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Design and control of reactive dividing-wall column for the production of methyl acetate

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ABSTRACT

A reactive dividing-wall column (RDWC) is developed for the production of methyl acetate (MeAc) in this work. Both design and control of the RDWC are investigated by using commercial chemical simulator Aspen Plus and Aspen Dynamics. The optimum RDWC design in terms of total annual costs (TAC) is screened based on the proposed optimization procedure. The results show that about 7.7% savings in energy consumption, 8.3% reduction in operating cost and 15.5% decrease in capital investment can be achieved by the RDWC design compared to the corresponding two-column design. Two control structures (i.e., basic control structure and improved control structure) for the RDWC are presented. The results indicate that the improved control structure can handle disturbances in ±20% feed flow rate and −5 wt% feed composition effectively.

1. Introduction

Methyl acetate (MeAc) is a widely-used solvent in the production of cementing compound, coating materials, nitrocellulose, cellulose acetate, cellulose ethers, and celluloid [1]. In addition, MeAc as an intermediate is used in the production of a variety of polyesters [2]. Traditionally, MeAc is synthesized through esterification of acetic acid (HAc) and methanol (MeOH). Rönnback et al. developed a kinetic model for the esterification of acetic acid with methanol in the presence of a homogeneous acid catalyst [3]. Tesser et al. studied the kinetics of oleic acid esterification with methanol by using an acid ion-exchange polymeric resin, and obtained a second-order pseudo-homogeneous model [4]. Altıokka and Çıtak studied the kinetics of the esterification of acetic acid and isobutanol in a stirred batch reactor with and without heterogeneous catalysts [5]. Peters et al., however, made a comparison between homogeneous catalysts and heterogeneous catalysts, and the results indicated that Amberlyst 15 is very effective for the esterification [6]. Traditional strong acids are highly active catalysts in esterification and transesterification reactions, but they usually suffer from corrosive nature, uncontrollable side reactions and difficult recovery. Heterogeneous catalysts can overcome the above-mentioned defects, and are attractive alternatives to homogeneous catalysts [7,8].

Reactive distillation provides an attractive alternative for process intensification to achieve capital and energy costs reduction. Traditional reactive distillation columns (RDCs) mainly involve one-column or two-column process. The former process is stabilized for neat operation by composition controls, which need on-line composition analyzers that are usually costly and introduce large lags. The latter is operated by temperature inferential control for one reactant excess. For two columns process, a reactant recovery column is needed, leading to a higher operation and capital cost [9]. Kiss and Bildea reviewed the industrial applications of DWCs and related research activities, including column configuration, design, modeling and control issues [10–12]. Asprion and Kaibel summarized the fundamentals and advances of DWC [13]. Ramona and Megan presented a rapid conceptual design of single-feed hybrid reactive distillation, and the methodology was illustrated for MTBE production [14,15]. Generally, reactive distillation can achieve high conversion and selectivity than traditional reaction and separation process [16]. DWCs usually can offer about 30% costs savings in capital and energy compared to conventional configurations.

Reactive dividing-wall column (RDWC) integrates a reactor and a separator in one DWC [17]. In such a column, reactive systems with more than two products, non-reacting components or excessive reagents can be separated. Kiss et al. studied the RDWC for the production of FAME with methanol and fatty acids, and the results indicated that 25% of energy savings could be realized compared with the base case design [18]. Mueller et al. developed a special two-step to decompose the RDWC into simple column sequences [19,20]. Fig. 1(a) shows the integration scheme of an

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Nomenclature

C_1	Reactive distillation column
C_2	Rectifying column
CDC	Conventional distillation column
CRDC	Conventional reactive distillation column
DWC	Dividing-wall column
HAc	Acetic acid
k_1	Forward rate constant
k_{-1}	Backward rate constant
K_{eq}	Equilibrium constant for the esterification reaction
L_1	Reflux flow rate in the reactive distillation column
L_2	Reflux flow rate in the rectifying column
m_{cat}	Catalyst-weight
MeAc	Methyl acetate
MeOH	Methanol
N_{HAc}	Acetic acid feed location
N_{MeOH}	Methanol feed location
N_R	Rectifying stages for the reactive distillation column
NRDC	Net reactive distillation column
N_{RX}	Reactive stages for the reactive distillation column
N_S	Stripping stages for the reactive distillation column
N_{T2}	Total stages for the rectifying column
N_{VR}	Withdrawal location of the vapor sidestream
Q_R	Reboiler heat input
r	Reaction rate
RCM	Residue curve map
RDWC	Reactive dividing-wall column
RGA	Relative gain array
RR_1	Reflux ratio in the reactive distillation column
RR_2	Reflux ratio in the rectifying column
SVD	Singular value decomposition
TAC	Total annual cost
V	Flow rate of the total rising vapor from the bottom
V_R	Vapor sidestream flow rate
X_{B3}	Mass fraction of water in the bottom of reactive distillation column
Y_1	Mass fraction of methyl acetate in the vapor sidestream
α_v	Vapor split ratio
β_L	Liquid split ratio

