Supplementary Information (SI) for Energy Advances.

A Cradle-to-Gate Life Cycle Assessment of Green Methanol Production Using Direct Air Capture

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Supplementary Information 1

Additional Life Cycle Inventory Analysis Information

DAC Construction and EOL

While detailed construction inventories are not generally published by DAC development companies due to the potential for release of proprietary information, Deutz and Bardow[1] have released some information regarding the types of materials used by Climeworks, and Madhu et al.[2] has performed calculations as well at the component level based on pre-existing processes in ecoinvent[2]. The inventories from these studies form the basis of this study. Construction has been shown to play only a minimal impact on overall impacts according to research by NETL[3], at just 0.0002 kg CO_2e per kg CO_2 captured at a 1 Mton/yr DAC facility; therefore, the impact to the results due to uncertainty in construction inventory is anticipated to be low but will be confirmed in the sensitivity analysis performed in the supplemental information.

Due to still being new technology, the plant life is assumed to be 20 years, which aligns with previous studies published[1,2,4]. For the 4,000 ton/year facility, the contributions of construction are amortized over the lifetime of the plant per the following equation:

$$\frac{Mass\ of\ emissions}{Functional\ unit} = \frac{Total\ emissions\ from\ construction}{Integrated\ facility\ design\ capacity * Capacity\ factor * Operational\ lifetime}$$

where a capacity factor of 0.95 is assumed to account for maintenance [5].

Sorbent Production & EOL Waste Treatment

The sorbent selected for all cases of DAC is Zeolite 13X based on its strong ability to absorb microwaves; Ellison et al.[6] states that zeolites have been often used in microwave regeneration studies because they have excellent microwave absorption and a relatively high CO_2 adsorption capacity[6]. Because zeolite 13X is cation-rich, it possesses local dipole moments which can absorb the microwave energy effectively[7]. Zeolite has also been demonstrated as a favorable sorbent for more conventional heat sources as well[8–13]. Hence, this sorbent is assumed for all DAC configurations considered in this study.

Zeolite 13X is expected to be replaced at regular intervals during the life cycle of the DAC facility due to performance degradation. The rate of depletion is assumed to be 0.788 g per kg CO_2 captured[14]. Since the functional unit (FU) of this LCA relates to the amount of synthetic methanol produced, this value is updated to 1.139 g sorbent per kg methanol produced based on the ratio of methanol production to CO_2 consumption.

Although the material and chemical makeup of zeolite 13X is available in the literature[15–17], the manufacturing life cycle of zeolite 13X to include energy consumption is not well documented. To determine the impacts of zeolite 13X, the inventory for zeolite powder in ecoinvent 3.8 was used, which represents the market for generic "zeolite, slurry, without water, in 50% solution state" [18]. A similar method for zeolite inventory was conducted by Gonzalez-Olmos et al.[14]. Zeolite is considered an inert material, so EOL treatment for sorbent is as municipal solid waste in a landfill[14].

Identification of Significant Issues

Based on the results of the LCI phase, the most significant issues related to the development of our model stem from uncertainties in the selection of certain parameters. These parameters include the energy inputs of DAC, the material and process assumptions for construction, sorbent depletion rate, and the pipeline travel distance for geological storage. These issues will be explored in the sensitivity analysis.

Evaluation

Completeness Check

This life cycle assessment study includes the full boundary suggested by the US DOE[5], to include energy generation, DAC construction and EOL activities, DAC operational processes, sorbent production and EOL activities, PV construction and EOL, CO_2 compression and transportation, and geological storage. In some cases, such as while developing the LCI for construction, we made logical assumptions based on similar LCAs[1,2,4]. Some uncertainty is present in the study, particularly in the construction inventory. Sensitivity analysis was performed to highlight the impact this could have on the final results.

Consistency Check

The goal and scope of this study is to analyze the implementation of renewable power sources and regeneration heat sources with synthetic methanol production and low temperature solid sorbent DAC using LCA methodology and a cradle-to-gate system boundary. The life cycle inventory represents all inputs included in the system boundary. The results are consistent with the assumptions made in the study and with the goal and scope.

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