Contents lists available at ScienceDirect

Chemical Engineering Research and Design

journal homepage: www.elsevier.com/locate/cherd

A generalized method for the synthesis and design of reactive distillation columns

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ABSTRACT

Owing to the combination between the reaction operation and the separation operation involved, it is extremely difficult to determine in advance the optimum configuration of a reactive distillation column and this makes process synthesis and design a great challenging task. Currently, no easy-to-use and yet effective methods are available to guide process synthesis and design, restricting considerably the applications and therefore the impacts of reactive distillation columns to the chemical process industry. In this paper, a generalized method is proposed for the synthesis and design of reactive distillation columns in terms of the insights from process intensification. The method is initiated from a simple process design with all feeds of reactants at the middle of the process and all stages as reactive ones. In terms of an economical objective function, it can be evolved into the optimum process design via sequential structure adjustments, including reactive section arrangement, feed stage relocation, feed splitting, and catalyst redistribution. The generalized method proposed is characterized by great simplicity in principle, the capability to tap the full potentials of process intensification, and the high robustness to the initial guess of process configuration as well as the thermodynamic properties of the reacting mixtures separated. Four example systems are employed to evaluate the generalized method proposed and the obtained outcomes demonstrate its effectiveness and applicability to the synthesis and design of various reactive distillation columns.

Keywords: Reactive distillation; Process intensification; Mass integration; Heat integration; Process synthesis; Process design

1. Introduction

The key for the synthesis and design of a reactive distillation column lies on the correct determination of the combination between the reaction operation and the separation operation involved (Malone and Doherty, 2000). Although the issue seems to be an ordinary combinatorial problem, it indicates essentially the great differences from that of a conventional distillation column. The combination should follow the stringent requirements of process intensification and could influence considerably the thermodynamic efficiency of a reactive distillation column. So far many methods have been developed for the synthesis and design of reactive distillation columns and they can generally be classified into three broad categories (Almeida-Rivera et al., 2004): (i) Graphical methods; (ii) Heuristic evolutionary methods; and (iii) Optimization-based methods. For the graphical methods, considerable attention has been paid over the past 20 years and the most representative ones should be the residue curve mapping techniques (Doherty and Buzad, 1992; Ung and Doherty, 1995) and conventional graphical techniques including the modified Ponchon-Savarit and McCabe-Thiele methods (Lee et al., 2000a, 2000b). Although these graphical methods appear extremely helpful in understanding the fundamental insights of reactive distillation columns, they are rather complicated in the case of a multi-component reaction system because of the increased dimensionality (Lee and Westerberg, 2000, 2001). Moreover, these methods can only yield rough process designs that need further refinement through rigorous computation with commercial software or other simulation programs (Barbosa and Doherty, 1988). For the heuristic evolutionary methods, they are generally based on available heuristics or an economical objective function to guide process synthesis and design (Subawalla and Fair,

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Received 7 November 2010; Received in revised form 19 June 2011; Accepted 30 June 2011

doi:10.1016/j.cherd.2011.06.020