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Design and optimization of isopropanol process based on two alternatives for reactive distillation

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ABSTRACT

Isopropanol, also known as isopropyl alcohol (IPA) is an important solvent used in many industries. It is mostly produced by direct hydration of propylene involving reversible reaction and azeotropic distillation in separate equipment. There have been many studies on separation of IPA and water azeotropic mixture but very few studies on the use of reactive distillation (RD), for improving overall efficiency of the entire process. RD can be used for IPA production in two different ways: with excess propylene to avoid azeotropic separation, and with excess water to achieve near complete conversion of propylene. The present work investigates both these options by design and optimization of complete IPA process for minimizing capital and operating costs. The results show that the RD process with excess water has lower costs compared to the RD process with excess propylene; but the former incurs small loss of propylene.

1. Introduction

Isopropanol or isopropyl alcohol or 2-propanol (IPA) with the chemical formula C_3H_7OH, is commonly used as a solvent in many industries as well as in household and medical applications like disinfectants. Global capacity for IPA is estimated to be 2.7 million tons per annum, mainly concentrated in North America, East Asia and Europe [1]. It is generally available in two grades: anhydrous composition of 99.8 wt.% (99.3 mol%) IPA and azeotropic composition of 87.4 wt.% (67.5 mol%) alcohol. IPA is manufactured by two major routes: indirect and direct hydration of propylene, of which the latter is common due to less corrosion in process equipment [2].

Direct hydration of propylene is an exothermic, reversible reaction carried out in the presence of an acid catalyst, which could be cation-exchange resins such as molybdophosphoric acid, titanium and zinc oxides [2]. The main reaction is:

$$CH_3CH = CH_2 + H_2O \rightleftharpoons (CH_3)_2CHOH. \quad (1)$$

The side product is diisopropyl ether (DIPE) formed by the reaction:

$$2(CH_3)_2CHOH \rightleftharpoons H_2O + [(CH_3)_2CH]_2O. \quad (2)$$

Conventional IPA process consists of 7 main unit operations, namely, trickled bed reactor, propylene–propane splitter, lights column, pre-concentrator, ether column, extractive distillation column and regenerator for solvent recovery [2]. Thus, the main steps in IPA process are reaction and separation in sequence.

Separation of IPA and water mixture in the downstream of a conventional IPA process has been studied by many researchers, partly due to the challenge posed by azeotrope of IPA and water (with 87.4 wt.% IPA [2]). Heterogeneous azeotroic distillation (HAD) was investigated for IPA production by, for example, Chien et al. [3], Arifin and Chien [4] and Chang et al. [5]. Separation of IPA and water by extractive distillation (ED) was studied by, for example, Luyben [6], Arifin and Chien [7] and Liang et al. [24]. Although purity of IPA produced in these studies is similar around 99.9 wt.% (99.7 mol%), feed composition and flow rate to the separation process are not the same in all of them. Arifin and Chien [7] compared HAD and ED for separation of 77 wt.% (50.1 mol%) IPA in water, and their results show that ED is better with 32% lower total annual cost (TAC). Besides distillation for IPA and water separation, pervaporation in combination with distillation was studied by Sommer and Melin [8]. Sharma and Wankat [9] examined hybrid processes of distillation and adsorption. Liu et al. [10] designed a comprehensive pressure swing adsorption process using a two-bed system packed with 3A molecular sieve adsorbent.

Compared to the studies on separation of IPA and water, there are fewer studies on reactive distillation (RD) for IPA production. Xu et al. [11] studied an IPA process, which requires only two unit operations, namely, RD column with excess propylene and the propylene–propane splitter, rather than seven units in the conventional process. However, simulation of the splitter was not included in the study of Xu et al. [11]. Further work by Wang and Wong [12] proposed a control strategy for