RDWC consisting of two columns separated by a dividing wall (vertical wall). Fresh feed A and B are fed into the left of RDWC, where A reacts with B generating C and D. The lightest component C is withdrawn from the top of the left part of the column and the heavier product D is obtained from the bottom of the column. D and the excess B are separated in the right part column, and as a result, almost pure B escapes from the top of the right column and then recycled back to the left part. It is noticed that the dividing wall top has no internal liquid split because it joins with the inner side wall at a certain location. At the dividing wall bottom, the vapor split ratio is determined by the cross-sectional area and hydraulics of each side of the wall. The scheme illustrated in Fig. 1(b) is equivalent to Fig. 1(a), which is made up of a reactive distillation column and a rectifying column. It is also the integration scheme applied in this study.

Due to the strong interaction among control loops, control problem for RDWC is a challenge. In 1995, Wolff and Skogestad first studied the control of a Petlyuk column for separating an ethanol–propanol–butanol ternary system [21]. Serra et al. studied the control of DWCs in a thorough way [22]. Ling and Luyben proposed a new control structure through manipulating liquid split β_L to realize minimized energy consumption for the separation of a benzene-toluene-*o*-xylene ternary mixture in a DWC [23,24]. Lee et al. studied the control of thermally coupled reactive distillation for the production of isopropyl acetate, and 23.14% energy savings compared to the conventional process can be realized [25]. Abdul Mutalib and Smith investigated the operation and control of the dividing wall column, and presented two different control configuration using temperature control [26,27]. Mueller et al. [19,20] studied the transesterification of acetates process with three types of configurations. They concluded that the RDWC configuration could realize half of the total costs savings in contrast to others.

So far, the study of reactive distillation in one divided wall column is scarce, especially for the control. The purpose of this work is to combine the benefit of reactive distillation with DWC to produce MeAc, and then investigate the design and control of a RDWC with special focus on the establishment of control structures. First, qualitative relationship between process flowsheet and phase equilibria is established and then a RDWC flowsheet is established. Next, a systematic procedure is proposed to obtain the optimum design on the basis of total annual cost (TAC). Finally, two control structures for the RDWC are presented.

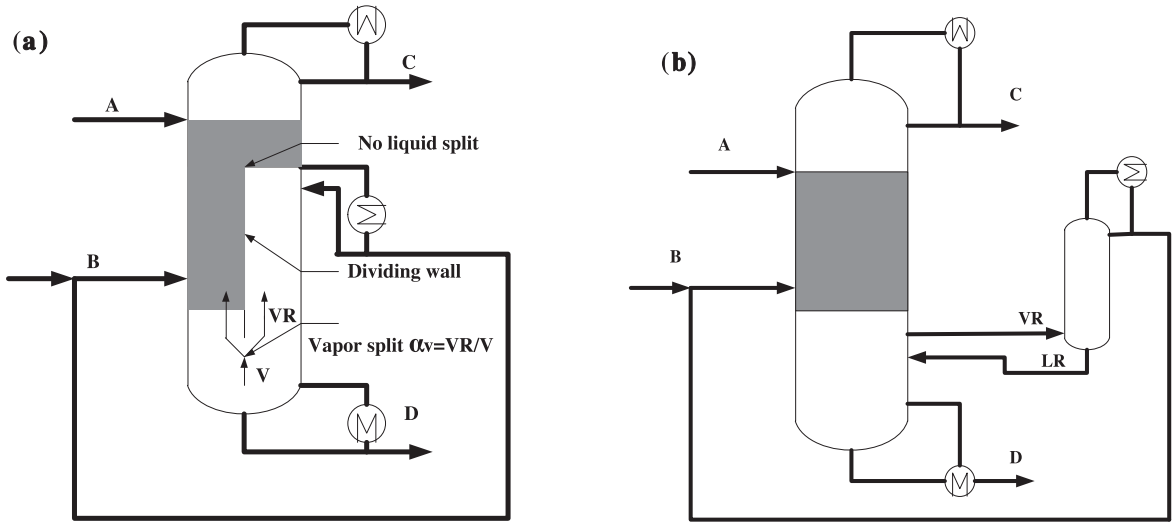

Fig. 1. (a) Integration scheme (b) equivalent scheme for a reactive dividing-wall column.