Available online at www.sciencedirect.com
SCIENCE DIRECT®

Chemical Engineering and Processing 45 (2006) 140–149

Chemical Engineering and Processing

www.elsevier.com/locate/cep

Impact of disturbance magnitudes and directions on the dynamic behavior of a generic reactive distillation

Moshood J. Olanrewaju, Muhammad A. Al-Arfaj *

Department of Chemical Engineering, King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia

Received 7 February 2005; received in revised form 23 June 2005; accepted 23 July 2005
Available online 15 September 2005

Abstract

The dynamic behavior for a high-purity/high-conversion reactive distillation is investigated. The impact of disturbance magnitudes and directions on both open loop and closed loop stability of the system is studied. Excess of less volatile reactant in two-reactant-two-product generic reactive distillation is found to enhance open loop stability, but decreases the products purity. However, excess of more volatile reactant trigger the system to another steady-state. Open loop changes in the manipulated variables (i.e. vapor boilup from the reboiler and reflux rate from the condenser) in certain directions are found to be intolerable due to their effect on both the reaction kinetics and the fractionation capacity of the column. The performance of the open loop system is improved significantly with the inclusion of internal inventory control of one of the reactants but this has been found to be insufficient when there is a change in some inputs in certain directions. Steady-state rating analysis on the system suggests that the limitations on certain inputs could be resolved by including a single-end controller, which will act to maintain the separation capacity of the column and thus stabilizes the system.

Keywords: Reactive distillation; Dynamic simulation; Nonlinear dynamics

1. Introduction

Because of environmental and economic considerations, researchers in both industry and academia have put tremendous efforts in process intensification. Reactive distillation is one of such promising operations where by reaction and distillation takes place in a single distillation column. Reactive distillation can, in some systems, provide an alternative to conventional multiunit flowsheets, which typically include a reactor followed by a separation section with recycles back to the reaction section. Some of reactive distillation advantages can be summarized as follows:

- Product selectivity can be improved due to a fast removal of reactants or products from the reaction zone.
- Reactive distillation could lead to capital savings as two process steps can be carried out in the same vessel.
- If reactive distillation is applied to exothermic reaction, the reaction heat can be used for vaporization of liquid, thus leads to savings of energy costs.
- Reactive distillation conditions could allow azeotropes to be reacted away.

Although reactive distillation might be an attractive alternative to the conventional multiunit processes, it can be effective for only a fairly small class of chemical systems because of some inherent limitations. Reactive distillation is particularly possible when reactants and products have suitable volatility to maintain high concentrations of reactants and low concentrations of products in the reaction zone. The reaction rates must be comparable to those in the reactor at temperature suitable for distillation.

The potential advantages of reactive distillation could be negated by improper choice of reactant to be run in excess in the reactive zone whenever it is needed to avoid substoichiometry balance. Thus, it is possible to decrease conversion by increasing the amount of catalyst under

* Corresponding author. Tel.: +966 3 860 1694; fax: +966 3 860 4234.
E-mail address: maarfaj@kfupm.edu.sa (M.A. Al-Arfaj).

0255-2701/$ – see front matter © 2005 Elsevier B.V. All rights reserved.
doi:10.1016/j.cep.2005.07.001

certain circumstances [1]. Increased separation capability could decrease process performance [2].

Numerous studies have been conducted on understanding the fundamental thermodynamics and kinetics in the operation of the columns [3–6]. Steady-state model analysis as well as steady-state multiplicities has been considered in detail by many researchers. Taylor and Krishna [7] presented a detailed review on the modeling of various reactive distillation processes. Recently, several papers have emerged in literature on closed loop performance of reactive distillation system [8–11].

However, successful commercialization of reactive distillation technology requires careful attention to the modeling aspects, including column dynamics, even at the conceptual design stage [12]. The design and operation issues for reactive distillation systems are considerably more complex than those involved for either conventional reactors or conventional distillation columns. The introduction of an in situ separation function within the reaction zone leads to complex interactions between thermodynamic vapor–liquid equilibrium, intra-catalyst dilution (for heterogeneously catalyzed processes) and chemical kinetics.

Another area of concern in the study of reactive distillation system is the impact of disturbance magnitudes and directions in dynamic behavior of both open loop and closed loop model of reactive distillation. In a typical reactive distillation column, the regions of intense mass transfer are in the middle of the column where the reactive zone is usually located, while the ends of column are essentially used for purification. These regions are more sensitive to disturbance directions as compared to the ends of columns.

The aim of this paper is to investigate the dynamic behavior of high-purity/high-conversion generic reactive distillation system. The effect of disturbance magnitudes and directions on the stability of both open loop and closed loop system of reactive distillation is quantitatively explored. The open loop performance of the system is explored with and without the inclusion of internal composition inventory controller. The impact of certain inventory control loops on the dynamic stability of the system is studied. This investigation is essential to gain a better understanding of this generic class of reactive distillation. In addition, the study will facilitate a better understanding of a similar system and will help in the application of an advanced process control.

For an effective control of a reactive distillation system, the process control engineer needs to understand the impact of disturbance magnitudes and directions on the dynamic behavior of the system. This is because the effectiveness of disturbance suppression in a multivariable control system depends strongly on the direction of disturbance [13]. This study will also provide valuable information on the importance of maintaining a correct stoichiometric balance between the feeds in both open and closed loop multi-feed reactive distillation column.

2. Process description

Among several chemical systems, two-reactant-two-product reactions have received wide application in reactive distillation technology [14]. In this work, we consider an ideal two-reactant-two-product reactive distillation column. The reactive column is shown in Fig. 1. It consists of a reactive section in the middle with nonreactive rectifying and stripping sections at the top and bottoms, respectively. The

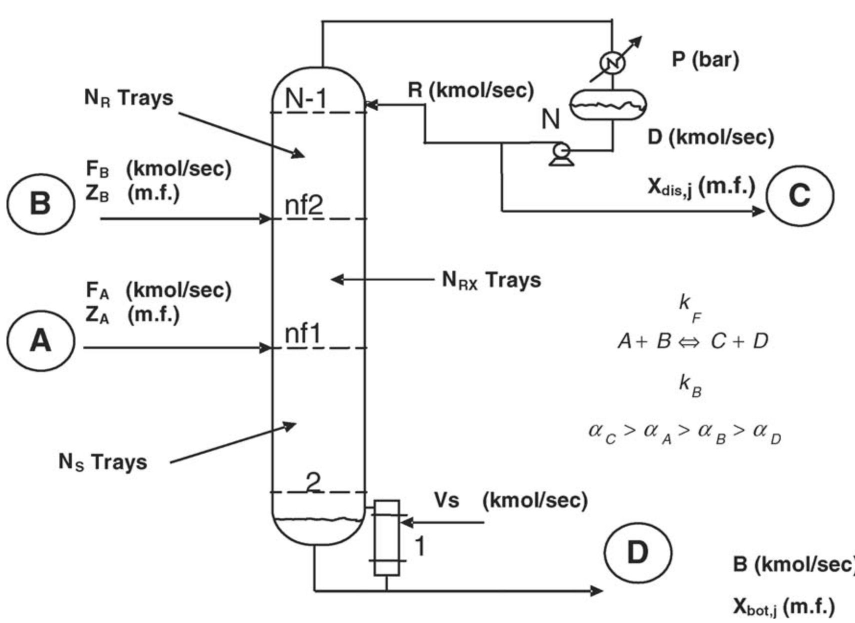

Fig. 1. Distillation column.