



A Systematic Process Design for Sustainable Dimethyl Carbonate Production through Carbon Dioxide Utilization

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With greenhouse gas emissions becoming an increasing global concern and environmental laws becoming more stringent, processes that produce carbon dioxide should ensure minimal emissions.

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In this work, the systematic hierarchical decomposition design method consisting of twelve tasks as described by Babi et. al [2] is employed to design a process producing 100,000 metric tons of 99% pure DMC per year with an additional production of 73,000 metric tons of ethylene glycol (EG) of 91% purity. This method assists in constructing the process initially obtaining a base case and subsequently developing an optimized rigorous design. Data required to develop a plant of the desired capacity is assimilated in tasks 1-3 to facilitate preliminary design decisions. Those are then verified through a mass balance in task 4 employing the commercial design simulator PROII. The simulation is extended from the initially simple model to a rigorous one in tasks 5-6 leading to a full fledged rigorous model where mass and energy balances are confirmed in task 7. The process is then sized and an economic analysis is carried out with the software ECON in task 8-9 leading to a base case for the process. Through that, targets for improvement are identified and the process is improved through optimization and heat integration in tasks 10-12. This is followed by an environmental impact analysis after each improvement step, to assess the overall sustainability of the final design. Applying these last tasks enables the design of an economically viable and simultaneously sustainable process obtaining DMC.

DMC can be produced from methanol (MeOH) and CO₂ through an intermediate alkylene carbonate production route. In this mechanism, CO₂ reacts with EO to form ethylene carbonate (EC) in a reaction under elevated pressure. Subsequently, MeOH is added and a transalkylation of the cyclic intermediate occurs to form DMC and EG as a byproduct at near ambient conditions. Azeotrope formation between DMC-MeOH and EG-EC is a crucial part of the separation sequence in the process. DMC is obtained at high purity from the pressure sensitive DMC-MeOH azeotrope operating at 15 atm. The purity of byproduct EG coming from a regular distillation is further increased by hydrothermal conversion of the remaining EC and separated using a flash [3].

From an environmental standpoint, apart from the utilization of CO₂, equivalent with a net reduction of CO₂ emissions, a main focus is set to reducing waste. This is achieved by handling the azeotropes by minimizing the use of solvents which makes the separations environmentally benign. The process is made economically more attractive by mass integration through recycling EC and heat integration to use energy efficiently. Through this hierarchical decomposition method, a potential zero discharge closed loop system is designed through the recycle of CO₂ produced from the hydrothermal decomposition of EG-EC azeotrope.

[1] Ullmann, Fritz, et al. Ullmann's encyclopedia of industrial chemistry. Vol. 7. Weinheim, Germany: Vch, 2012.

[2] D. K. Babi, "Teaching Sustainable Process Design using 12 systematic Computer Aided Tasks". Computer Aided Chemical Engineering, 2015, vol. 37, pp. 173-178.

[3] Seader, Junior D., and Ernest J. Henley. Separation process principles. Hoboken, NJ: Wiley, 2011.

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