CHEMICAL ENGINEERING RESEARCH AND DESIGN 90 (2012) 1856–1870

Contents lists available at SciVerse ScienceDirect

Chemical Engineering Research and Design

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

Analysis and prediction of input multiplicity for the reactive flash separation using reaction-invariant composition variables

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ABSTRACT

In this study, we introduce a new approach for predicting and analyzing the input multiplicity in reactive flash separation processes. Specifically, we have identified necessary conditions to detect these multiple states in reactive flash separations using reaction-invariant composition variables. The presence of the input multiplicity is studied for the reactive systems of MTBE and TAME production to illustrate the capabilities of our methodology. For these reactive systems, we report the existence of multiple states for different operating conditions. In summary, our strategy can be applied with any reactive system and thermodynamic model, assuming that all reactions are reversible and in thermodynamic equilibrium and the operating conditions are away from the retrograde region. In general, our method is a robust procedure for the multiplicity analysis in flash separation of multi-reactive and multi-component systems.

Keywords: Reactive flash separation; Input multiplicity; Reaction-invariant composition variables

1. Introduction

Reactive separation schemes (e.g., reactive distillation, extraction and crystallization) are integrated unit operations widely used in the current chemical industry due to their well-known economical and operational advantages. Specifically, these separation systems may improve the process performance via the reduction of capital cost, the increment of selectivity and conversion, the decrement of heat demand, the suppression of side reactions and the avoidance of undesirable phase equilibrium conditions such as homogeneous azeotropy (Taylor and Krishna, 2000). However, the reliable modeling of reactive separation process is difficult due to the multicomponent nature of the reactive systems, the nonlinearity of the thermodynamic models caused by the interaction of simultaneous chemical and physical equilibrium, and also by the type of variables involved in defining the mathematical model, which are generally composition variables in molar units and extents of reaction. In particular, reactive separation processes exhibit a high non-linear behavior and, as a consequence, the multiplicity of solutions is often possible during the design and modeling of these separation schemes (Taylor and Krishna, 2000; Chen et al., 2002).

Multiplicity of solutions is an important feature of industrial processes and plays an important role in design, simulation and control of separation units (Monroy-Loperena, 2001). In process system engineering, it is important to predict all multiple states within the practical domain of operating variables, to know whether they are desirable, and to understand how the separation scheme responses to changes in the operating conditions (Tiscareño et al., 1998; Yang et al., 2006). According to the literature, reactive separation systems can exhibit two types of multiplicity: input and output multiplicity (Singh et al., 2005a; Malinen and Tanskanen, 2010). Input multiplicity occurs when two or more sets of input variables produce the same output conditions, while output multiplicity occurs when one set of input variables results in two or more independent sets of output variables (Singh et al., 2005a,b;

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Received 27 August 2011; Received in revised form 13 December 2011; Accepted 29 February 2012

doi:10.1016/j.cherd.2012.02.017