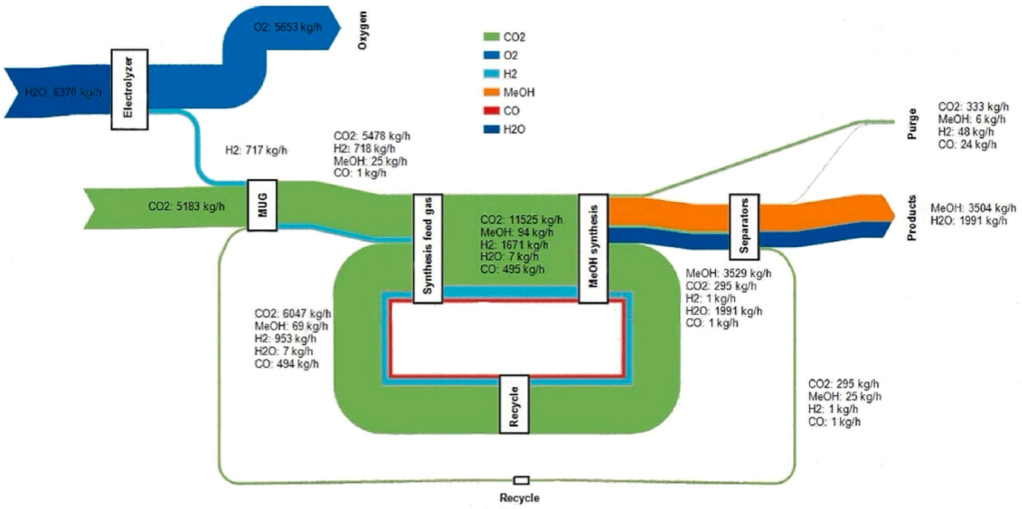


Fig. 3. Material flows Sankey diagram of the process.

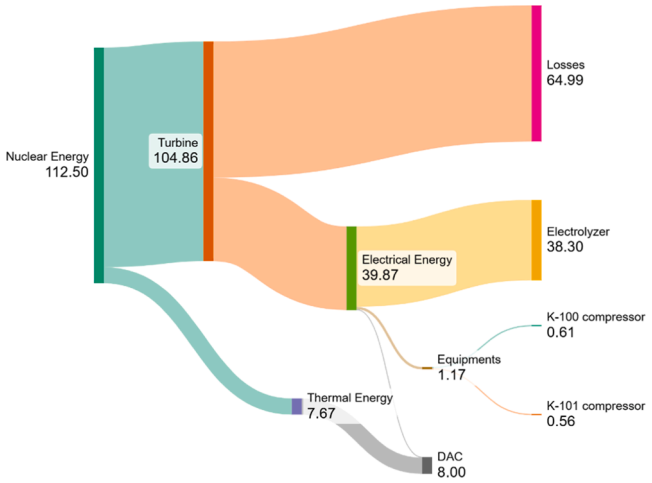


Fig. 4. Energy Sankey diagram [MW].

Table 6
Additional power required by the plant in DAC case.

Equipment	Power [kW]
E−101	227.5
E−104	159.6
K−102	4.803
T−101 reb	271.7
T−103 reb	2358
Heat reactor 1	936.5
Heat reactor 2	929.5

Table 7
CapEx comparison (10 years plant lifetime).

	DAC	FLUE GAS	Benchmark
3 Empty nuclear reactor [M$]	150	150	150
3 recharges [M$]	105	105	105
Alkaline electrolyzer [M$]	30.60	31.95	33.26
Equipments [M$]	9.82	10.07	10.22
DAC [M$]	90.20	-	-
CCU [M$]	-	3.72	-
Grassroot cost [M$]	392.51	307.72	305.54

Table 8
Steam and cooling water consumption.

