



## Optimal design of mixed acid esterification and isopropanol dehydration systems via incorporation of dividing-wall columns



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### ABSTRACT

This study explores the design of a reactive distillation system and that of a heterogeneous azeotropic system by incorporating dividing-wall column (DWC). The first system involves the esterification of mixed acid (acetic acid and propionic acid) with methanol. Simulation studies are carried out for conventional reactive distillation sequence as well as for reactive dividing-wall distillation system. Both systems are optimized by an iterative optimization procedure. Optimal design results show that the reactive dividing-wall system saves steam consumption by 45.2% and reduces total annual costs (TAC) by 34.5%. The second case investigated is a heterogeneous azeotropic distillation system involving dehydration of crude isopropyl alcohol with cyclohexane as entrainer. Two optimal separation systems are generated, including one with a single-dividing wall column and one with a double-dividing wall column. In comparison with an energy-efficient azeotropic distillation sequence containing two stripping columns by Chang et al. (2012) [1], simulation results show that the former two systems can cut steam usage further by 6.0%. The two systems save about 5.4–6.1% in terms of TAC. DWCs prove to be superior to the convention distillation systems with respect to both cost and energy efficiency.

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### 1. Introduction

Process intensification is a design philosophy that deliberately integrates different processes into a single operation to reduce energy consumption and capital investment, as well as to achieve environmental and safety benefits. It represents an important trend in chemical engineering and process technologies and has attracted increasing attention in the industry and research community. Due to dwindling energy supplies and fluctuating oil prices in recent years, the development of energy-saving processes has become an important issue. In the chemical process industry, distillation is undoubtedly the most energy-intensive separation process utilized in practice. It consumes approximately 3% of the energy in the world [2]. Motivated by this large energy requirement for distillation, much research effort has been focused on the thermal coupling between the distillation columns in series for the separation of multi-component mixtures. Thermally coupled distillation provides potential energy saving of around 30% with respect to conventional distillation trains by

implementing the interconnection of liquid and vapor streams between two columns. Capital cost can be further saved if these two columns with thermal coupling are integrated into one shell. This alternative to conventional columns is recognized as a dividing wall column (DWC). A DWC is achieved by inserting a vertical partition wall in a column shell. It is thermodynamically equivalent to the Petlyuk distillation column. Because of the considerably low requirement on capital investment and operating cost, the DWC has received increasingly more attention since the world's first DWC was successfully established by BASF in 1985 [3,4]. Recently, Dejanović et al. [5] gave a comprehensive overview of DWCs, covering both the theoretical description and the patent area. Yildirim et al. [6] reviewed current industrial applications of DWCs and related research activities. According to Schultz et al. [7], the DWC will become a standard distillation tool in the next 50 years.

Reactive distillation (RD) has attracted much attention in the last two decades due to its potential for improved capital productivity, improved selectivity, increased reaction conversion, and reduced energy usage by combining reaction and separation into a single column. Research on RD has been comprehensively reviewed [8–10]. More than 100 industrially or potentially important reactions for RD applications were surveyed [9]. From

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the book of Luyben and Yu [10], there were 1105 related publications and 814 U.S. patents between 1971 and 2007. Luyben and Yu also highlighted 236 reaction systems, which can be designed by RD configurations. The above references show the importance of RD technology in industrial applications. This useful technology is now being applied for any scale of operation from manufacture of fine chemicals to that of bulk chemicals.

RD and dividing wall distillation are two promising technologies achieving substantial economical benefits from process intensification. Recently, a new intensification scheme known as reactive DWC (R-DWC) has been proposed by combining these two technologies. R-DWC represents a combination of a reactor and a separation unit in one DWC. It is a highly integrated operation and has been investigated in numerous reaction systems, such as fatty ester synthesis [11–15], transesterification reactions [16–21], ethyl acetate synthesis [22], isopropyl acetate synthesis [23], DMC synthesis [24], methyl acetate hydrolysis [25]. In reactive DWCs, reactive systems with more than two products, non-reacting components or excess reactants can be separated.

Heterogeneous azeotropic distillation is commonly used in industries to separate close boiling point mixtures and azeotropes by using an additional entrainer to alter the relative volatility of the components to be separated. The conventional heterogeneous azeotropic distillation sequence usually includes an azeotropic column and a recovery column. In principle, it is possible to combine heterogeneous distillation with the DWC concept. Up to now, only few papers about azeotropic DWC (A-DWC) have been published [26–28].

