Achieving a More Sustainable Design for the Production of Di-Methyl Carbonate Via CO2 Utilization

Jhamb, Spardha; Hurley, Dane ; Sobczyk , Pawel ; Anantpinijwatna, Amata

Publication date:
2015

Document Version
Publisher's PDF, also known as Version of record

Citation (APA):
Jhamb, S., Hurley, D., Sobczyk , P., & Anantpinijwatna, A. (2015). *Achieving a More Sustainable Design for the Production of Di-Methyl Carbonate Via CO2 Utilization*. Abstract from 2015 AIChE Annual Meeting, Salt Lake City, United States.

(426d) Achieving a More Sustainable Design for the Production of Di-Methyl Carbonate Via CO2 Utilization

Conference: AIChE Annual Meeting

Year: 2015

Proceeding: 2015 AIChE Annual Meeting

Group: Computing and Systems Technology Division

Session: Interactive Session: Systems and Process Design

Time: Monday, November 9, 2015 - 6:00pm-8:00pm

Authors:

Jhamb,
S., Technical University of Denmark

Hurley,
D., Technical University of Denmark
Sobczyk,
P., DTU
Anantpinijwatna,
A., Technical University of Denmark

Carbon dioxide (CO_2) emissions are a great concern for the environment resulting in many new technologies and policies in order to mitigate these emissions. This ongoing issue has gained significant attention in recent years and poses a challenge for the 21st century. CO_2 utilization can be achieved in three ways; conversion into a fuel, a feedstock for producing important chemical compounds and lastly via non-conversion utilization such as for enhanced oil recovery and as a solvent [1].

One particularly important chemical which CO_2 can be converted into is dimethyl carbonate (DMC). DMC is a good replacement for toxic methylating agents and phosgene. Additionally, it can also be used as an octane booster in fuel as it significantly increases the octane number due to the high oxygen content (53.3 wt%) in comparison to other alkylcarbonates [2]. DMC can be produced from CO_2 by either reacting CO_2 directly with methanol or by firstly reacting ethylene oxide with CO_2 to produce ethylene carbonate as an intermediate followed by a subsequent reaction with methanol [4].

In this project, a process plant was designed using the two step reactions utilising CO_2 to produce DMC as well as the by-product ethylene glycol and any unconverted ethylene carbonate. A hierarchical decomposition approach was used for designing the process, by decomposing the synthesis into 12 hierarchical tasks. According to the design, the process will produce on a yearly basis around 15,000 metric tonnes of DMC (10% of the Chinese market, excluding the largest producer).

This design of the process is unique as it does not use conventional separation procedures like pressure-swing, reactive distillation or extractive distillation to break azeotropes that are commonly encountered during the separation of products, hence, avoiding the use of toxic chemicals. Instead, the separation of DMC and methanol utilises a pressure distillation column as the azeotrope is pressure sensitive and can be broken at 20 bar. Additionally, the azeotrope between ethylene glycol and ethylene carbonate is not sensitive to pressure so the possibilities of membrane separation were explored. A membrane that could separate the two compounds based on polarity was chosen, which could result in pure ethylene carbonate and almost pure ethylene glycol. Further, this membrane separation also reduces the consumption of energy in comparison to the installation of distillation columns.

Heat integration and process optimisation were then performed in attempt to reduce energy consumption and unnecessary costing according to the economic evaluation of the process. In order to meet the design targets these limitations need to be eliminated. Finally, a LCA and sustainability analysis were performed in order to reduce other limitations in the process design [3], [5].

This poster will present the 12 step hierarchical approach to synthesise a more sustainable process design for utilising CO2 to produce DMC. The results from each task and the important considerations for each stage will be highlighted.

References

[1] Michele Aresta. Carbon dioxide recovery and utilization. Springer Science & Business Media, 2003.

[2] Fredrik Bertilsson and Hans T Karlsson. Co 2 utilization options, part ii: Assessment of dimethyl carbonate production. Energy conversion and management, 37(12):1733–1739, 1996.

[3] Ana Carvalho, Henrique A Matos, and Rafiqul Gani. Sustainpro—a tool for systematic process analysis, generation and evaluation of sustainable design alternatives. Computers & Chemical Engineering, 50:8–27, 2013.

[4] Daniele Delledonne, Franco Rivetti, and Ugo Romano. Developments in the production and application of dimethylcarbonate. Applied Catalysis A: General, 221(1):241–251, 2001.

[5] Sawitree Kalakul, Pomthong Malakul, Kitipat Siemanond, and Rafiqul Gani. Integration of life cycle assessment software with tools for economic and sustainability analyses and process simulation for sustainable process design. Journal of Cleaner Production, 71:98 –109, 2014.