	DAC	FLUE GAS	Benchmark
steam			
E−101 (heater) [kt/y]	3.9	4.1	4.2
E−104 (heater) [kt/y]	2.7	2.9	3.0
cooling water			
E−102 (cooler) [kt/y]	836.6	878.5	908.9
E−105 (cooler) [kt/y]	345.0	362.3	376.0
condenser 1 [kt/y]	4.2	4.2	4.5
condenser 2 [t/y]	504.2	504.2	490.8

Table 9
OpEx costs.

	DAC	FLUE GAS	Benchmark
steam			
E−101 (heater) [k$/y]	59.9	63.1	65.6
E−104 (heater) [k$/y]	42.0	44.4	46.2
cooling water			
E−102 (cooler) [k$/y]	49.8	52.3	54.1
E−105 (cooler) [k$/y]	20.5	21.6	22.4
condenser 1 [k$/y]	0.25	.25	.26
condenser 2 [k$/y]	30.0	30.0	29.2
CO_2 sources OpEx [M$ /y]	0.95	1.09	-
Total utilities costs [M$ /y]	1.16	1.31	0.22
COM without depreciation [M$ /y]	5.95	6.19	4.88
COM with depreciation [M$ /y]	7.11	7.37	6.09

used, the annual costs would have been 47 M$ (considering electricity price of equal to 11.6c€/kWh). Therefore, it can be concluded that, in addition to environmental benefits, nuclear energy also leads to lower costs compared to fossil resources. In comparison with other renewable resources, modular nuclear energy offers the advantage of a continuous and reliable supply at a relevant scale for methanol synthesis, without being more expensive than solar or wind power [22]. Table 11 illustrates the payback period of each case in three different lifetime scenarios (considering the discount rate).

Fig. 7 illustrates the cost components contributing to the levelized cost of methanol production, along with the positive impacts of the sale of oxygen and carbon credits. the revenue generated from carbon credits and oxygen sales contributes significantly, amounting to approximately 230$ per ton of methanol. Conversely, nuclear reactors and batteries account for around 60 % of the levelized production cost. In addition, Table 12 shows the financial metrics chosen for each case, and with and

