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# Applications of dividing wall column technology to industrial-scale cumene production

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## ABSTRACT

Recent advances in dividing wall column (DWC) have led to renewed interest in the design or redesign of many industrial processes. For the distillation system of cumene production, the existing design alternatives have the potentials of energy savings and consequently the reduction of total annual cost (TAC) and energy consumption. In this paper, cumene production based on the real industrial process is simulated in a conventional process using commercial process simulator Aspen Plus, and two DWC distillation processes are introduced. Then optimization study for the proposed DWC distillation processes is performed based on the TAC calculation with sensitivity analysis to investigate the effects of operating parameters. The results indicate that the optimum DWC distillation process works well for the production of cumene, and the corresponding TAC is reduced significantly accompanied by substantial energy savings.

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## 1. Introduction

As an important organic material, cumene is not only used as the thinner for paints and varnishes, but also can be used as the component of aviation fuel. Moreover, cumene is an industrial intermediate mainly used for the production of phenol and acetone, which is produced in a high-temperature and high-pressure gas phase reactor by the reaction of benzene and propylene (Sharma et al., 2013). The Friedel-Crafts alkylation of benzene with propylene is carried out to produce cumene in the chemical industry. The cumene manufacturing process has received a lot of attention in recent years and effort was invested in developing alternative catalyst systems in order to optimize the cumene production (Perego and Ingallina, 2002; Degnan, 2003). Turton (2009) described the cumene process in detail without considering the optimization. Luyben developed a steady-state economic optimum design of the cumene process (Luyben, 2009). Nevertheless, Turton et al. and Luyben didn't use a transalkylation reactor to convert the di-isopropyl benzene (DIPB) back to cumene,

and the DIPB was discarded as a byproduct stream without being processed further. However, the use of transalkylation reactor is a standard practice in a conventional cumene manufacturing process (Pohl and Ram, 2005). Pathak et al. (2011) developed a reactive distillation process with transalkylation reactor for cumene manufacture, which was about 47% cheaper for the total annual cost (TAC) compared with the corresponding conventional distillation process design. Flegiel et al. (2015) modified the cumene process design for reducing the raw materials, product losses, and energy integration. Both two designs they proposed are optimized using multiobjective optimization method which required less energy requirement than other literature designs. Much work was invested in developing the cumene production, nevertheless few flow-sheet based on the heat integration has been announced.

Distillation, as a workhorse of chemical process industries, is an energy-intensive process and, therefore, it is the first to be addressed to improve the energy efficiency over the short- and long-term. Dividing wall column (DWC) distillation, which is thermodynamically equivalent to the Petlyuk column, has

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## Nomenclature

### Greek letters

|             |                                      |
|-------------|--------------------------------------|
| $h_T$       | height of the tower                  |
| $\lambda_V$ | the latent heat of the steam (kJ/kg) |

### Abbreviations

|                     |                                                                  |
|---------------------|------------------------------------------------------------------|
| C-1                 | first column of the separation unit of the whole process         |
| C-2                 | second column of the separation unit of the whole process        |
| C-3                 | third column of the separation unit of the whole process         |
| CC                  | capital cost (\$)                                                |
| $C_p$               | specific heat capacity of the cooling water                      |
| $D$                 | diameter of the column                                           |
| DIPB                | di-isopropyl benzene                                             |
| DWC                 | dividing wall column                                             |
| $F$                 | fresh feed flow rate (kg/h)                                      |
| $F_{L1}$            | flow rate of the liquid stream withdrawn from main column (kg/h) |
| $F_{V2}$            | flow rate of the vapor stream withdrawn from main column (kg/h)  |
| ID                  | industrial data                                                  |
| $L_C$               | height of the column (m)                                         |
| M&S                 | Marshall & Swift index                                           |
| $N_1$               | the number of C-1                                                |
| $N_2$               | the number of C-2                                                |
| $N_3$               | the number of C-3                                                |
| $N_{\text{actual}}$ | the number of actual stages                                      |
| $N_F$               | feed tray location of the DWC                                    |
| $N_{F1}$            | feed tray location of C-1                                        |
| $N_{F2}$            | feed tray location of C-2                                        |
| $N_{F3}$            | feed tray location of C-3                                        |
| NHV                 | the net heating value of a fuel (kJ/kg)                          |
| $N_{L1}$            | source stage of the liquid stream withdrawn from main column     |
| NRTL                | non-random two liquid                                            |
| $N_S$               | side stream tray location of the DWC                             |
| $N_{T1}$            | number of stages in the main column                              |
| $N_{T2}$            | number of stages in the prefractionator                          |
| $N_{V2}$            | source stage of the vapor stream withdrawn from main column      |
| OP                  | operating cost (\$/year)                                         |
| PIPBs               | polyisopropyl benzene                                            |
| $P_1$               | operating pressure of the main column (MPa)                      |
| $P_2$               | operating pressure of the prefractionator (MPa)                  |
| $P_{T1}$            | operating pressure of C-1 (bar)                                  |
| $P_{T2}$            | operating pressure of C-1 (bar)                                  |
| $P_{T3}$            | operating pressure of C-1 (bar)                                  |
| $Q_C$               | condenser heat duty (kW)                                         |
| $Q_R$               | reboiler heat duty of the DWC (kW)                               |
| $Q_{R1}$            | reboiler heat duty of C-1 (kW)                                   |
| $Q_{R2}$            | reboiler heat duty of C-2 (kW)                                   |
| $Q_{R3}$            | reboiler heat duty of C-3 (kW)                                   |
| $R$                 | reflux ratio in the main column                                  |
| $R_1$               | reflux ratio in C-1                                              |
| $R_2$               | reflux ratio in C-2                                              |
| $R_3$               | reflux ratio in C-3                                              |
| SR                  | simulated results                                                |
| TAC                 | total annual cost (\$/year)                                      |
| $U$                 | heat transfer coefficient (kW/(K m <sup>2</sup> ))               |

