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Chemical Engineering Science 61 (2006) 4432–4450

Chemical Engineering Science

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Evaluation of a two-temperature control structure for a two-reactant/two-product type of reactive distillation column

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Received 4 June 2005; received in revised form 10 January 2006; accepted 30 January 2006
Available online 31 March 2006

Abstract

Several different control structures have been proposed for reactive distillation columns. The appropriate control structure depends on the flowsheet and on the type of reactions occurring in the column. If two reactants are involved and if it is desirable to operate the process without any excess of reactant, it is necessary to manage the fresh feed streams so that the stoichiometry is exactly balanced. A composition analyzer that measures an internal composition in the column is often required. However, if two products are produced, it is possible to avoid the use of an analyzer by using two temperatures in the column to adjust the two feed streams. This type of structure was proposed by Roat et al. [Roat, S., Downs. J., Vogel, E., Doss, J., 1986. Integration of rigorous dynamic modeling and control system synthesis for distillation columns. In: Chemical Process Control—CPC III. Elsevier, Amsterdam.] for the ideal reaction $A + B \leftrightarrow C + D$ in one of the earliest papers dealing with reactive distillation control.

The purpose of this paper is to explore the effectiveness of this two-temperature control structure for various column designs (number of reactive stages) to quantify the impact of design on controllability. We also discuss the issues of the selection of the trays whose temperatures are to be controlled and the tuning of the two interacting temperature controllers. Disturbances in production rate and fresh feed compositions are made to examine the rangeability of this control structure. Both an ideal reaction system and the methyl acetate system are studied. One of the main conclusions is that the locations of the temperature control trays should be made such that the two temperature controllers both have direct action (an increase in temperature increases feed), which requires negative openloop process gains for both loops.

Keywords: Reactive distillation; Process design; Process control; Simulation; Separation; Methyl acetate

1. Introduction

In the last decade, the number of papers that deal with the closedloop control of reactive distillation column has increased from a mere handful to over a dozen. Several types of controllers have been studied, ranging from simple proportional-integral (PI) controllers to complex nonlinear model predictive controllers. Even if we limit ourselves to PI controllers, there has been a variety of alternative control structures studied.

There also has been a variety of chemical systems studied and a number of types of flowsheets. For example, some of the common types of reactions are:

1. Reactions with two reactants and two products.
2. Reactions with two reactants and one product.
3. Reactions with one reactant and two products.

The flowsheet for the third type of chemistry listed above is usually a single reactive column with reactant fed in and the two products removed in the distillate and bottoms streams. The control of this type of system is usually quite simple because the feed is a single reactant. Unlike the two-reactant chemistry, there is no need to precisely adjust the two feed streams so as to balance the stoichiometry.

However, the flowsheets for the first and second types of chemistry listed above come in two flavors. The flowsheet can consist of either a single reactive column. Or it can be a two-column system with a reactive distillation column followed by

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0009-2509/$ - see front matter © 2006 Elsevier Ltd. All rights reserved.
doi:10.1016/j.ces.2006.01.050

a recovery column and recycle of excess reactant back to the reactive column. The type of flowsheet depends on whether we want to operate the reactive distillation column "neat", i.e. no excess of either reactant. The "excess-reactant" flowsheet has higher capital and operating cost, but its control is easier (Luyben, 2000).

The "neat" flowsheet is more difficult to control because the two reactants must be fed in exactly the correct amounts to satisfy the stoichiometry *down to the last molecule*. This places a heavy demand on the control structure and requires some type of feedback of information from within the process to indicate the accumulation or depletion of at least one of the reactants. In some chemical systems the only way this can be achieved is by the use of a composition analyzer.

Al-Arfaj (2002) studied a number of types of reactions and a number of control structures. An empirical finding from the many case studies is that a composition analyzer may not be required in the two-reactant case if there are *two* products produced.

If only *one* product is produced, the temperature profile does not display enough information to enable the use of inferential control for component inventory control purposes. There is only one product leaving the column, and information can be extracted from a limited region where the concentration of this product becomes large. Industrial examples of this type of system are MTBE, ETBE and TAME.