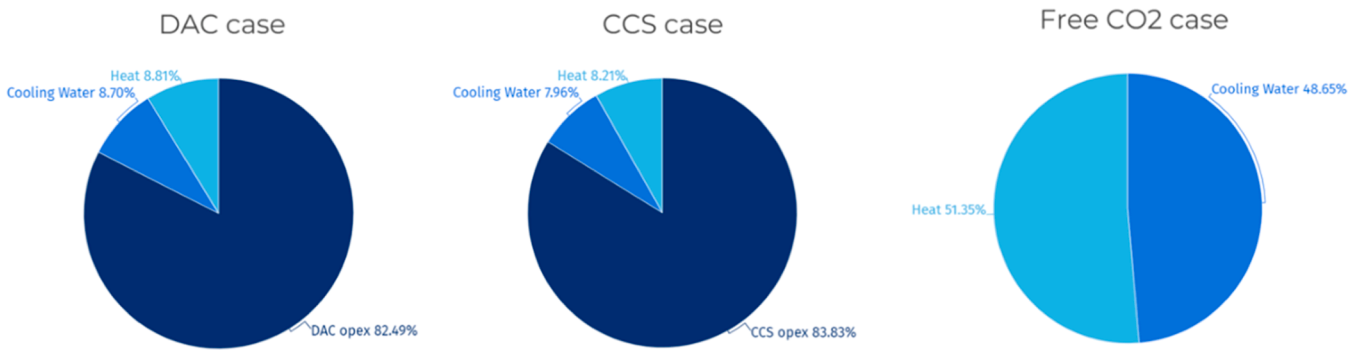
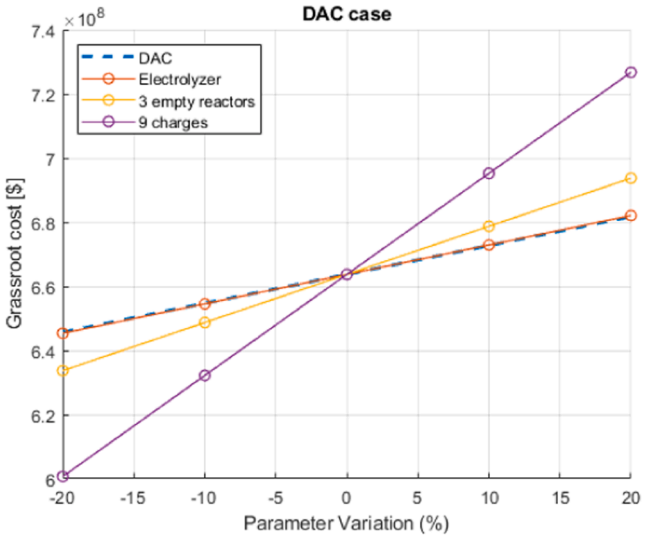
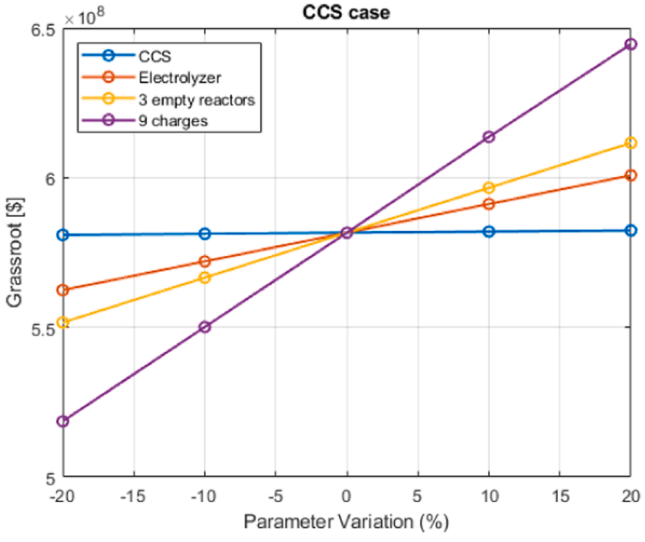


Fig. 5. Total utilities costs comparison.



(a) *Sensitivity analysis for DAC case*



(b) *Sensitivity analysis for CCU case*

Fig. 6. Sensitivity analysis for DAC and CCU cases.

Table 10
Production and revenues of DAC, FLUE GAS, and Benchmark cases.

	DAC	FLUE GAS	Benchmark
Methanol production [kt/y]	28.1	29.4	30.5
Oxygen production [kt/y]	45.2	47.5	49.4
Methanol revenues [M$ /y]	36.5	38.2	39.6
Oxygen revenues [M$ /y]	4.1	4.4	4.5
Total revenues [M$ /y]	40.6	42.5	44.2

Table 11
Payback Times considering the sale of carbon credits.

	DAC	FLUE GAS	Benchmark
10 years plant lifetime [year]	10.4	7.7	7.1
20 years plant lifetime [year]	14.0	10.8	10.4
30 years plant lifetime [year]	17.6	14.1	13.6

without carbon credits and oxygen selling.

Comparing the LCOP values with the equivalent for a conventional methanol plant (402$ per ton of MeOH) and the value according to Cameli et al. (2024) one [34] (1809$ per ton of MeOH), the nuclear energy-based method is cost competitive with the renewable energy-based e-MeOH but it is significantly higher than the conventional synthesis method (from natural gas).

The cleaner production route selected for the e-MeOH plant relies on expensive technologies that affect the selling price. This can be attributed to the high costs of batteries, direct air capture equipment, and electrolysis, as well as the low energy efficiency of the process. The sensitivity of the annual revenues of the DAC case on the cost of carbon credits, methanol and oxygen is illustrated in Fig. 8. The sensitivity of the other cases is similar to what has already been reported.

