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A generic methodology for the design of sustainable carbon dioxide utilization processes using superstructure optimization

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Global warming and other environmental concerns are fueling increased focus on sustainability resulting in new and stringent guidelines, especially with regard to emissions [1]. Greenhouse gases are prevalent and among harmful emissions that are targeted to be reduced; carbon dioxide (CO₂) is the primary greenhouse gas that is targeted via carbon capture and storage (CCS) as well as carbon capture and utilization (CCU) [1]. Carbon capture and utilization is showing promise because, in contrast with carbon capture and storage, it takes the captured carbon dioxide and makes further use of it, including as an extractive agent or raw material. Chemical conversion, an important element of utilization, involves the use of carbon dioxide as a reactant in the production of chemical compounds [2]. However, for feasible implementation, a systematic methodology is needed for the design of the utilization, especially chemical conversion, processes. To achieve this, a generic methodology has been developed, which adopts a three-stage approach consisting in (i) process synthesis, (ii) process design, and (iii) innovative and sustainable design [3]. This methodology, with the individual steps and associated methods and tools, has been developed and applied to carbon dioxide utilization networks.

This work will focus on the first stage, process synthesis, of this three-stage methodology; process synthesis is important in determining the appropriate processing route to produce products from a selection of feedstock [4], in this case carbon dioxide. This stage contains three steps, each incorporating relevant methods and tools. First, with the help of user specifications, the problem is specified. Then, the processing routes linking feed and product are represented via a superstructure. This is performed with the help of a software interface, Super-O, guiding through the steps of the methodology related to superstructure development and optimization [5]. The data necessary to perform this step is extracted from an especially structured database ontologically designed for the easy extraction and addition of data. This database contains information on the raw material (including different carbon dioxide emission conditions), the products and the reactions linking these. With this help of the database it is possible to quickly compare utilization processes for a specific problem as the information is easily accessible; thereby, for the problem of certain products and given a specific feed it becomes easy to say which conversion processes are most promising to sustainably reduce emissions.

This methodology, the software interface and the database will be presented together with validation results from a conceptual example. Using the methodology a network of conversion reactions from carbon dioxide to various carbon, hydrogen and oxygen containing compounds, such as methanol, dimethyl ether and dimethyl carbonate, is developed; using ProCARP [6], a software tool for reaction path synthesis, the network is created containing the feasible reactions. Using the developed database, the data needed, including reaction conversions and separation factors, for the superstructure is extracted. The optimization gives the selection of the best processing routes. These are subsequently designed rigorously and analyzed for economic and environmental sustainability. The resulting design and analysis show the use of the methodology and the opportunity for sustainable reduction of emissions using conversion processes to produce chemical products.

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