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Life Cycle Assessment of Synthetic Methanol Production: Integrating Alkaline Electrolysis and Direct Air Capture Across Regional Grid Scenarios

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ABSTRACT

A transition to low-carbon fuels is integral in addressing the challenge of climate change. An essential transformation is underway in the transportation sector, one of the primary sources of global greenhouse gas emissions. The electrofuels that represent methanol synthesis via power-to-fuel technology have the potential to decarbonize the sector. This paper outlines a critical comprehensive life cycle assessment for electrofuels, with this study focusing on the production of synthetic methanol from renewable hydrogen from water electrolysis coupled with carbon from the direct air capture (DAC) process. This study has provided a comparison of the environmental impacts of synthetic methanol produced from grids of five regions (India, the US, China, Switzerland, and the EU) with conventional methanol from coal gasification and natural gas reforming. The results from this impact assessment show a high dependency of environmental scores on the footprint of the grid. Switzerland, with its limited usage of fossil fuels in grid electricity, has shown the least environmental damage in most of the impact categories in comparison to more non-renewable grids like India and China. Interestingly, conventional methanol has proved to be more environmentally friendly when compared with non-renewable grids like India and China in most of the impact categories.

Keywords: Alternative Fuels, Aspen Plus, Carbon Dioxide Capture, Energy, Environment, Hydrogen

INTRODUCTION

The drive for reducing greenhouse gas (GHG) emissions has resulted in a global focus on sustainable fuels, with synthetic methanol among other potential alternatives to fossil fuels. Synthetic methanol combined with hydrogen (H_2) and carbon dioxide (CO_2) can be a pathway for decarbonizing the transportation and chemical feedstock production sector. Sustainable methanol paths rely on hydrogen generation by alkaline electrolysis and CO_2 capture through direct air capture (DAC) technologies. At the same time, fossil fuels demonstrate their continued relevance to world economies, and despite global endeavors to slash emissions, those typical mitigation methods are falling short of the ambitious targets set by the Paris Agreement. Synthetic fuel production is a promising avenue of study to fill this gap when paired with net carbon-negative technologies like DAC [1]. With ubiquitous CO_2-scrubbing technology, concentrated CO_2 streams are achievable for fuel production. Carbon dioxide is hence considered a renewable feedstock since it is non-depleting [2], [3], [4]. However, extraction and refining of the isolated carbon dioxide stream requires a significant amount of energy, which can further contribute to environmental damage scores. Hence, it can be stated that carbon capture and utilization (CCU) methods do not explicitly yield the environmental benefits one might assume, necessitating careful assessment. This often stems from the fact that these processes generally require substantial input energy. A detailed life cycle assessment (LCA) will be essential for elucidating the environmental footprints of synthetic methanol and discovering sustainable production pathways.

The studies at carbon capture plants combined with renewables for methanol manufacture present an intentional approach to reduce GHG emissions and transition to sustainable production of chemicals. The studies [5], [6] analyze the economic and environmental performance of DAC and its environmental guide in the field of methanol production. In the work by [7] more of these arguments are fleshed out by comparing power-to-fuel and power-to-DAC approaches and providing evidence for the efficiency of DAC to facilitate climate change mitigation in Ireland. Biernacki et al. [8], who also consider the environmental impacts of using renewable electricity to produce methanol, further demonstrate the integration of renewable energy into the chemistry industry. Through a detailed assessment of CCU technology development, the research by [9] emphasizes that life cycle assessment (LCA) is fundamental to maximizing these technologies for environmental and economic sustainability. The research publications [10], [11], [12], [13] have examined green methanol production from CO_2 and renewable hydrogen, highlighting the significance of process design and the use of renewable energy sources in fuel production.

The literature thus far has much interest in the LCA of synthetic methanol and its precursors. However, most of these studies are too geographically limited, neglecting to model changes in grid mixes and lacking sufficient attention to the co-optimization of end-use electricity use. Most importantly, the differences in the carbon intensity of the electricity grid between countries and the resulting variability in environmental impacts remain largely unaddressed.

