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In the past several decades, there has been a growing awareness and an increasing concern in the public

As a potential strategy to reduce carbon dioxide emissions into the atmosphere, CO_2 utilization processes have gained much attention in recent times as means to produce fine chemicals. Dimethyl carbonate (DMC) is one such product that can be synthesized by utilizing CO_2.

Dimethyl carbonate is a non-toxic, readily biodegradable chemical that exhibits high reactivity [1]. DMC received its VOC exemption under the Clean Air Act on January 13, 2009 by the US EPA. While the traditional production from phosgene and methanol uses toxic and hazardous chemicals, DMC can now be produced via the transesterification of ethylene carbonate (EC) and methanol. EC is obtained from reacting ethylene oxide (EO) with CO_2. Ethylene glycol (EG) is a valuable product that is coproduced in this process.

A sustainable process is developed to produce DMC and EG using a systematic framework [2]â€”a twelve-step hierarchical decomposition method. Using this approach, a plant with an annual production capacity of about 100,000 tonnes of DMC is designed. EO, CO_2, and methanol are the raw materials. EO and CO_2 are first reacted at 120 ^{o}C and 20 bar to form EC. A flash is used to separate EC from impurities and unreacted components. The EC stream is sent into the second reactor to react with methanol at 60 ^{o}C and atmospheric pressure to produce DMC and EG. The outlet of this reactor contains DMC-methanol and EG-EC azeotropes that are separated in a distillation column at atmospheric pressure. The overhead stream of DMC and methanol is separated in a high-pressure distillation column at 40 bar while the bottoms stream of EC and EG are separated using a membrane. Once the sizing and costing are done, a base case design is obtained.

An economic analysis is performed on the base case design to identify process hotspots that are translated into design targets for process integration and optimization. The resulting process is then put through sustainability analysis [3] and life cycle assessment [4] to refine it further with respect to environmental impact. In this project, PRO/II is used as the simulation tool. The final objective is to obtain a more sustainable process design that is also able to achieve a negative net CO_2 emission.

[1] P. Tundo and M. Selva, â€œThe Chemistry of Dimethyl Carbonateâ€. Acc Chem Res, 2002, vol. 35 (9), pp 706â€“716.

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

[3] A. Carvalho, H. A. Matos, and R. Gani, â€œSustainProâ€”A tool for systematic process analysis, generation and evaluation of sustainable design alternativesâ€.Â Comput. Chem. Eng.Mar. 2013, vol. 50, pp. 8â€“27.

[4] S. Kalakul, P. Malakul, K. Siemanond, and R. Gani, â€œIntegration of life cycle assessment software with tools for economic and sustainability analyses and process simulation for sustainable process designâ€.Â J. Clean. Prod.May 2014, vol. 71, pp. 98â€“109.

Topics: Process Design & Development | Sustainable Engineering

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