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Design of an Energy Saving ACN-based Butadiene Production Process by Using Dividing Wall Columns

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Butadiene (normally refers to 1,3-butadiene), separated from C4 mixture, is a major petrochemical product and an important feedstock for downstream polymerization processes. Because each component of the C4 mixture has very similar relative volatilities, extractive distillation is usually used to separate butadiene from the other C4 components, with the aid of some solvents such as acetonitrile (ACN), dimethylformamide (DMF), N-methyl-2-pyrrolidone (NMP). This study considers the ACN-based butadiene production process, which contains several extractive distillation columns (EDCs) and conventional distillation columns (CDiCs). To obtain an energy saving process, the concept of dividing wall column (DWC) is introduced to redesign the conventional flowsheet. That is, two EDCs and two CDiCs are replaced by an extractive dividing wall column (EDWC) and a simple DWC, respectively. With using Aspen Plus, it is observed that the new process design requires less energy consumption as well as less space than the conventional design.

1. Introduction

Distillation, as one of the most important and widespread thermal separation methods in modern chemical process industry (Liu et al., 2017), has been widely used in petrochemical, chemical, metallurgic, food, and textile industries (Cui et al., 2017a). It was shown by researches that approximately 43% of thermal energy is used for industrial applications representing a large part of the global energy usage (Bor et al., 2015). Despite accounting for around 50% of the operational costs of chemical plants (Cui and Sun, 2017), distillation is still one of the most popular separation technologies (Cui et al., 2017b).
Butadiene (normally refers to 1,3-butadiene) is a major petrochemical product and an important feedstock in the production of rubbers and plastics, such as styrene butadiene rubber (Cui et al., 2017c), polybutadiene rubber, and styrene butadiene latex (White, 2007). It is mainly contained in C4 mixture, a by-product from naphtha crackers. Before using in downstream polymerization processes, butadiene must be separated from the C4 mixture. Generally, the C4 mixture contains butane, butene, 1,2-butadiene, 1,3-butadiene and acetylene, etc. Since these C4 components have very similar volatilities, conventional distillation can hardly separate them into each purified component (Cui et al., 2017d). Industrially, extractive distillation can be used to obtain butadiene from the C4 mixture (And et al., 2007). The other C4 components demonstrate different volatility compared with butadiene in some solvents such as acetonitrile (ACN), dimethylformamide (DMF), N-methyl-2-pyrrolidone (NMP), because the presence of solvent varies the polarity between each component as well as corresponding relative volatility.
The basic principle of extractive distillation processes using different solvents is identical, but each process has its own advantages and disadvantages due to different solvent physical properties. Among the abovementioned solvents, the column operating temperature of ACN-based process is the lowest, lowering the possibility of butadiene self-polymerization and increasing operation period. In addition, the lower solvent viscosity and less corrosive property of ACN increase the column tray efficiency, thus the corresponding column investment is relatively lower than other processes. Based on the above advantages, this study focuses on ACN-based butadiene production process.
The conventional ACN-based butadiene production process is shown in Figure 1, including two main sections – extractive distillation section and ordinary distillation section. There are two extractive distillation columns (EDCs) and a side rectifier in the extractive distillation section. The first EDC is used to separate the light

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compounds such as butane, butylene etc as distillate. The second EDC is used to separate crude butadiene product overhead, with the heavier components separated in bottoms. A side rectifier is used to separate vinyl-acetylene as a main side product. In addition, there are two conventional distillation columns (CDiCs) in the ordinary distillation section. The first one is used to separate heavy compounds (heavier than butadiene) like cis-2-butene and C5 components, and the second one separates light compounds (such as propyne) in distillate, leaving the high purity butadiene product in bottoms.

