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Design and control of hybrid heat-integrated configuration for an ideal indirect reactive distillation process

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ABSTRACT

A hybrid configuration can simultaneously improve the energy efficiency and reduce the overall energy requirement of the ideal IIp reactive distillation (RD) process reported by Weng and Lee [1]. This hybrid heat-integrated configuration can save 50.4% of the energy used in the conventional configuration; moreover, the remixing effect can be eliminated. Energy waste in the condenser of the second column is lower than that in the thermally coupled configuration, and the additional energy transfer area in the heat exchanger is smaller than that in the double-effect configuration. In this study, three control structures: thermally coupled configuration, and hybrid configuration with/without pressure-compensated temperature control structures are demonstrated to evaluate the control performance. When a pressure-compensated temperature control is provided, an equation can give a satisfactory correlation between column pressure and control temperature. Compared with the control performance of the two hybrid configurations, the pressure-compensated temperature control structure is capable of maintaining specifications during ±20% throughput disturbances.

1. Introduction

For centuries, the products of the chemical industry have been widely used as raw materials for industrial and consumer goods. A typical, traditional chemical process usually consists of numerous units, which can be divided into two categories, reaction and separation. One of the most energy-intensive units of separation processes is distillation column. As environmental issues are increasingly receiving public attention, traditional chemical processes that have low energy efficiency and high energy consumption are gradually being phased out. Agreda and Partin [2] reported the application of a reactive distillation (RD) process, which combines reaction and separation in a distillation column, to industrial production. Luyben and Yu [3] presented updated summaries. Moreover, numerous studies (*e.g.*, Wright [4], Andrecovich and Westerberg [5], Robinson and Gilliland [6], and Jiao et al. [7]) have discussed energy saving by using heat-integrated designs such as thermally coupled configurations and multi-effect configurations. Several articles have explored the benefits of combining RD and heat-integrated designs to reduce energy use [8,9].

Conventional ternary components in the distillation configurations are usually used in two types of routes, direct and indirect sequences to separate the components in the process. In these configurations, a crucial phenomenon—the remixing effect—can be observed when the composition with middle relative volatility first rises and then descends. The remixing effect may occur at the top or bottom of a column. A thermally coupled distillation configuration can eliminate the remixing effect. A direct-sequence thermally coupled configuration removes the reboiler from the bottom of the first distillation column and provides the necessary energy from the second distillation column. An indirect-sequence thermally coupled configuration removes the condenser from the top of the first distillation column, and the overhead of the first column is fed into the second column.

A conventional distillation column wastes energy extravagantly when it adds energy to a reboiler at the bottom of a column and removes energy from a condenser at the top; a transfer of energy from the condenser to the reboiler can improve energy efficiency. The double-effect configuration is derived from this concept. The pressure in a high-pressure distillation column is controlled to get the necessary temperature difference between the top of the high-pressure column and the bottom of the low-pressure column; thus, energy can be transferred from the high-pressure column to the low-pressure column. Although this approach improves energy efficiency, it requires an additional column and thus entails relatively high capital costs. Therefore, it presents a trade-off between energy savings and capital costs.

Studies have reported that a double-effect configuration can increase energy efficiency without eliminating the remixing effect.

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Table 1
Thermodynamic parameters of an ideal RD process.

Heat of vaporization (kJ/mol)	ΔH_v	29			
Relative volatility (*LLK/LK/HK/HHK*)		8/4/2/1			
Vapor pressure constant		*LLK*	*LK*	*HK*	*HHK*
$\ln P_i^s = A_{VP,i} - B_{VP,i}/T$	A_{VP}	13.04	12.34	11.65	10.96
	B_{VP}	3862	3862	3862	3862

Table 2
Kinetics parameters of the ideal RD process.

Reaction	$A + B \Leftrightarrow C + D$	
Reaction rate	$R_{j,i} = \upsilon_i M_j (k_{Fj} x_{j,A} x_{j,B} - k_{Bj} x_{j,C} x_{j,D})$	
k_{Fj}	$k_{Fj} = A_F e^{-E_F/RT_j}$	A_F (kmol/kmol s) = 0.008 E_F (kJ/kmol) = 50160
k_{Bj}	$k_{Bj} = A_B e^{-E_B/RT_j}$	A_B (kmol/kmol s) = 0.004 E_B (kJ/kmol) = 71060

Weng and Lee [1] combined double-effect and thermally coupled configurations; they proposed a hybrid heat-integrated configuration that simultaneously eliminated remixing, improved energy efficiency, and reduced overall energy requirements.