The present work can contribute to overcoming the existing research gaps by providing a detailed cradle-to-grave LCA of synthetic methanol and emphasizing the evaluation of electricity sources used for hydrogen production from alkaline electrolysis. This research analysis focuses on the impacts of electricity grids of five large-scale regions, namely India, China, Switzerland, Europe, and the USA, representing a wider range of electricity grid carbon intensities. Combining Aspen Plus modeling for process-level simulations with region-specific LCA data, this research depicts the regional environmental trade-offs related to electricity utilization depending on the grid. Moreover, this study seeks other routes for reducing ecological footprints, such as renewable energy incorporation and optimized electrolysis performance.

This work is significant because it features both the methodological rigor of high-resolution integration of Aspen Plus process simulations with geographically explicit LCA and the scenario-based assessment of regional electricity grids, yielding actionable insights for policy-makers and industrial stakeholders. Instead of generalizing a single electricity input or assumed constant, this research serves as a dynamic model of grid mixes to enable a more realistic evaluation of the environmental viability of synthetic methanol.

This study is critical in closing urgent knowledge gaps in the literature. This work leverages advanced modeling and assessment tools to help inform sustainable energy pathways and aid in the decision-making for the low-carbon transition.

METHODOLOGY

The methodology for assessing the environmental sustainability of synthetic methanol production combines process simulation, life cycle assessment (LCA), and comparative analysis. Hydrogen from alkaline electrolysis and subsequent conversion to methanol through hydrogen and CO_2 was modeled in Aspen Plus for process simulation and energy balance calculations. Parameters like electrolyzer operations, energy requirements, and process operations efficiency were specifically modeled to simulate hydrogen production in Aspen Plus.

The carbon dioxide used for methanol manufacturing was obtained from direct air capture (DAC) technologies. Plant data for DAC was imported from several literature sources ([14], [15], [16]), which allowed us to quickly disaggregate energy usage, material requirements, and CO_2 capture efficiencies. Using the LCA methodology, the above inputs were parametrically modeled to account for realistic operating situations, allowing for a comprehensive analysis of DACs' contribution to the overall environmental footprint.

Life cycle assessmentAn LCA was conducted following the ISO 14040 and 14044 frameworks using the SimaPro 9.6.0.1 software and various Ecoinvent databases. A cradle-to-grave system boundary was defined, including all stages from raw material extraction and energy inputs through methanol production and final use. Environmental impacts were evaluated using the ReCiPe 2016 impact assessment method with GWP, fossil resource depletion, and other impact categories of interest. The electricity consumption for hydrogen production has been modeled under five regional grid scenarios, i.e., India, China, Switzerland, Europe without Switzerland (EU), and the United States of America (USA) using the Ecoinvent database for country energy mix. The above geographical areas were chosen to capture a wide range of carbon intensity of the electricity grid, from coal-heavy grids to high-renewable generation grids across the globe.

The results from the LCA were contextualized by evaluating the LCA outcomes for synthetic methanol against conventional methanol production pathways, namely coal gasification and natural gas reforming. All these conventional pathways data were obtained from the Ecoinvent database in SimaPro to ensure consistency and comparability. Combining Aspen Plus simulations with region-specific life cycle assessment (LCA) enabled a high-fidelity examination of the environmental trade-offs of synthetic methanol production. This study draws

