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Control of a reactive distillation column with double reactive sections for two-stage consecutive reactions

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ABSTRACT

In this study, the control performance of a reactive distillation column with double reactive sections is evaluated. The reactions taking place in the column are two-stage consecutive reversible liquid-phase reactions. A hypothetical ideal reaction system is selected as case study. Different control structures including temperature and/or composition control loops are developed and tested for different load disturbances. The closed loop results of different control structures demonstrate that a workable control structure should include direct control of compositions. A control structure with two temperature controllers and two composition controllers provides an effective control for the column with double reactive sections.

1. Introduction

Process intensification appears as one of the most promising tools in chemical industry, because increasing economic and safety considerations force the industry to focus on smaller scale and more energy-efficient technologies. One of the most glaring examples of this tool is the reactive distillation column which combines both the reaction and separation units into a single vessel. Recent design studies have indicated the advantages of reactive distillation columns such as the decrease of investment and operating costs, and the increase of conversion and selectivity, compared to the conventional multi-unit processes, when used for suitable chemical systems.

An overview on chemical reaction types shows that single-stage reversible reactions including quaternary systems (two reactants and two products) and ternary systems (two reactants and one product) lead the studies on reactive distillation columns [1]. Processes including etherification and esterification reactions could be given as the well-known industrial examples of these systems. On the other hand, the third type of reactions widely found in the industry is the two-stage consecutive reversible reactions. However, there are only a few studies reported in the literature for the separation of this type of reactions, and reactive distillation columns with a single reactive section (RDC-SRC) have been used in almost all of these studies [2–6]. Only one of them focused on the control of a reactive distillation process including two consecutive trans-esterification reactions [7].

Recently, a novel reactive distillation column with double reactive sections (RDC-DRS) has been proposed for the separations of the two-stage consecutive reversible reactions [8]. Results of this study indicate better steady-state performance than the RDC-SRC, but the dynamic performance and controllability of the RDC-DRS has not been studied.

The aim of this study is designing effective and robust control structures for the RDC-DRS. The example used in this study is the same hypothetical ideal two-stage consecutive reversible reaction, $A + B \leftrightarrow C + D$ and $C + B \leftrightarrow E + D$, used in the literature [8].

Although the dynamic controllability must be taken into account at the steady-state design stage, there is no relevant study in the literature on the controllability of the RDC-DRS including two-stage consecutive reversible reactions. Since nothing is known on the controllability of this process, it is believed that the contributions of this study will close a lack in the field as a novel work.

2. Process studied

The two-stage consecutive reversible liquid-phase reactions considered in this study are

$$A + B \Leftrightarrow C + D \quad (1)$$

$$C + B \Leftrightarrow E + D \quad (2)$$

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Nomenclature

A_{VP}	Vapor pressure constant
B	Bottoms flow rate in the column (mol/s)
B_{VP}	Vapor pressure constant
D	Distillate flow rate in the column (mol/s)
F_j	Fresh feed flow rate of reactant j (mol/s)
k_F	Specific reaction rate of forward reaction ($mol\,s^{-1}\,mol^{-1}$)
k_R	Specific reaction rate of reverse reaction ($mol\,s^{-1}\,mol^{-1}$)
K	Steady-state gain
N_T	Number of trays
P	Column pressure (bar)
R	Reflux (mol/s)
T_i	Column temperature on tray i (K)
V_S	Vapor boilup (mol/s)
$x_{n,j}$	Composition of component j in liquid on tray n
$x_{B,j}$	Bottoms composition of component j in liquid
$x_{D,j}$	Distillate composition of component j in liquid

The net reaction rates for component j on tray i are given by

$$R_{1,i,j} = \nu_{1,j} M_i \left(k_{F,1} x_{i,A} x_{i,B} - k_{R,1} x_{i,C} x_{i,D}\right) \quad (3)$$

$$R_{2,i,j} = \nu_{2,j} M_i \left(k_{F,2} x_{i,C} x_{i,B} - k_{R,2} x_{i,E} x_{i,D}\right) \quad (4)$$

where $\nu_{m,j}$ is the stoichiometric coefficient of component j in m^{th} stage reaction. The rate law is based on concentrations in mole fractions and liquid holdups in kmoles. The forward and backward specific reaction rates follow the Arrhenius Law

$$k_{F,m} = a_{F,m} e^{-E_{F,m}/RT} \quad (5)$$

$$k_{R,m} = a_{R,m} e^{-E_{R,m}/RT} \quad (6)$$

respectively, where m is the stage number of the reaction. The steady-state vapor and liquid rates are constant through the non-reactive sections, since equimolal overflow is assumed. This is also the case for reactive trays, because average heat of reaction is assumed negligible.