3.3. KPI

Table 13 shows the KPIs of the three cases analyzed, compared to the conventional standards. In particular, the comparison was made with a natural-gas-based process currently employed for large-scale production of methanol [47] and a process that uses direct air capture as a carbon source, a PEM electrolyzer, and renewable electricity [34]. The different processes have different production capacities; however, the performance indicators are normalized to the mass of the product, allowing for a consistent comparison.

Comparing the energy efficiency values, it can be seen that the energy efficiency of the natural-gas-based process currently employed for large-scale production is 23 % higher compared to the e-MeOH process. The main reason is the energy efficiency of the electrolyzer (which is in the range of 70–80). Additionally, the efficiency of the process is affected by the thermodynamic cycle used to produce electricity from the nuclear heat (Brayton turbine, with an efficiency of 38 %). An

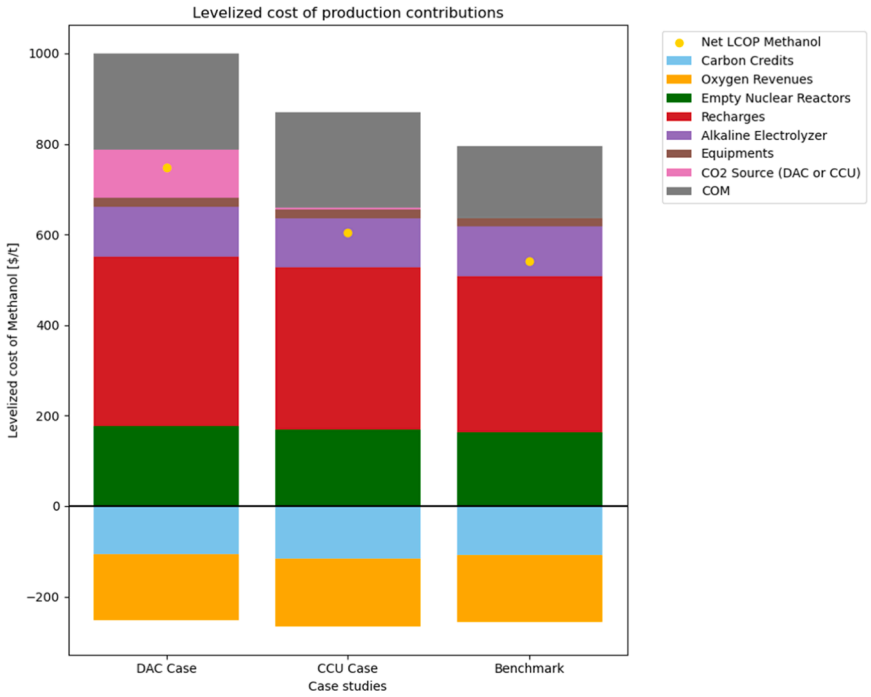


Fig. 7. Methanol levelized cost of production contributions.

Table 12
Financial metrics for different CO_2 sources.

	DAC	FLUE GAS	Benchmark
IRR [%]	3.26	5.33	6.18
IRR [%] with credits	3.63	6.27	7.14
LCOP (NPV) [$ /tMeOH]	852	722	648
LCOP (DNPV) [$ /tMeOH]	1914	1509	1400
LCOP (NPV) [$ /tMeOH] without selling O_2	1000	870	796
LCOP (DNPV) [$ /tMeOH] without selling O_2	2062	1657	1549
LCOP (NPV) [$ /tMeOH] with credits	747	605	541
LCOP (DNPV) [$ /tMeOH] with credits	1809	1392	1283

Table 13
Comparison of Key Performance Indicators for different technologies.

