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Application of a systematic methodology for sustainable carbon dioxide utilization process design

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As concerns about the environment are growing, new efforts are needed to achieve more sustainable processes. One such environmental concern is global warming, which is primarily caused by the greenhouse effect or the increase in concentration of greenhouse gases [1]. The most significant greenhouse gases are carbon dioxide, methane and nitrous oxide, of which carbon dioxide is the highest constituent at 82%. Furthermore, the amount of carbon dioxide emissions is growing with time. These trends make it evident that there is a need for methods to reduce these greenhouse gases emissions. While there are two methods of reducing carbon dioxide emissions, carbon capture and storage (CCS) and carbon capture and utilization (CCU), CCU is considered promising as it makes further use of the carbon dioxide as a solvent, raw material, and reagent to produce valuable products [1]. Using such utilization processes, the emissions can be reduced as they are being utilized and profit can be obtained, or the cost of operation for the carbon dioxide treatment can be returned, through this utilization process.

In order to systematically reduce such emissions, carbon capture and utilization is considered rather than carbon capture and storage. To achieve this a methodology is developed to design sustainable carbon dioxide utilization processes. First, the information on the possible utilization alternatives is collected, including the economic potential of the process and the carbon dioxide emissions. The carbon dioxide emissions can be classified as direct and indirect emissions in a chemical process. The net carbon dioxide is determined for the utilization processes as the indirect carbon dioxide emissions minus the carbon dioxide utilized. Processes that presents zero or negative net carbon dioxide emission are desired in order to reduce the carbon dioxide emissions. Using this estimated preliminary evaluation, the top processes, with the most negative carbon dioxide emission are investigated by rigorous detailed simulation to evaluate the net carbon dioxide emissions. Once the base case design is established and evaluated, targeted improvements are made by exploiting opportunities, for example, optimization, heat integration and improved design decisions so that more sustainable and lower net carbon dioxide emission alternatives are obtained.

This method is applied to various processes where carbon dioxide is used as raw material. First, the process data are collected and compared. The economic feasibility is evaluated. From this, five processes are selected and analyzed in detail: the production of dimethyl carbonate, succinic acid, propylene carbonate, dimethyl ethylene and methanol. Not all the studied processes could be designed for zero or negative net carbon dioxide emission. Propylene carbonate production is found to have a negative net carbon dioxide, where, implementing targeted process improvements minimized the net carbon dioxide emission to -0.389 kg of carbon dioxide per kg of propylene carbonate. On the other hand, for succinic acid production, even after targeted improvements, the net carbon dioxide remained

positive, even though compared to the existing industrial processes there is a relative reduction of upto 85%.

What this study shows is that for meaningful net carbon dioxide reduction, the carbon dioxide utilization processes need to be selected very carefully to obtain the best results. However, the opportunity to potentially reduce the net carbon dioxide emissions for the production of some bulk chemicals with carbon dioxide as feedstock exists.

- [1] Yuan, Z., Eden, M.R., Gani, R., 2016. Toward the Development and Deployment of Large-Scale Carbon Dioxide Capture and Conversion Processes. *Ind. Eng. Chem. Res.* 55, 3383–3419.
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