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Heat-Integrated Reactive Distillation

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Significant advances have been made by industry and academic research organizations to establish the commercial advantages of Reactive Distillation (RD). It is an effective but challenging technique for energy-efficient synthesis of major commodity chemicals. However, the number of actual reactive distillation installations is quite small despite a large number of patents and extensive academic and industrial research. The main reason for this is that it is difficult to match the optimum conditions for distillation, reaction, and scale up of experimental test data to commercial units [1]. Pressure is the primary variable that affects efficient separation and many reactive distillation processes are not very flexible due to the interactive effects of reaction and separation on each reactive stage.

This project focuses on the opportunities provided by heat-integration to expand the applicability of reactive distillation by providing an additional adjustment to match the optimum conditions for distillation, reaction, and scale-up of experimental test data to commercial units. This will investigate: a) thermal management for optimum global temperature profiles that would also influence global distribution reactants and localized temperature distribution in the catalyst bed; b) effective ways to improve contacting of the reactive phases with the catalyst; and c) a rate-based model to account for localized reactive multi-phase flows.

A rigorous and critical review of the literature data and analysis was carried out and an analysis was performed to select industrial processes that can be further advanced by addressing these three technical barriers. The resulting industrial processes selected for further developments are: a) production of cyclohexanol representing hydration/esterification process; b) isomerization process; and c) production of alkyl carbonate (e.g., di-methyl carbonate - DMC) representing emerging market. This project focuses on simulation of esterification of cyclohexene with acetic acid. Additionally, single- and two-phase flow through a Katapak-SP11 structured packing was modeled using ANSYS FLUENT 12.1. The purpose of this analysis is to determine the liquid flow distributions interior and exterior to the catalyst baskets, catalyst wetting, and hence reaction effectiveness. From this, a full process design using both Aspen and ICAS simulations were performed using available kinetic data to establish the benchmark. Subsequently, distributed heat removal and addition was investigated to optimize the catalyst loading and total reboiler heat duty. The analysis also considered thermal management by application of heat pumps for transferring latent heat from rectifying section to the stripping section. The project plans include validation using 10 m high, 50 mm diameter reactive distillation column equipped with Sulzer Katapak SP-11.

REFERENCES

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