	Energy Efficiency	CO_2 Emissions ($kgCO_2$, eq $kgMeOH^{-1}$)	Levelized Cost of Product ($\$\ t^{-1}MeOH$)	Cost of CO_2 Avoided ($\$\ tCO_2^{-1}$)
DAC	0.18	−0.94	1809	860
CCU Flue Gas	0.19	−1.06	1392	563
Benchmark	0.19	−1.06	1283	506
e-MeOH (Cameli)	0.42	−0.61	1809	1071
Conventional	0.65	0.5–4.3 (0.7 median)	402	

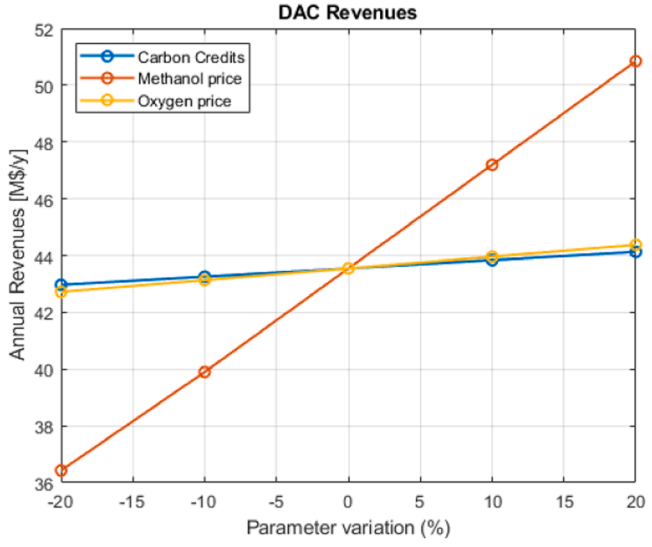


Fig. 8. Sensitivity analysis of the revenues for DAC case.

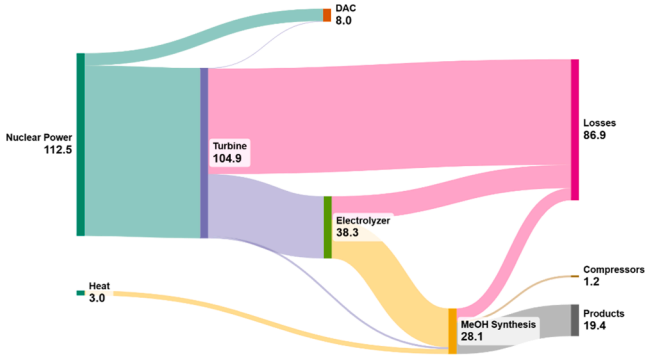


Fig. 9. Energy Sankey diagram (DAC case).

energy balance of the designed methanol plant is reported in the Sankey diagram in Figs. 9 and 10.

When comparing the GHG values, it is evident that facilities working with direct air capture, CCU and cheap CO_2 show a negative value, highlighting that the carbon dioxide emitted for methanol production is less than what is stored in the product. This presents an advantage from both environmental and economic points of view, allowing companies to

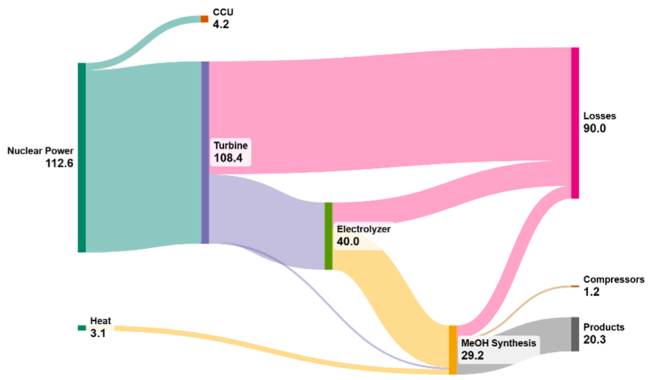


Fig. 10. Energy Sankey diagram (CCU case).

obtain additional benefits from carbon credits. Lastly, the cost per ton of CO_2 avoided by the simulated plant in all three cases is lower than that of the e-MeOH plant. This shows that despite suboptimal energy efficiency and high production costs, the processes are highly effective in reducing CO_2 emissions, making them more cost-effective in terms of CO_2 reduction.