Ideal vapor-liquid equilibrium is assumed with constant volatilities. The volatilities of components are $\alpha_E > \alpha_A > \alpha_C > \alpha_B > \alpha_D$. Since the final products are the most and least volatile components, it is the ideal system for reactive distillation. Kinetic and physical properties and vapor-liquid equilibrium parameters given in Table 1 are taken from Yu et al. [8].

A schematic of the RDC-DRS is given in Fig. 1. The column consists of five sections; stripping, lower reactive, middle non-reactive, upper reactive and rectifying sections. The numbering of the trays is bottom-up excluding the reboiler and condenser. Although both reactions occur on both reactive sections, the first stage reaction is dominant in the upper reactive section, while the second stage reaction mainly takes place in the lower reactive section. The heavy reactant A, which is the reactant of the first stage reaction, is fed to the top tray of the upper reactive section. On the other hand, the light reactant B is introduced from the bottom of both reactive sections, because it is the common reactant of first and second stage reactions. The light product D leaves in the distillate, while the heavy product E is removed from the bottoms. Because the light reactant goes up through the column after being fed on the bottom trays of reactive sections, there will be very little of component B in the bottoms. Likewise heavy reactant goes down through the column after being fed on the top tray of the upper reactive section, and there will be very little of component A in the distillate. Intermediate boiling component C will appear in both product streams as trace. The steady-state values of holdups are kept constant at 1000 mol on reactive trays and at 400 mol in other sections of the column.

Table 1
Kinetic and physical properties.

Parameter	Value
Column pressure (bar)	10
First stage activation energy ($kcal\,mol^{-1}$)	
forward	30
reverse	30
Second stage activation energy ($kcal\,mol^{-1}$)	
forward	30
reverse	30
First stage specific reaction rate at 366 K ($kmol\,s^{-1}\,kmol^{-1}$)	
forward	0.008
reverse	0.004
Second stage specific reaction rate at 366 K ($kmol\,s^{-1}\,kmol^{-1}$)	
forward	0.0008
reverse	0.0016
First stage chemical equilibrium constant at 366 K	2
Second stage chemical equilibrium constant at 366 K	0.5
Heat of reaction ($kcal\,mol^{-1}$)	0
Heat of vaporization ($kcal\,mol^{-1}$)	6.944
Vapor pressure constants[a] ($A_{VP,j}$–$B_{VP,j}$)	
A	10.96–3862
B	2.351–3862
C	11.65–3862
D	13.04–3862
E	10.27–3862

[a] $\ln P_j^s = A_{VP,j} - B_{VP,j}/T$ with temperature in K and vapor pressure in bar.

The number of trays in each section, the feed locations of reactants, the feed splitting ratio of the common reactant B and the operating pressure are kept same as those of the paper written by Yu et al. [8]. First, the RDC-SRS is designed using initial guessed values of mole fractions and temperature throughout the column. Then, the steady-state design of the RDC-SRS is used as the initial guess to obtain the steady-state design of the RDC-DRS. Relaxation method is used to calculate mole fractions and temperature

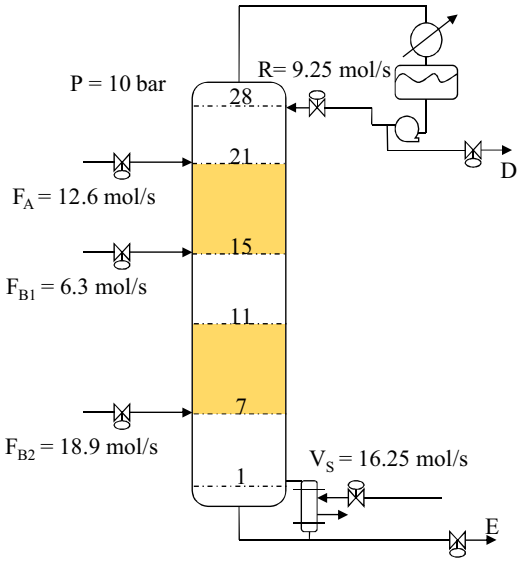

Fig. 1. Flowsheets of reactive distillation column.

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