Sustainable process design with process intensification - Development and implementation of a framework for sustainable carbon dioxide capture and utilization processes - DTU Orbit (05/10/2019)

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Due to environmental concerns, greenhouse gas emissions, particularly carbon dioxide, need to be reduced. There are numerous methods being discussed, one of which is carbon dioxide capture and utilization (CCU). Carbon dioxide capture and utilization removes the carbon dioxide from the offgas streams and transforms it into commercial products, for example the conversion to value-added chemicals. While CCU is promising, especially as the commercial products provide an economic incentive, the sustainability needs to be ensured. Assuring the sustainability of carbon dioxide capture and utilization processes is a challenge as the energy requirements result in indirect emissions that should not exceed the utilization. In this work, therefore, a framework for the sustainable design of carbon dioxide capture and utilization (with a focus on conversion) processes is developed and implemented.

The developed framework adopts a 3-stage approach for sustainable design, which is comprised of: (1) synthesis, (2) design, and (3) innovation. In the first stage, the optimal processing route is obtained from a network via a superstructure-based approach. This stage incorporates a structured database for the storage and retrieval of data, reaction path synthesis for the generation of reaction pathways and products, and a user interface, Super-O, which facilitates the implementation of Stage 1 of the framework. Then, the output of this stage is used as the input to the second stage, where the optimal route is rigorously designed, simulated, and analyzed. Stage 2 provides detailed equipment design and stream information, which is used in the analysis to provide targets for improvement. In Stage 3, the targets are addressed by finding innovative alternatives via hybrid methods, process integration, and process intensification. The end result is a more sustainable carbon dioxide capture and utilization process. The developed framework is then applied to the design of sustainable processes using carbon dioxide captured from a coal-fired power plant (as these represent almost 30% of global emissions). In the first stage, seven scenarios are considered to evaluate the influence of different parameters (such as prices and conversion) in finding the optimal processing route(s). The results show a trade-off in the reduction of carbon dioxide and the profit for the different routes. From Stage 1, four processes are considered and are designed and simulated in detail:

1. Dimethyl ether from methanol via combined reforming
2. Dimethyl ether from methanol via direct hydrogenation
3. Dimethyl carbonate via ethylene carbonate and methanol from combined reforming
4. Dimethyl carbonate via ethylene carbonate and methanol from direct hydrogenation.

Through the analysis of the processes, it can be seen that the methanol distillation and the dimethyl carbonate downstream separation contribute to large amounts of the utility consumption and therefore costs. Therefore, the reduction of the utility consumption of the methanol distillation and dimethyl carbonate downstream process are targeted for improvement. In Stage 3, the targets are addressed by introducing a hybrid distillation-membrane process and an intensified, reactive distillation dimethyl carbonate process. The result is four improved, more sustainable processes for the production of dimethyl ether and dimethyl carbonate from carbon dioxide. However, while it is possible to design carbon dioxide reducing processes, the amount of emissions that can be offset by these processes is small. Therefore, these carbon dioxide capture and utilization or conversion processes should be considered in conjunction with methods to improve efficiency and other alternative, sustainable processes.