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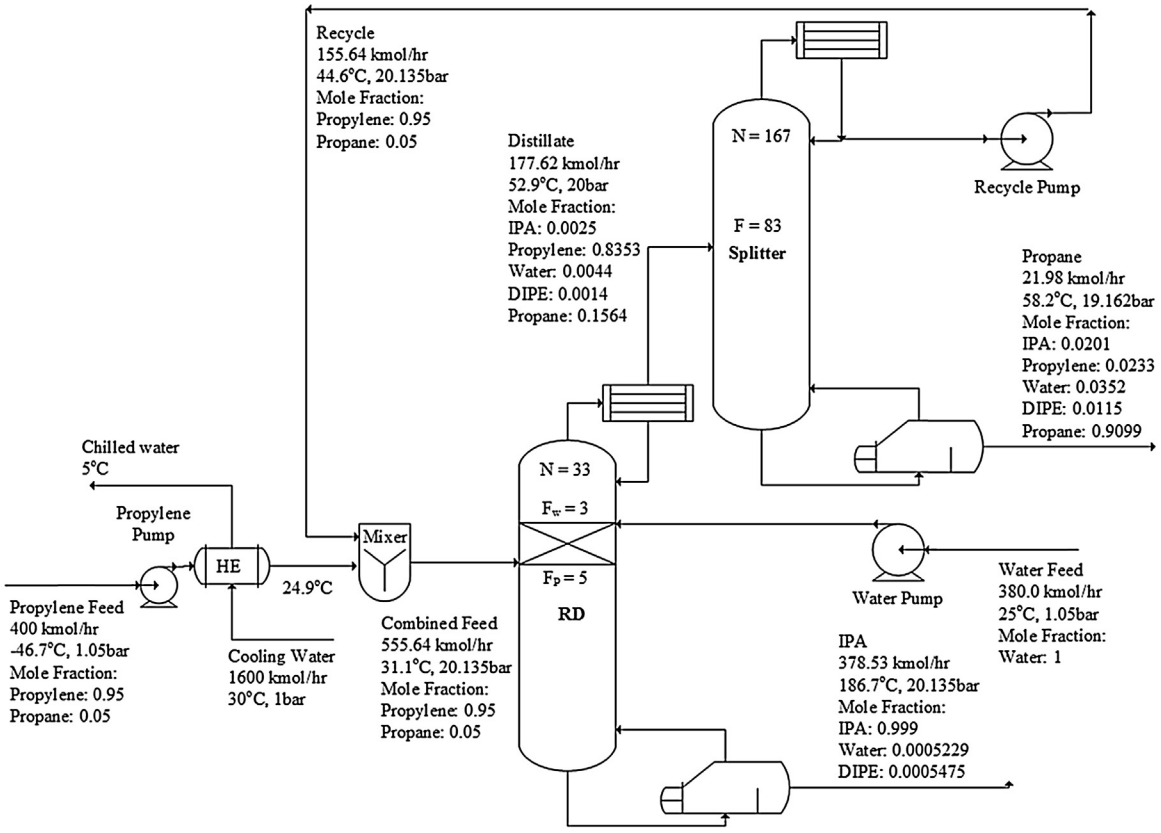

Fig. 1. RD-splitter process flow diagram with stream data for the optimal solution with the lowest TAC.

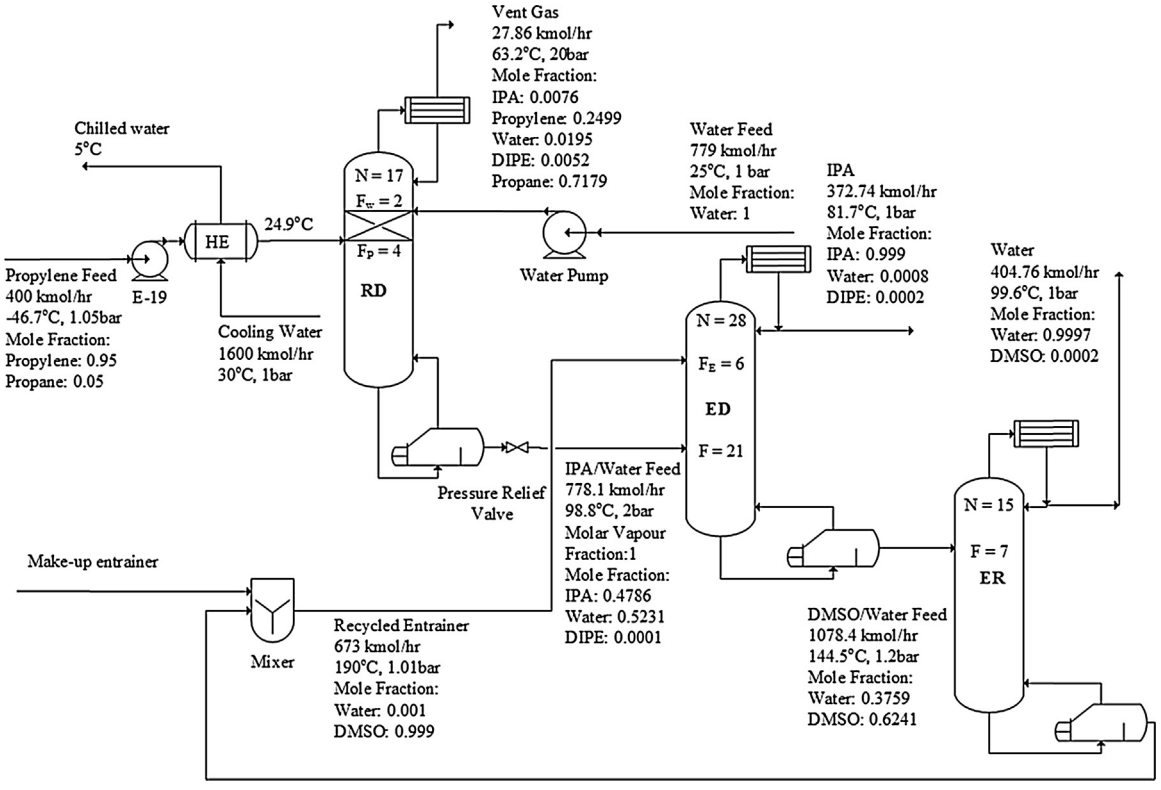

Fig. 2. RD-ED process flow diagram with stream data for the optimal solution with the lowest TAC.