Journal of Membrane Science 497 (2016) 108–119

Contents lists available at ScienceDirect

Journal of Membrane Science

journal homepage: www.elsevier.com/locate/memsci

Vapor permeation–distillation hybrid processes for cost-effective isopropanol dehydration: modeling, simulation and optimization

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ARTICLE INFO

Article history:
Received 13 June 2015
Received in revised form
31 August 2015
Accepted 14 September 2015
Available online 16 September 2015

Keywords:
Membrane-distillation hybrid
Isopropanol dehydration
Vapor permeation
Azeotropic distillation
RSM optimization

ABSTRACT

This study reports the advantages of a cost-effective unit process using a hybrid distillation and vapor permeation unit for isopropanol dehydration. The feasibility of numerous hybrid membrane distillation schemes for isopropanol dehydration was evaluated by simulation and optimization in Aspen Plus. A built-in model for a membrane separation system was proposed by developing a mathematical model in an Aspen Custom Modeler and integrating it simultaneously with an Aspen Plus. The output results of the rigorous membrane models were consistent with the experimental data from the literature. The influence of the decisive operational parameters, which will be used as an optimization variable to examine the different configurations of hybrid systems, was analyzed. Furthermore, this study also employed the response surface methodology (RSM) to optimize the economical calculation and find the best design for the desired product. The RSM optimization effectively connected the interception of the optimizing variables and its predictions agreed well with the results of rigorous simulations. The most significant savings in the total costs could be achieved by applying a distillation–vapor permeation configuration (approximately 77% compared to azeotropic distillation). Therefore, it is economically beneficial to employ distillation–vapor permeation over the previously proposed hybrid systems of the distillation–pervaporation and distillation–pervaporation–distillation.

1. Introduction

Isopropanol is used extensively as a solvent in the automotive and pharmaceutical industries [1]. Most applications require high purity isopropanol, which makes it necessary to remove the water contents. The removal of water from a mixture of isopropanol and water to achieve high purity isopropanol is difficult. Considering the VLE diagram, the formation of an azeotrope occurs at a pressure of 1 bar with a composition of 87 wt% IPA and 13 wt% of water and with a boiling point of 80 °C [2,3].

Azeotropic distillation is a widely applied separation technique for the dehydration of isopropanol [4–6]. Because azeotropic distillation for achieving high purity isopropanol is highly cost-energy intensive, this paper proposed a new combination of distillation and membrane process. The membrane process was chosen to replace the conventional methods due to the increasing applications in process industries [7–9]. In particular, as alternative technologies for azeotropic separation problems, there are two types of membrane processes that have a good impact when combined with a distillation column. These two cases were differentiated due to the phases when entering the membrane, saturated liquid is entering the pervaporation process while in vapor permeation, saturated vapor enters the membrane surface [10].

The economic benefits of the dehydration of isopropanol using hybrid distillation and pervaporation have been reported [11–13]. On the other hand, there no reports on the design and optimization aspects of hybrid distillation with vapor permeation for isopropanol dehydration. The opportunity of the vapor permeation process is where saturated vapor streams are readily usable. This will ward off the phase changes across the membrane surface, which appears simpler than the pervaporation process.

In addition to its simplicity, vapor permeation is less sensitive to concentration polarization on the feed side of the membrane; the membrane lifetime is expected to be longer than pervaporation, due to the low degree of membrane-swelling [14]. Furthermore, the hollow fiber module is used because of its wide applications and large membrane area packed into a small volume [15–17], and it is also capable when combined with a distillation column [18].