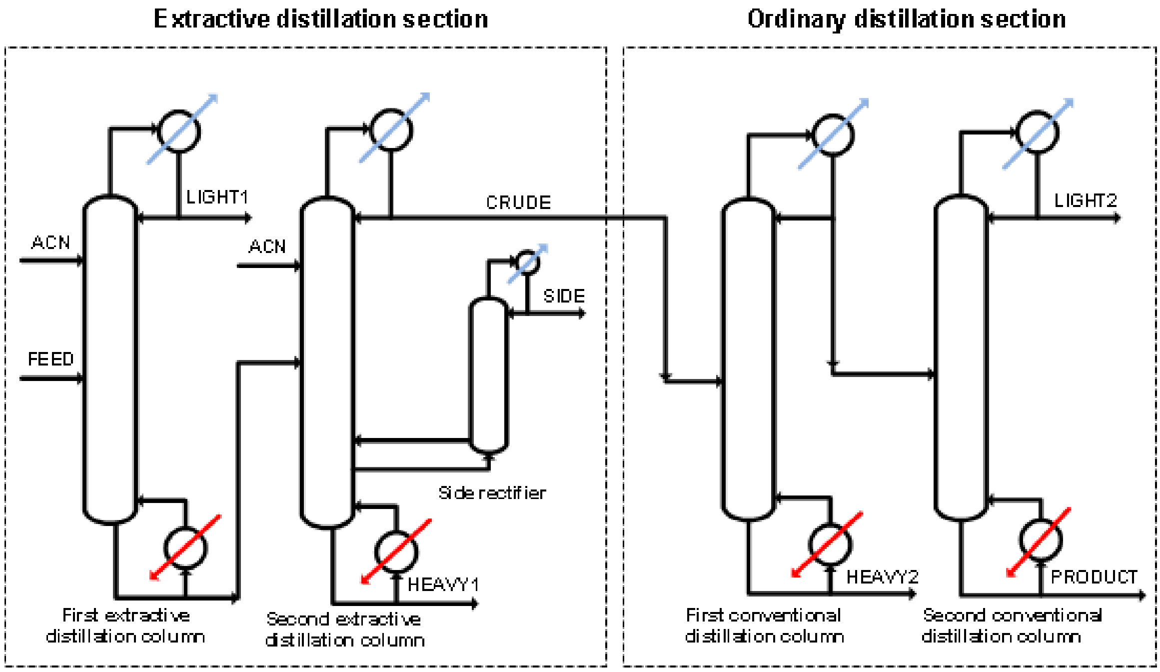

Figure 1: Conventional ACN-based butadiene production process

On the other hand, the conventional ACN-based butadiene process suffers some disadvantages such as high energy consumption, large number of devices, and high investment. To improve the process performance, the concept of dividing wall column (DWC) is used to redesign the conventional process. In detail, two EDCs are redesigned as an extractive dividing wall column (EDWC). Two CDiCs are replaced by a simple DWC.

2. Energy-saving measures

2.1 Dividing wall column

For a ternary mixture, in the presence of a vertical wall, three pure fractions can be obtained in a single distillation column. As shown in Figure 2, two types of DWC configuration can be applied. The first type is middle DWC in which the dividing wall is in the middle section (Figure 2a). For this configuration, the feed and side draws are placed close to the middle section (Asprion et al., 2010). The second type is shown in Figure 2b and Figure 2c where a bottom or top split is employed, and the dividing wall is located either at the upper or at the lower part of the column. The column shown in Figure 2b is referred to as split shell column with common bottoms section and divided overhead section, while the column in Figure 2c is known as split shell column with divided bottoms section and common overhead section (Schultz et al., 2006). With multiple vertical walls, crude feed of ternary system can be separated in a single DWC (Cui et al., 2016). As one of the most important advanced distillation technologies, DWC has been widely used for industrial separation (Li et al., 2018). Due to no back-mixing advantage of a DWC, it has been shown that a DWC can achieve up to 30% of energy saving over conventional distillation sequences (Long et al., 2013). Furthermore, capital investment and space savings can be achieved based on the reduced number of columns, reboilers, condensers, and associated equipment like pumps, pipes, and their supports (Kiss et al., 2012). Therefore, DWC is attractive to many chemical and related industries.

