**Analyses of a non-isothermal simulated moving bed reactor based on Multi-objective optimization**

Jian Wang, Weifang Yu\*, Jin Xu\*

*College of Chemistry and Material Engineering, Wenzhou University*

*\*Corresponding author: [ywf@wzu.edu.cn;](mailto:ywf@wzu.edu.cn;) [xujin@wzu.edu.cn](mailto:xujin@wzu.edu.cn)*

**Highlights**

* Non-isothermal operations of an SMBR for methyl acetate synthesis were evaluated by multi-objective optimization.
* In addition to unit throughput and product purity, solvent consumption was also considered.
* Effects of kinetic parameter and adsorption strength of reactant were investigated by sensitivity study.
* The feasibility of applying non-isothermal operations was systematically investigated.

**1. Introduction**

Simulated moving bed reactor (SMBR) couples in-situ adsorptive separation with chemical reaction. Conversion of a reversible reaction can be increased beyond the limit of thermodynamic equilibrium and, as the same time, pure product can be directly collected, simplifying the downstream purification processes [1]. SMBR consists of a series of columns packed with solid phase materials with both catalytic activity and adsorptive selectivity. Typically, inlet and ourlet ports divide the columns into four zones, each playing a specific functional role.

Efficiency of the onsite separation is crucial for the success an SMBR. VariCol and PowerFeed technologies that have been originally developed for SMB separation were proven to be effective for the improvement of SMBR performance [2,3]. Gradient operation by introducing different adsorptive strength into different zones according to their functions has been extensively used to reinforce SMB separation processes.

The ongoing work in this group and colleagues is aimed at examining the feasibility of applying temperature variance on an SMBR. For this purpose, synthesis of methyl acetate catalyzed by amberlyst 15 was used as the model reaction. It has been shown by both theoretical and experimental studies that complete conversion and separation can be achieved [4,5].

One of our previous study investigated the effects of temperature gradient under the frame of Triangle Theory [6]. Maximum unit throughput for complete conversion and separation was acquired by fixing conservative flowrates in zones I and IV and searching the two dimensional parametric plane consisting of flworates in zones of II and III. In this work, zones I and IV were also taken into consideration. Multi-objective optimizations were carried to evaluate SMBR performance in terms of unit throughput, product purity and solvent consumption as well.

**2. Methods**

Mathematical model and model parameters for the simulation of an SMBR reactor were established in previous publications [5,6]. A four zone SMBR has five independent operating parameters, namely, switching time and the four flowrate. The maximum flowrate that is limited by column pressure was assigned to zone I as a scaling factor. Simultaneous maximization of unit throughput and product purity was pursued by tuning the other four parameters that had been converted to dimensionless flowrate ratios. As in general, operating conditions have contradicting effects on these two objectives and the solutions form a pareto curve. Non-dominated sorting genetic algorithm (NSGA-II) was used to acquire the solutions.

**3. Results and discussion**

Pareto solutions of an SMBR operated under various modes are compared in Figure 1. Minimization of solvent consumption was then pursued by both parametric sensitivity analyses and 3-objective optimizations. Using the same procedure, effects of kinetic rate, adsorption strength of reactant and reaction heat on the SMBR performance were also investigated. More detailed results and discussions omitted here for conciseness will be presented in the conference.



**Figure 1.** comparison of pareto solutions acquired for SMBR with several temperature distributions

**4. Conclusions**

Temperature may have both synergy and contradicting effects on reaction kinetics and separation in different zones. As a result, temperature gradient operation can be conditionally but not generally applied to improve SMBR performance.

**References [Calibri 10]**

1. A.K. Ray, R.W. Carr, Chem. Eng. Sci. 50 (1995) 3033–3041.
2. W. Yu , K. Hidajat , A.K. Ray, Chem. Eng. J. 112 (2005) 57-72.
3. J.S. Hariprasad , K. Hidajat , A.K. Ray, Comput. Chem. Eng. 27 (2003) 1883–1901.
4. W. Yu , K. Hidajat , A.K. Ray, Ind. Eng. Chem. Res. 42 (2003) 6743–6754.
5. W. Yu , K. Hidajat , A.K. Ray, Appl. Catal. A: Gener. 260 (2004) 191–205.
6. J. Xu, Y. Liu, G. Xu, W. Yu, A. K. Ray, AIChE J., 59 (2013) 4705-4714.