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Methanol production via CO_2 hydrogenation optimization using response surface methodology

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In the recent years, climate change has become more concern. Carbon dioxide (CO_2) is one of the greenhouse gas which contributes to the global warming. Many researches and developments have been conducted to mitigate CO_2 in the atmosphere. Among the studies, conversion of CO_2 into value added chemicals, i.e., methanol, with low operating cost is of interest. Methanol is considered as alternative fuel which is one of options for renewable energy resources. The reactions involving the conversion of syngas to methanol is as below.

Reverse water gas shift:

$$CO_2 + H_2 \leftrightarrow CO + H_2O$$

Methanol synthesis:

$$CO + 2H_2 \leftrightarrow CH_3OH$$

Reverse methanol steam reforming:

$$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O$$

In this presentation, optimization of CO_2 conversion to methanol via hydrogenation [1] for minimum methanol production cost is studied. The response surface methodology [2] is used as the optimization tool for this problem. The economic analysis involves all major equipment (excluding pump) costs, utilities cost, and cash flow analysis. The equations and the data from capital equipment – costing program (CAPCOST) is used to estimate the capital cost. The process is simulated using Aspen Hysys process simulator.

In the conversion to methanol via hydrogenation process, 1,000 kg mol/h of 21% water and 79% CO_2 at 1 bar is compressed and sent to two reactors in series for CO_2 hydrogenation. The product streams leaving reactors is then cooled and sent to two distillation columns in series to purify methanol product to 99.8 %w/w.

There are five decision variables for optimization of the process which are the temperature after cooler of each product streams leaving the reactor (total of three streams), and the temperature inlet to each distillation column.

For the response surface methodology (RSM), the objective is to minimize methanol production cost ($/ kg produced methanol). The local first - order regression model is performed to find the significant decision variables, and the second - order regression model of the objective function is performed to search for the local minimum point using Solver in Microsoft Excel.

The results show that response surface methodology can be used to minimize the methanol production cost in CO_2 hydrogenation process. The obtained optimum temperatures (decision variables) yields lower methanol production cost compared to base case.

References

[1] I. L. Wiesberg, J. L. de Medeiros, R. M. B. Alves, P. L. A. Coutinho, O. Q. F. Araujo, *Energy Convers. Manag.* **2016**, 125, 320.
[2] A. Nuchitprasittichai, S. Cremaschi, Comput. Chem. Eng. **2011**, 35, 1521