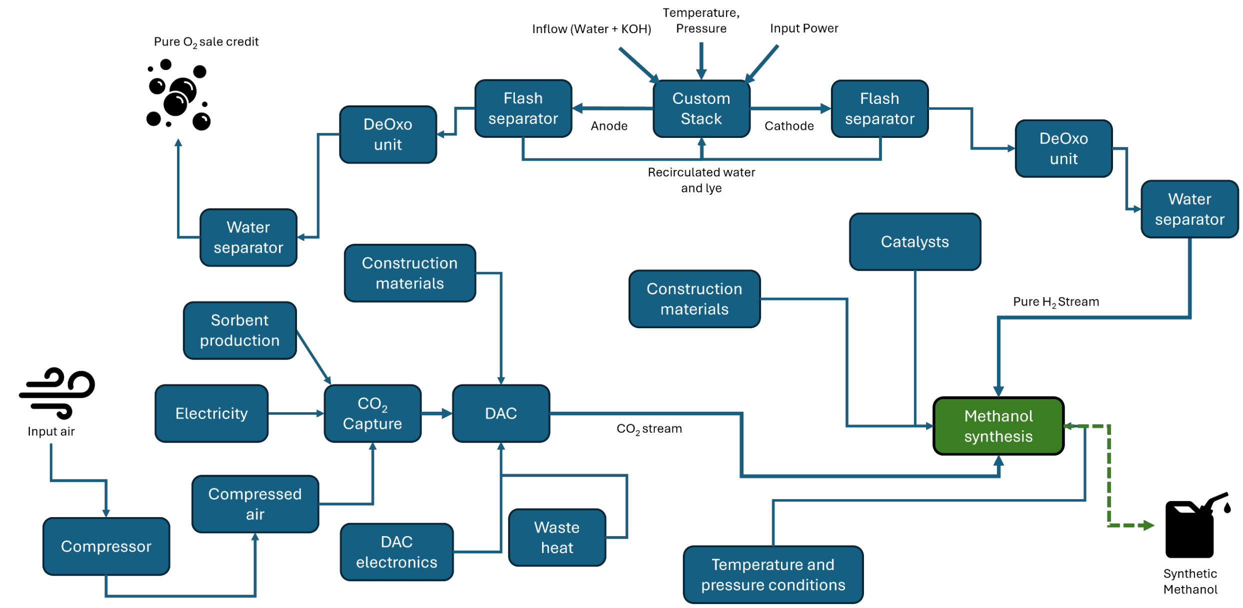

Figure 1: Overall methodology adopted for synthetic methanol production.

on available DAC data from credible literature sources and compares the results across regional grid scenarios and conventional production pathways to inform comprehensive insights into the potential for decarbonization and the hazards associated with transitioning to sustainable methanol production. The overall production methodology is depicted in Figure 1.

Hydrogen production

The hydrogen production for this study has been modeled as a 500 kW electrolyzer in Aspen Plus, along with various balance of plant components. The hydrogen production modeling aims to obtain a purity greater than 99.99% to make industrially suitable hydrogen. As shown in Figure 1, the stack has been custom-modeled using the Aspen Custom Modeler at 25 bars of pressure and at a temperature of 75°C. This work has significantly used the semi-empirical polarization curve model developed by Sánchez et al. [17], [18] to generate a customized model for an alkaline electrolyzer stack in the Aspen Custom Modeler. This model has robustly described the electrochemical behavior of the alkaline water electrolyzers, incorporating critical resistive, kinetic, and thermodynamic phenomena for hydrogen production.

The Aspen Plus model is focused on efficiency and environmental effects, simulating the combined alkaline electrolysis for hydrogen production. Water and a lye solution are electrolyzed at the system's cathode and anode, producing hydrogen and oxygen molecules. This approach recycles the leftover water and lye produced at the two electrodes back to the stack (B1) to minimize the waste of resources and to maintain permanent operation. During recirculation, the recirculating streams are cooled using two shell-and-tube heat exchangers (IC-R1 and IC-R2) to maintain ideal operating temperatures for the stack to enhance system performance.

A de-oxygenation kinetic reactor unit operates on the cathode side to remove any oxygen impurities from the hydrogen product stream. This reactor facilitates the controlled reaction of surplus hydrogen and oxygen impurities to create water. This process creates high-purity hydrogen at 99.9958% purity that has high industrial utilization after extraction from the water stream. For oxygen purification at the anode side, a similar purification process is implemented via oxygen extraction as a product for real-world use. This recovery not only provides a potential financial benefit by valuing the by-product oxygen, but it also reduces the environmental impacts associated with the oxygen production processes, aligning with sustainable and resource-efficient concepts.

The model results show that approximately 59 units (kWh) of electricity are required to produce 1 kg of pure hydrogen. Similarly, 9.3 kilograms of makeup water is required to produce one kilogram of pure hydrogen.