This study summarizes several configurations, including the conventional ideal RD [10], thermally coupled [11], and double-effect configurations, and evaluates the energy savings of the hybrid heat-integrated configuration by Weng and Lee [1]. A suitable control structure is proposed and analyzed for proper controllability under various throughput disturbances. To evaluate the effect of the hybrid configuration on an ideal RD process, this study compares the control performances of three control structures: a thermally coupled configuration, and hybrid configurations without/with pressure-compensated temperature control. The characteristics of relevant control structures are also explained.

2. Thermodynamic and kinetic models

Insofar as it is possible, every simulation must be made as realistic as possible; in the simulation of distillation, calculation of phase equilibrium is the core function, and that calculation must proceed from an appropriate thermodynamic model. This section illustrates the thermodynamic model for this research.

Our ideal system references the results of IIp RD processes from Lin [10], and our thermodynamic model uses the hypothesis by Tung and Yu [12]. Four virtual components were labeled A, B, C, and D. Their relative volatilities were as follows (high to low):

$$\alpha_C > \alpha_D > \alpha_A > \alpha_B$$

This ideal RD process is assumed to be an extremely exothermic reaction. The relative volatility is assumed to be invariant with temperature. It is assumed that neither azeotrope status nor liquid–liquid equilibrium occurs. Simulation of the thermodynamic model is used to our ideal IIp RD process. The vapor pressure of each component can be calculated with the Antoine equation. The relevant thermodynamic parameters are listed in Table 1.

The reaction kinetics model references Tung and Yu [12]. The two components with higher boiling points, A and B, are reactants, and the two components with lower boiling points, C and D, are products. This chemical reaction is reversible and exothermic:

$$A + B \Leftrightarrow C + D$$

The reaction rate of each component (R_i) can be calculated as follows:

$$R_i = \nu_i M (k_F x_A x_B - k_B x_C x_D)$$

where the subscript i represents the components involved in it, ν_i is stoichiometric coefficient, M is the liquid holdup in the reaction, x_i represents the molar fraction of the ith component, k_F (forward) and k_B (backward) are the reaction rate constants. Using the Arrhenius equation, it can be calculated as following two equations.

$$k_F = A_F e^{-E_F/RT}$$

$$k_B = A_B e^{-E_B/RT}$$

A_F and A_B are the pre-exponential factors; E_F and E_B are the forward and backward activation energy, respectively; T is temperature (K), and R is the ideal gas constant (kJ/(kmol K)). Table 2 lists the kinetic parameters of this ideal RD process.

3. Reactive distillation process

3.1. Conventional and thermally coupled RD configuration

The conventional IIp RD process was proposed by Tung and Yu [12], and the parameters were described by Lin [10]. The result of

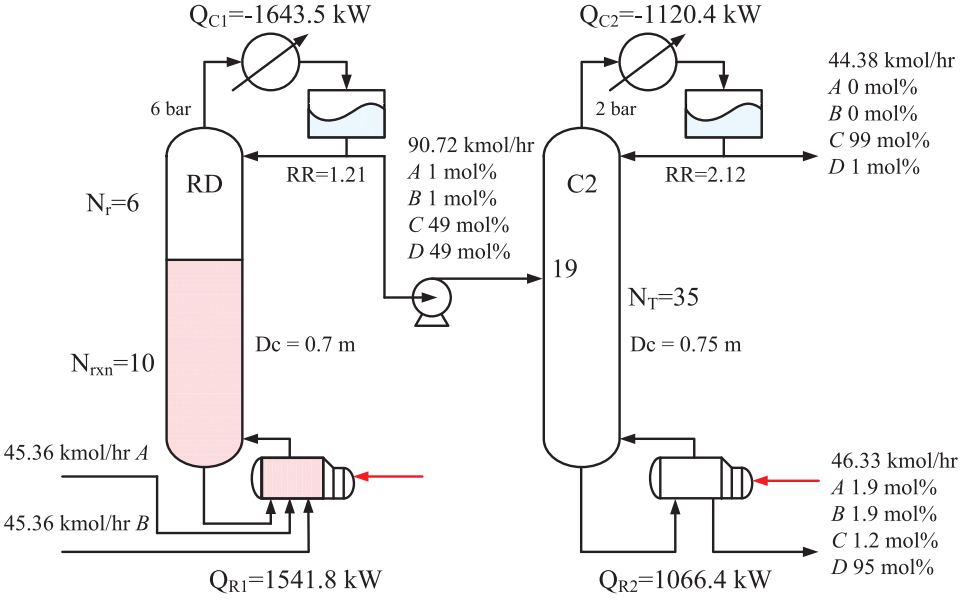

Fig. 1. Result of the ideal RD process with IIp conventional configuration [10].

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