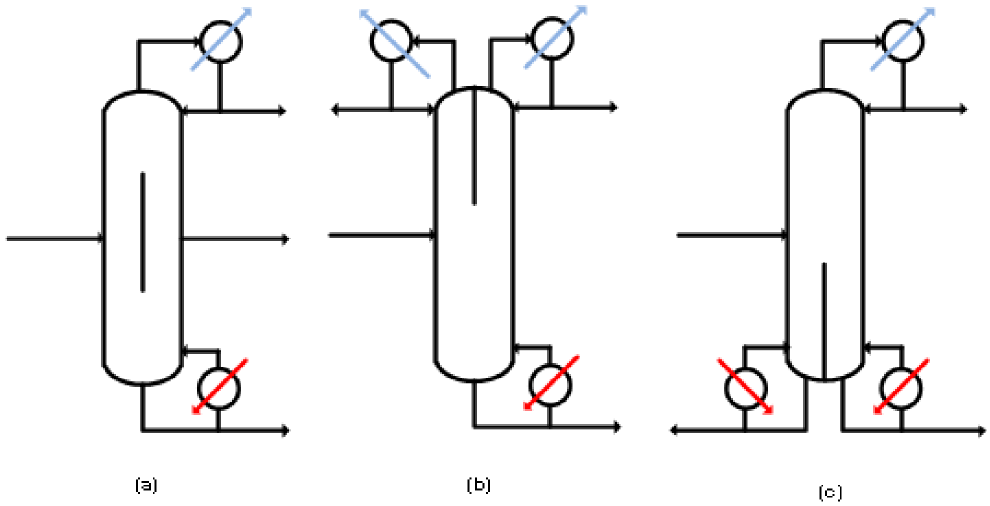

Figure 2: The scheme of three types of DWC with different wall positions

2.2 Extractive dividing wall column

Azeotropic or close-boiling mixtures can be separated using extractive distillation. In the conventional extractive distillation process as shown in Figure 3, an additional solvent S with a boiling point much higher than that of A and B is fed near the top of the first EDC. The relative volatility between the components varies due to the involvement of solvent. In the first EDC, the light component A can be obtained as distillate, whereas solvent S and heavy component B are further separated in the second EDC (Lei et al., 2004). The solvent withdrawn at bottom of the second EDC is recycled back to the first column. It is critical to choose an appropriate solvent in the design of EDCs since solvent selection strongly affects the energy consumption and capital investment of the process due to the differences in selectivity, capacity and boiling points (Luyben 2013).

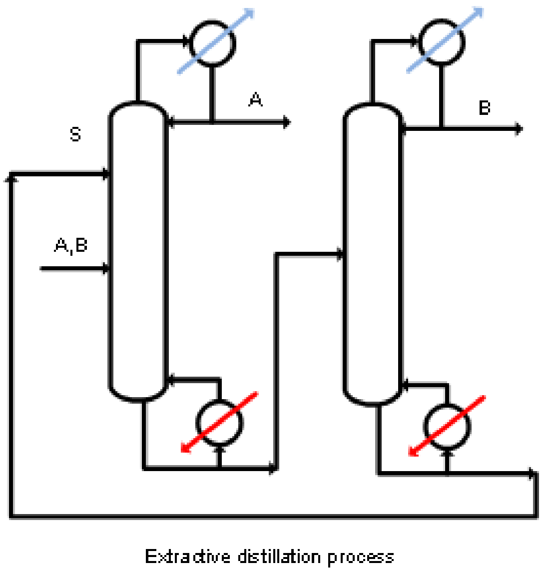

Figure 3: The conventional extractive distillation process

The conventional EDCs can be integrated as an EDWC (Yildirim et al., 2011), illustrating in Figure 4. The EDWC is divided into left and right parts by a vertical wall and a public solvent regeneration part. Mixture A-B and the solvent S are fed to the EDWC. A and B are obtained from the left and right parts of the EDWC, respectively, whereas S is obtained at the bottom of the EDWC and recycled back into the left part. Note that the left and right parts share one public stripping section and one reboiler (Xia et al., 2016), thus capital investment, space and energy cost can be reduced.