4. Conclusions

This study explores a sustainable process for the synthesis of methanol using low-carbon technologies, including direct air capture (DAC) and carbon capture systems (CCU) for CO_2 extraction, electrolysis for H_2 production, and batteries as an energy source. The techno-economic analysis, accounting for CapEx and OpEx, highlights H_2 production via alkaline electrolysis as the main electricity demand, while thermal energy losses occur due to Brayton turbine inefficiencies. The DAC unit dominates CapEx, followed by electrolyzer costs, while methanol plant equipment has minimal economic impact. Despite high costs and suboptimal energy efficiency, the plant significantly reduces CO_2 emissions compared to traditional methods, supporting cli- mate goals. The carbon-negative route achieves −0.94 to −1.6 $kgCO_2$-eq/kgMeOH emissions, substantially lower than conventional methods (0.5–4.3 $kgCO_2$-eq/kgMeOH). The Levelized Cost of Production (LCOP) is estimated at $ 1809 per ton of MeOH in the DAC scenario, decreasing with CCU and Benchmark cases. Lowering DAC CapEx is crucial to achieving competitive LCOP. Economic feasibility and process efficiency could be improved by optimizing energy use, reducing costs in DAC, electrolyzers, and nuclear batteries, and encouraging policy support. These improvements can make methanol production economically and environmentally sustainable, advancing global emission reduction efforts and promoting a low-carbon economy.

CRediT authorship contribution statement

Emanuele Moioli: Writing – review & editing, Writing – original draft, Supervision, Funding acquisition, Formal analysis, Data curation, Conceptualization. **Flavio Manenti:** Writing – review & editing, Writing – original draft, Conceptualization. **Bozzini Marcello:** Writing – review & editing, Writing – original draft, Visualization, Investigation, Formal analysis, Data curation, Conceptualization. **Margherita Signorelli:** Writing – review & editing, Writing – original draft, Formal analysis, Data curation, Conceptualization.

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.

Appendix A. Supporting information

Aspen HYSIS V11 does not support the direct implementation of Eqs. (5) and (6) because it only accepts specific types of kinetic models.

To develop a kinetic model that is compatible, the thermodynamic equilibrium equations were integrated into the kinetic constants and the equation units were adjusted to meet the de- mands of Aspen Plus. The modified kinetic model is displayed in Equations.

Table A.14 displays the model parameters for Eq. A.1, A.2 and A.3, with pressure in bar and temperature in K.

Methanol synthesis:

$$r_{CH_{3OH}} = \frac{k_1 P_{CO_2} P_{H_2} - k_6 P_{H_{2O}} P_{CH_{3OH}} P_{H_2}^{-2}}{\left(1 + k_2 P_{H_{2O}} P_{H_2}^{-1} + k_3 P_{H_2}^{0.5} + k_4 P_{H_{2O}}\right)^3} \left[\frac{\text{kmol}}{\text{kg}_{\text{cat}} \cdot \text{s}}\right] \tag{A.1}$$

Reverse water gas shift reaction:

$$r_{RWGS} = \frac{k_5 P_{CO_2} - k_7 P_{H_{2O}} P_{CO} P_{H_2}^{-1}}{1 + k_2 P_{H_{2O}} P_{H_2}^{-1} + k_3 P_{H_2}^{0.5} + k_4 P_{H_{2O}}} \left[\frac{\text{kmol}}{\text{kg}_{\text{cat}} \cdot \text{s}}\right] \tag{A.2}$$

Table A.14
Parameters of the rearranged kinetic model

i	A_i	E_i
k_1	7, 138	−36, 696
k_2	3453.6	0
k_3	0.499	−17, 197
k_4	$6.62E-11$	$-1.24E+5$
k_5	$8.14E+3$	94, 765
k_6	$2.79E+14$	21, 999
k_7	$7.61E+11$	55, 080

Temperature dependence of rate constants

$$k_i = A_i \cdot \exp\left(-\frac{E}{RT}\right) \quad \text{(A.3)}$$

Appendix B. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.jcou.2025.103186.

Data availability

Data will be made available on request.

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