Carbon capture

This analysis's DAC plant construction and operating data are based on Climeworks' work [14]. The carbon capture is based on the temperature-vacuum swing adsorption method. The plant's capacity is four kilotons (kt) CO_2 per year with an operational life of 20 years. The plant's construction is divided into collector, processing, land requirement, and hall and tank units. The land requirement for this 4-kt/year plant is taken as 1045 m^2. The LCI also considers the materials required to manufacture, operate, and maintain DAC systems. The existing plant comprises eight collection containers, each containing six CO_2 collectors and a processing unit. The materials are procured and processed according to industry requirements, including steel, stainless steel, aluminum, copper, concrete, insulation, and polymers. Considering global recycling rates (e.g., 70% for copper and 85% for steel), the LCI includes recycling rates for key metals, such as copper, steel, and aluminum. Plastics and insulation hand disposed of in landfilling or waste incinerator techniques are examples of non-metallic materials. For conventional production, end-of-life scenarios are considered to avoid burdens, accounting for the environmental credit through co-generated heat and energy in the waste treatment. The energy requirements for this plant have been fulfilled by waste heat from chemical industries and electricity. The waste heat requirement has been taken as 1.55 MJ and 0.55 kWh of electricity for extracting 1 kilogram of CO_2 [15], [16], [19]. The sorbent type for carbon capture was taken as zeolite powder. The solid low-temperature sorbent consumption requirement was 0.788 g/kg of CO_2 captured [19].

Methanol production

Several interconnected procedures are used in the CO_2 hydrogenation process to produce methanol, increase productivity, and reduce environmental effects. A low-temperature powder sorbent DAC system is used to capture CO_2 at the start of the process. The methanol production for this study is based on research done by [20]. For every kilogram of methanol produced, the process consumes 1.446 kg of CO_2, 0.208 kg of H_2, and 2.173 kWh of electricity. The product is 1 kg of 95.3% pure methanol [20]. In the synthesis of methanol, the streams of CO_2 and H_2 are compressed and heated to 6.5 MPa and 210°C, respectively, before being fed into an adiabatic fixed-bed catalytic reactor with a Cu/Zn/Al catalyst installed based on the Aspen model by [20]. The reaction produces water and methanol; unreacted gases are recycled to increase conversion efficiency. However, during the separation process, there are minor losses of CO_2 (36.32 kg/h) and H_2 (9.64 kg/h). The purification process involves treating about 281 kg of water every hour, and a distillation column refines the resulting methanol stream.

RESULTS, DISCUSSION, AND CONCLUSIONS

The underlying energy mix in each location drives notable trends in the Life Cycle Impact Assessment (LCIA) results for methanol production across different energy grids. In addition to traditional production techniques like coal gasification and natural gas reforming, the comparison covers the United States, Switzerland, India, the European Union, and China grids. Particulate matter generation, ionizing radiation, ozone depletion, global warming potential, and other essential impact categories were assessed. The observed differences in environmental impacts can be explained by the energy grid performance of each region, which reflects the proportion of nuclear, renewable, and fossil fuels in its electricity generation portfolio.

Compared to the grids in the United States, Switzerland, and the European Union, the global warming potential (GWP) of the Chinese and Indian grids is significantly more enormous. For instance, the Chinese grid records 11.51 kilograms CO_2 eq per kilogram of methanol, whereas the Indian grid displays 15.93 kg CO_2 eq. On the other hand, the Swiss grid exhibits a net carbon sequestration effect, with a negative GWP of -0.97 kg CO_2 eq. The negative values indicate the avoided emissions due to the sale of purified oxygen. This discrepancy can be linked to China's and India's heavy reliance on coal and other fossil fuels, which raise CO_2 emissions significantly when energy is generated. Coal makes up more than half of the electrical mix in China, and in India, it makes up around 70%. Conversely, Switzerland's energy mix is primarily composed of nuclear and hydroelectric power, which are nearly carbon-neutral and account for its negative GWP numbers.

Across all grids, stratospheric ozone depletion is typically minimal, but it is marginally higher in areas where a significant portion of fossil fuels are used. The Swiss grid reports 0.000002 kg CFC11 eq, while the Indian grid displays the highest amount at 0.000005 kg CFC11 eq. Though in small proportions compared to past emissions from refrigerants and aerosols, burning fossil fuels emits chlorinated chemicals that can damage the ozone layer. Switzerland contributes very little to ozone depletion because of its emphasis on clean energy sources, primarily hydropower and nuclear energy [21].