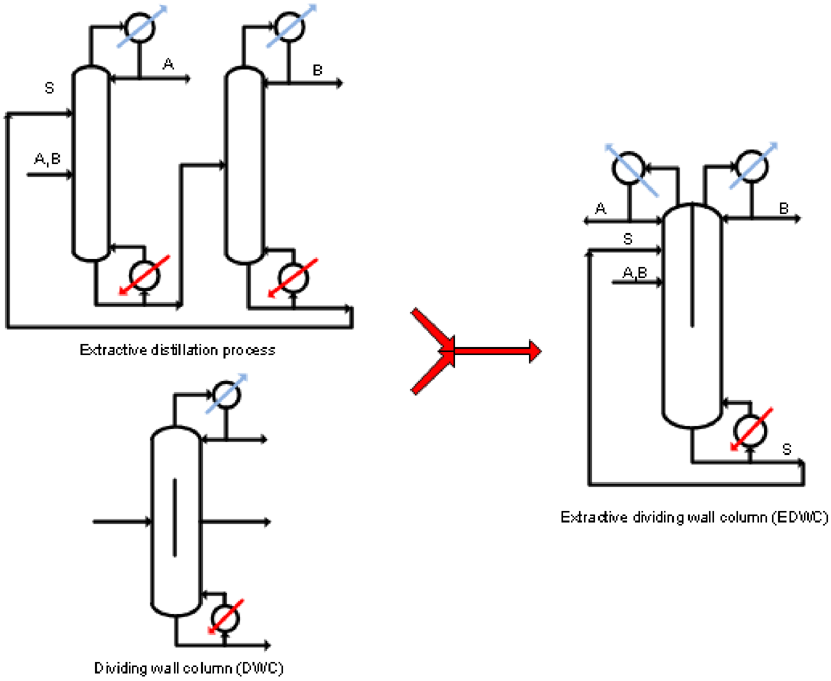

Figure 4: The formation schematic of an extractive dividing wall column

3. Novel butadiene production process

Two EDCs in the extractive distillation section are redesigned as an EDWC, and two CDiCs in the ordinary distillation section are replaced by a DWC. The novel ACN-based butadiene production process is shown in Figure 5. The C4 mixture is fed into the EDWC. The lighter components like butane and butylene are separated in the left part of the EDWC. The crude butadiene product is obtained from the right part of the column and then transferred to the subsequent refining process. The light hydrocarbon components like vinyl-acetylene are removed from the side stripper. The bottom public part of the EDWC is the regeneration section for ACN recovery. The regenerated solvent is then recycled back to the column. The crude butadiene obtained from EDWC is fed into a DWC: the lighter components are separated as distillate, the butadiene product with the required purity is obtained from the middle, and the heavier compounds are separated as bottoms.