|    |                                                     |
|----|-----------------------------------------------------|
| XD | cumene composition in the distillate of main column |
|----|-----------------------------------------------------|

received considerable attention as a means of process intensification in the field of chemical engineering (Dejanović et al., 2010; Staak et al., 2014). Since BASF in Ludwigshafen set up the first production scale column in 1985, many researches have been proposed to retrofit conventional columns to DWC (Premkumar and Rangaiah, 2009; Long and Lee, 2013a, 2013b; Chew et al., 2014; Staak et al., 2014). Apart from the potential of both energy and capital cost savings, DWC also requires less space, shorter piping and electrical runs, therefore, the DWC shows great advantages over conventional two-column configuration (Long et al., 2010; Cossio-Vargas et al., 2012; Sun et al., 2014). With the integration of azeotropic, extractive and reactive distillation principles, DWC can be utilized as azeotropic dividing wall column (A-DWC), extractive dividing wall column (E-DWC) and reactive dividing wall distillation (R-DWC) which shows a remarkable reduction in terms of total annual cost and energy requirement (Bravo-Bravo et al., 2010; Murrieta-Dueñas et al., 2011).

Fig. 1(a) illustrates the integration scheme of DWC for separating ternary mixtures, which consists of two parts separated by a dividing wall. Ternary mixtures are introduced into the left part of the column. The light component A and intermediate component B move upward, while component B and the heavy component C flow down out of the left part. These compounds move to the right part of the DWC for further separation. It is noticed that the left and right parts share the common rectifying and stripping sections, which consequently reduces the capital cost as well as the utility cost compared with the conventional distillation sequence.

Process simulation technology is an effective tool to analyze the performance of a chemical engineering process. Aspen Plus, which contains strong databases, complete sets of modules and flexible simulation tools, is one of the standard process simulators in chemical industries. Fig. 1(b) shows the equivalent scheme for DWC implemented in Aspen Plus, which consists of a prefractionator and a main column. This equivalent scheme is applied in the study of this paper for its feasibility of modeling in Aspen Plus. Schultz et al. (2009) proposed a process with the use of DWC for producing cumene, and the fresh benzene fed to the alkylation reactor directly doesn't have any impurities, however, the industrial feed benzene contains impurities such as inert *n*-propane and water, which has a significant influence on the activity and stability of catalyst (Van Bokhoven et al., 2002). The reduction of CO<sub>2</sub> emissions from distillation systems is an absolute necessity and an expensive challenge in the chemical industries (Gutiérrez-Guerra et al., 2009; Ibarra-Sánchez and Segovia-Hernández, 2010). It is desirable to find other feasible distillation systems for industrial cumene production that can achieve the optimum economic design.

Dividing wall columns (DWC) for the distillation of multi-component mixtures have received much attention in the past 15 years and have experienced a booming development. Since DWC demand higher efforts in equipment design and process control, few open literature can be found where DWC are used in industrial operation of cumene production.

Several schemes have been proposed to produce cumene (Lei et al., 2004; Pohl and Ram, 2005; Turton, 2009; Luyben,

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