Sustainable Design for Production of Dimethyl Carbonate from Ethylene Oxide, CO2 and Methanol - DTU Orbit (18/08/2019)

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There is a growing awareness and research into how to mitigate the carbon dioxide (CO2) emissions. Two attractive methods that can be applied in addressing this are, carbon capture and sequestration (CCS) (IPCC, 2005) where CO2 is captured at emission points, and deposited under a suitable geological formation, from whence it will not escape back into the atmosphere, or CO2 chemical utilization where CO2 is used as a raw material for producing a chemical compound. Dimethyl Carbonate (DMC) is an important bulk chemical because it is a viable substitute for methyl-tert butyl ether (MTBE) (F. M. Mei, 2009). DMC can be produced using different reaction pathways, for example, through the reaction of phosgene with methanol, which yields DMC and HCl. This method is the traditional route, but involves hazardous chemicals, and the product has high chlorine content. Another method is the alcoholysis of urea. First urea is produced from CO2 and ammonia. The urea then reacts with methanol to produce DMC. However, in this process, methyl carbamate is easily generated as mono-charged intermediate in the second reaction step, and this cannot be further reacted into DMC.

A more sustainable process design for the production of DMC is proposed using a systematic method that is based on a 12 task, hierarchal approach with CO2, ethylene oxide (EO) and methanol used as raw materials and ethylene glycol (EG) as the by-product. The production target is set at 100,000 metric tons with a product and by-product purity of 99% (w/w). The reaction path synthesis chosen consists of two steps. In the first step, EO and CO2 react (at a temperature of 110°C and pressure of 8 MPa) to produce ethylene carbonate and in the second step ethylene carbonate and methanol react (at a temperature of 90°C and pressure of 0.3 MPa) to produce DMC and ethylene glycol. The reaction path chosen produces a by-product that, at a given purity, can be sold.

A description of the process is as follows. The first reactor outlet consists of EO, CO2 and ethylene carbonate (EC). A flash separated as much of the CO2 as possible, and the rest of the stream is led into reactor 2, to which is added methanol as well. The outlet stream of the second reactor contains EO, CO2, EC, EG and DMC. First, a distillation column separates the rest of the EO and CO2 from the mixture, and recycles this back into reactor 1. A second distillation column separates DMC and methanol from EC and EG. Both these combinations form azeotropes. The DMC/methanol azeotrope is handled using a large distillation column at high pressure, from which 99% of the DMC can be extracted at high purity. The EG/EC stream is first cleaned of leftover methanol, hence fed into a distillation column, which separates as much of the EC as possible. The azeotrope cannot be broken through distillation, so a the difference in polarity between the two is taken advantage of, and a membrane is used to separate the rest of the EC from the EG. The EC is recycled back into the second reactor, and the EG has a high enough purity to be sold commercially.

The process described here is used as the reference design, that is, the base case design which is evaluated for process improvement related to process integration (heat integration), process optimization and sustainable improvement.

First, an economic analysis is performed for identifying process limitations that are translated into design targets used for heat integration and process optimization. If these limitations are minimized and/or eliminated the design targets are met. The design is then analyzed using a sustainability (Carvalho, 2012) and LCA (Kalakul, 2014) analysis in order to further identify process limitations and other design targets related to sustainability. In this poster, a more sustainable process for the production of DMC, through the utilization of CO2 will be presented. The 12 task-based approach will be presented and the input and output of each task will be highlighted.