With the continued growth of the chemical industry, disposal of an increasing quantity of hazardous industrial wastes oftentimes poses a challenge. In some cases, industrial wastes may contain appreciable concentration of mono-carboxylic acids such as acetic acid (HAc) and propionic acid (HPr). There is, in fact, a dire need in a local chemical plant to remove these substances. To efficiently recover these two acids from a waste stream in the plant, RD is used as the first investigated case in the study to yield methyl acetate (MeAc), methyl propionate (MePr), and water by reacting these two acids and methanol (MeOH). Simulation studies are carried out for conventional RD sequence as well as for reactive dividing-wall distillation system. Both systems are optimized by an iterative stepwise optimization procedure. The second case being investigated is the heterogeneous azeotropic distillation for the dehydration of crude isopropyl alcohol (IPA). IPA is widely used in the semiconductor industry as a cleaning agent, thus its recovery from a waste solvent stream is worthy of detailed study. This waste solvent stream contains mainly IPA and water which form a minimum-boiling azeotrope and, thus, is difficult to separate. In the heterogeneous azeotropic distillation, cyclohexane (CyH) is used as an entrainer. Two optimal separation systems are generated in a manner similar to that used for the RD system, including one with a single-dividing wall column and one with a double-dividing wall column. Our simulation results will demonstrate that a R-DWC and an A-DWC by incorporating dividing wall concept in a RD and an azeotropic distillation, respectively, are superior to their corresponding conventional distillation systems with respect to both cost and energy efficiency.

**2. Case 1: design of a mixed acid esterification and purification system**

**2.1. Problem statement**

The first process being looked into involves the esterification of a mixed acid feed with MeOH to yield MeAc, MePr, and water (H<sub>2</sub>O) through a conventional RD sequence system and a R-DWC system.

**Table 1**  
NRTL parameters for the system of esterification of mixed acids and methanol.

Comp. <i>i</i> Comp. <i>j</i>	HAc		HAc		HAc		HAc		HPr		MeOH		MeOH		MeOH		MeAc		MeAc		MePr	
	HPr	MeOH	MeAc	H <sub>2</sub> O	MePr	H <sub>2</sub> O	MeAc	H <sub>2</sub> O	MePr	MeOH	MeAc	H <sub>2</sub> O	MePr	MeOH	H <sub>2</sub> O	MePr	MeAc	H <sub>2</sub> O	MePr	H <sub>2</sub> O	MePr	
<i>a</i> <sub>ij</sub>	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-3.765252	2.278852	0	0	
<i>b</i> <sub>ij</sub>	-60.97606	-122.7962	-257.9757	-190.22	-191.0529	1296.574	-232.8317	-311.81	-84.651	240.3357	151.2656	-79.16406	0	0	0	0	0	1716.77	221.9769	1254.732	0.2	
<i>b</i> <sub>ji</sub>	94.7943	102.4353	448.2141	587.7127	587.7127	-694.3849	347.5604	611.89	879.7869	133.8708	306.3816	375.6612	16.72	107.4711	0.3	0.3	0.415	107.4711	1254.732	1254.732	0.2	
<i>α</i> <sub>ij</sub>	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	
Regression data source	VLE et al. [32]	Malijevka et al. [32]	Sawistowski et al. [33]	Gmehling et al. [34]	Hsieh et al. [35,36]	Gmehling and Onken [37]	Gmehling and Onken [37]	Hsieh et al. [35,36]	Hsieh et al. [35,36]	Ito et al. [38]	Gmehling and Onken [37]	Gmehling and Onken [37]	Gmehling and Onken [37]	Gmehling and Onken [37]	Gmehling and Onken [37]	Hsieh et al. [35,36]	Gmehling and Onken [37]	Gmehling and Onken [37]	Hsieh et al. [35,36]	Gmehling and Onken [37]	Hsieh et al. [35,36]	Srephenson et al. [39] Hsieh et al. [35,36]

$$\ln \gamma_i = \sum_k \frac{x_i \tau_{ki}}{x_i G_{ki}} + \sum_j \frac{x_j G_{ji}}{x_i G_{ji}} \left[ \tau_{ij} - \frac{\sum_k \sum_l \tau_{kl} G_{kl}}{\sum_k x_k G_{kj}} \right] \tau_{ij} = \exp(-\alpha_{ij} \tau_{ij}), \tau_{ij} = a_{ij} + b_{ij} / T, \alpha_{ij} = \alpha_{ji}$$

where  $\gamma_i$ : activity coefficient of *i*;  $x_i$ : mole fraction of *i*;  $\tau_{ij}$ : dimensionless interaction parameters;  $a_{ij}$ : non-randomness parameter;  $T$ : absolute temperature (K).

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