Impacts of ionizing radiation differ significantly; the EU grid has the second-highest figure at 2.84 kBq Co-60 eq, while the Swiss grid has the highest at 3.57 kBq Co-60 eq. Since ionizing radiation is released during the extraction, processing, and disposal of nuclear fuel, this pattern is consistent with the high percentage of nuclear power in Switzerland and the EU. On the other hand, because of its restricted use of nuclear energy, the Indian grid exhibits far lower ionizing radiation at 0.23 kBq Co-60 eq. There are noticeable differences in the creation of particulate matter and ozone, two processes that affect air quality and human health. The highest ozone generation values are seen in the Chinese and Indian grids, with the Chinese grid recording 0.03754 kg NOx eq and the Indian grid recording 0.04195 kg NOx eq. Similarly, the Indian grid has the largest particle matter generation

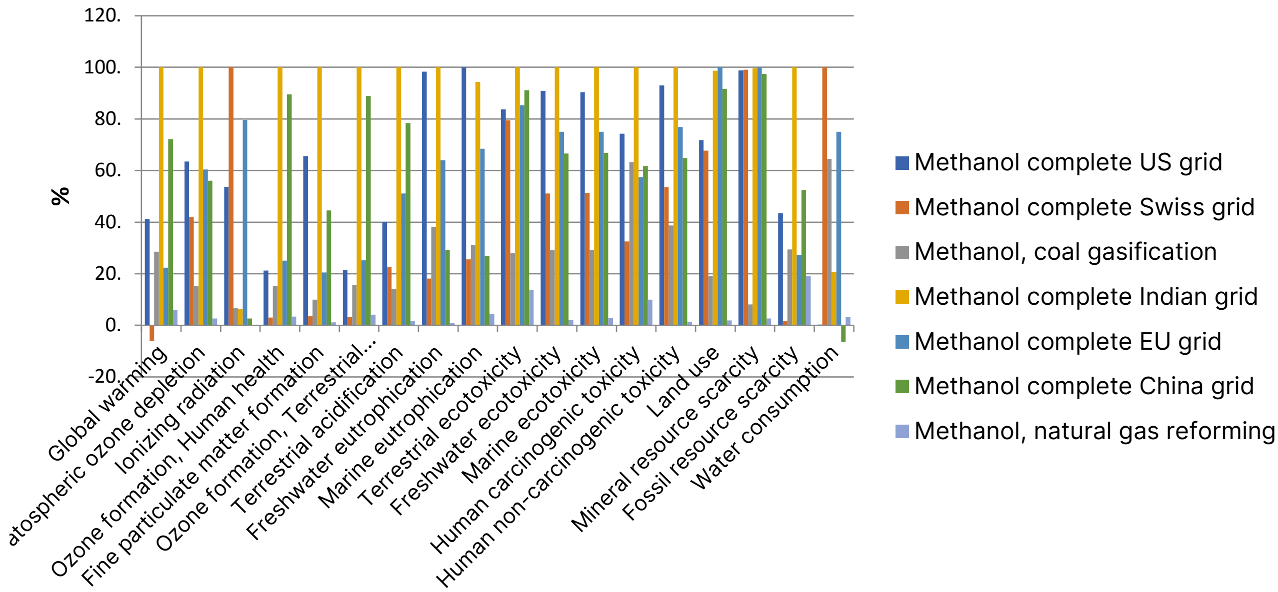

Figure 2: Life cycle impact results for synthetic and conventional methanol compared across various grids.

(0.04575 kg PM2.5 eq). These outcomes are caused by nitrogen oxides (NOx) and fine particles released while burning coal and other fossil fuels. With 0.00126 kg NOx eq for ozone formation and 0.00159 kg PM2.5 eq for particulate matter formation, the Swiss grid, on the other hand, has the lowest values in these categories because of its clean energy mix. An overall comparison of all the impact categories for various region-based grids for synthetic methanol and conventional methanol (natural gas reforming and coal gasification) is depicted in Figure 2. The significant impact that energy mixes have on environmental effects is highlighted by the comparative Life Cycle Impact Assessment (LCIA) for methanol production across several energy grids. Due to their carbon-intensive energy generation, grids that rely heavily on coal and other fossil fuels, like those in China and India, have far higher global warming potential (GWP), ozone formation, and particulate matter formation. On the other hand, networks that use cleaner energy sources—such as Switzerland's combination of nuclear and hydroelectric power—achieve low or even negative GWP values, which indicates net carbon sequestration. Furthermore, the effects of ionizing radiation and stratospheric ozone depletion correspond with the frequency of nuclear power and fossil fuel burning, respectively, in local grids. These results highlight how important it is to switch to low-carbon and renewable energy sources to lessen the adverse environmental effects of methanol production, especially in areas that rely significantly on coal and other fossil fuels.

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