However, if *two* products are produced, the temperature information may be rich enough to infer compositions with sufficient accuracy so that direct composition measurement is not absolutely necessary for "neat" operation. The ideal case considered by Roat et al. (1986) ($A + B \Leftrightarrow C + D$) and the production of methyl acetate (methanol + acetic acid $\Leftrightarrow$ methyl acetate + water) are examples of this type of chemistry. In our present study, we consider an ideal system and the methyl acetate system.

To summarize, the process under study is a reactive distillation column, operated without an excess of one of the reactants, in which there are two reactant feed streams and two products are produced.

In the paper by Roat et al. (1986), two PI temperature controllers are used to maintain two tray temperatures in the column by manipulating the two fresh feed streams. Production rate changes are achieved by changing the vapor boilup. Their paper gave very limited details about the system. They claimed that this scheme could handle only 5% increases in vapor boilup. They did not show results for other types of disturbances, and they only looked at a single reactive column with a fixed number of reactive, stripping and rectifying trays.

Al-Arfaj and Luyben (2002) studied several alternative control structures for both the ideal reaction case and the methyl acetate case, including the two-temperature structure. They used singular-value decomposition (SVD) methods to select trays for temperature control. They did not explore the effects of changing the number of reactive stages on dynamic controllability, nor were questions of rangeability addressed. Few details were provided for the two-temperature control scheme in the ideal case.

The purpose of this paper is to extend the analysis of the two-temperature control structure by quantitatively exploring the impact of design on controllability and addressing the issues of control tray selection, controller tuning and rangeability in the face of large disturbances.

2. Ideal process studied

The first process considered is taken from our previous paper (Kaymak et al., 2004) in which an ideal reversible liquid-phase reaction occurs on the reactive trays

$$A + B \Leftrightarrow C + D. \tag{1}$$

The forward and backward specific reaction rates follow Arrhenius equations

$$k_F = a_F e^{-E_F/RT}, \tag{2}$$

$$k_R = a_R e^{-E_R/RT}. \tag{3}$$

The rate law is based on concentrations in mole fractions and liquid holdups in kmoles. The forward reaction rate is specified as $0.008\,\mathrm{kmol\,s^{-1}\,kmol^{-1}}$ at 366 K. The reverse reaction rate at this temperature is calculated by taking a specific value of $(K_{EQ})_{366}$

$$(k_R)_{366} = \frac{(k_F)_{366}}{(K_{EQ})_{366}}. \tag{4}$$

Both reaction rates are temperature dependent, and the ratio of k_F to k_R is not equal to $(K_{EQ})_{366}$ at temperatures different than 366 K due to the difference of activation energies. The reverse reaction rate is more temperature dependent than the forward reaction rate since the reaction is exothermic.

Kinetic and physical properties and vapor–liquid equilibrium parameters are taken from our previous paper (Kaymak et al., 2004). Details of the design equations, procedures, optimization strategies, assumptions and numerical methods are also given in the same paper. A single value of the chemical equilibrium constant is used in this paper: $(K_{EQ})_{366} = 2$.

Ideal vapor–liquid equilibrium is assumed with constant relative volatilities. The lightest component is one of the products (C) and the heaviest component is the other product (D). Reactant component A is lighter than the other reactant B. Thus, the relative volatilities are

$$\alpha_C = 8, \quad \alpha_A = 4, \quad \alpha_B = 2, \quad \alpha_D = 1. \tag{5}$$

The design objective is to obtain 95% conversion for pure reactant fresh feed flowrates of $12.6\,\mathrm{mol\,s^{-1}}$. Essentially all of C leaves in the distillate and all of D leaves in the bottoms because of the relative volatilities. The specifications for the product impurities are assumed to be 5 mol% B in the bottoms and 5 mol% A in the distillate. A reactive tray holdup M_i of 1000 mol is used, which gives reasonable tray liquid heights (0.1 m) for the column diameters calculated from flooding calculations (0.8 m).

There are three design optimization variables: (1) the column pressure P (2), the number of reactive trays N_{RX}, and (3) the