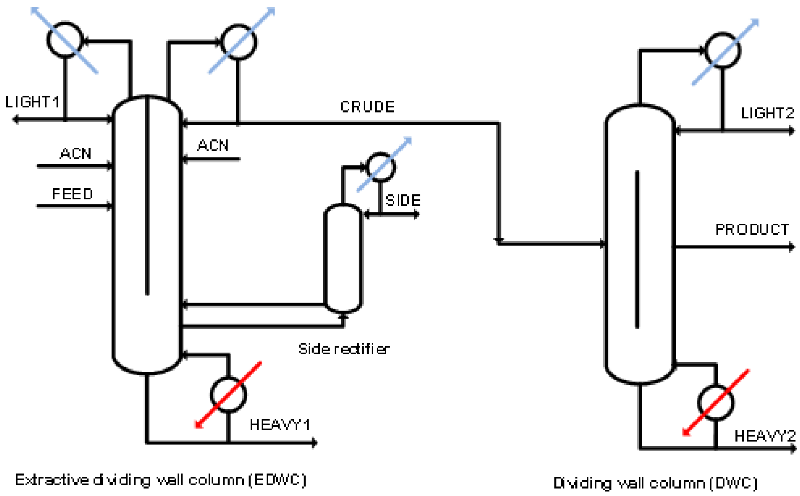

Figure 5: The novel ACN-based butadiene production process

4. Simulation results

Figure 6 shows the equivalent scheme of the novel process in simulation mode. In this work, the simulation was performed on Aspen Plus. The flow rates and composition of the C4 mixture are from on-site data (Table 1). The process consists of 3 columns, an EDWC, a side rectifier, and a DWC. There are three main sections in the EDWC, C11 is the left part, Cl2 the right part and C13 the public stripping section. The side rectifier is connected to the EDWC via thermally coupled stream, drawn out from the 12nd stage of C13 (stage is numbered from top). There are four main sections in the DWC, C31 is the prefractionation section, C32 the public rectifying section, C33 the public stripping section, and C34 the main section. The operation conditions of each column section are shown in Table 2. The mass purity of butadiene product is set as 99.5%. Through Aspen simulation, we observed that the butadiene purity and yield of the novel process are close to the conventional process. The EDWC can achieve 11% of energy saving over the conventional extractive section, whereas the DWC can save up to 20% of energy consumption over the ordinary distillation section.

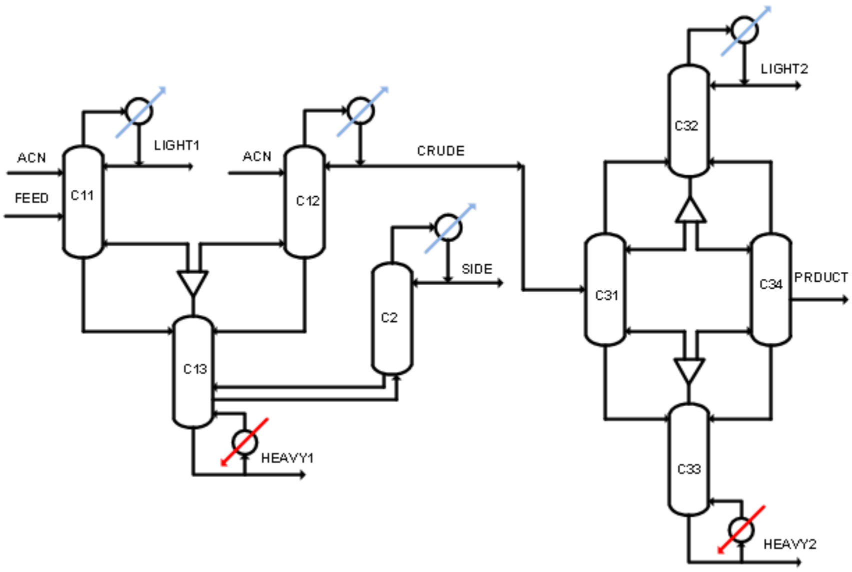

Figure 6: The equivalent scheme *of novel ACN-based butadiene production process*

Table 1: The flowrate and mass fraction of the main components of C4 mixture

Components	Flowrate (kg/h)	Mass fraction (%)
PROPYNE	71.87	0.1732
VINYL-ACETYLENE	172.60	0.4160
1,3-BUTADIENE	8155.35	19.6585
N-BUTANE	7171.03	17.2858
ISOBUTANE	5620.04	13.5472
N-BUTENE	11666.56	28.1223
ISOBUTYLENE	6290.72	15.1638
N-PENTANE	55.39	0.1335

Table 2: Operation conditions of novel ACN-based butadiene production process

Section	Number of stage	Overhead Temperature (°C)	Overhead Pressure (bar)
C11	80	48.60	5.81
C12	62	47.17	5.41
C13	20	92.19	6.51
C2	50	51.80	1.11
C31	40	45.09	5.01
C32	13	29.88	4.81
C33	40	45.18	5.01
C34	66	46.88	5.11

5. Conclusions

This study proposes a novel ACN-based butadiene production process for saving equipment, space, and energy. The conventional extractive distillation section is replaced by an EDWC, and the ordinary distillation section is replaced by a DWC. With using Aspen Plus, the novel process can achieve required product purity and yield. In terms of the energy consumption, EDWC and DWC can save 11% and 20% of energy compared to the corresponding conventional sections. Furthermore, the new design needs lower investment than the conventional design Therefore, the concept of DWC is recommend to be applied in the butadiene production process.

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