Moreover, optimization approaches are promising for process

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http://dx.doi.org/10.1016/j.memsci.2015.09.032
0376-7388/

design studies. Sosa and Espinosa developed rigorous optimization approaches in their conceptual models of hybrid distillation and pervaporation [12]. In the present article, a more detailed total annual cost optimization was performed using a response surface methodology (RSM) technique based on the central composite design method. RSM is one of many techniques for an empirical study of the relationships between the measured responses and independent input variables [19]. RSM used the developed model to optimize the conditions of the process under various conditions. RSM is used widely for many applications because it is efficient and easier to arrange and interpret than other methods [20–22]. RSM uses quantitative data from a proper experimental design to determine and simultaneously solve multivariable problems. Central composite design method proposed three levels (low, medium, and high, coded as -1, 0, $+1$) that required few experimental and simulated runs [23].

Conventionally, the dehydration of isopropanol occurs through azeotropic distillation. The azeotropic distillation process will be used as a base case in this study. In this study, the feasibility of numerous hybrid membrane distillation schemes for isopropanol dehydration was examined by simulation and optimization in Aspen Plus. A built-in model for membrane separation system is not available in Aspen Plus. Therefore, it was implemented by building up a mathematical model in Aspen Custom Modeler and integrating it with Aspen Plus simultaneously. In the commercial use, isopropanol sells at approximately 99.0 and 99.9 wt% IPA. Hence, the objective of this case study was to achieve at least 99.5 wt% isopropanol as the final product.

The feed composition and operating conditions for the separation of an isopropanol–water mixture are same for the azeotropic distillation (base case), previous hybrid system and the proposed design in this work. This work has the advantage of being a cost-effective unit process using a simple configuration without entrainers (compared to azeotropic distillation) and phase changing (compared to pervaporation). To assess the potential of this technique, fair total annual cost comparison between the hybrid distillation–pervaporation and hybrid distillation–vapor permeation is reported. Overall, the total annual cost optimization using RSM can achieve a final optimal design of hybrid distillation vapor permeation for isopropanol dehydration. The decisive variable in the total annual optimization is the isopropanol mass fractions in the interface (top stream of first column) and retentate. The influence of each variable in the hybrid distillation–vapor permeation performance was also examined.

2. Mathematical model of a membrane module

In this case, solution–diffusion model was employed because of its reliability. Fig. 1 presents a schematic diagram of the solution–diffusion model in membrane from feed to downstream. Using this model, the permeate components dissolve in the membrane material and further diffuse throughout the membrane along a concentration gradient. Separation occurs due to the difference in rates of diffusion that each component has through the membrane's material as well as the solubility of each component in the membrane's material.

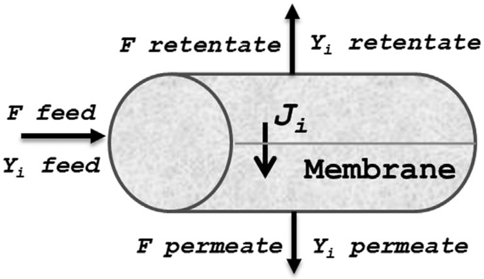

Fig. 1. Schematic of membrane model through the solution–diffusion model.

The mathematical model used is a combination of models proposed by Ji et al. [24] and Wijmans and Baker [25]. This solution–diffusion model consists of two parts. The first is the general mass balance equations at the feed side.

For the total feed flow,

$$\rho_L dq = -J dA_m \tag{1}$$

For organic compounds (component i),

$$dqC_i = -J_i dA_m \tag{2}$$

The second is the equations for calculating the permeation flux. The organic flux can be expressed in terms of the overall permeability or overall mass transfer coefficient as follows:

$$J_i = \frac{D_i \cdot K_i \cdot (p_{io} - p_{il})}{t} \tag{3}$$

The product of the diffusion coefficient by the sorption coefficient (solubility) is the permeability coefficient, leading to

$$J_i = \frac{P_i \cdot (p_{io} - p_{il})}{t} \tag{4}$$

This equation indicates that the flow rate across a membrane is proportional to the difference in partial pressure and inversely proportional to the membrane thickness. The ideal selectivity is applied by the ratio of permeability coefficients between the two elements.

$$\alpha_{i/j} = \frac{P_i}{P_j} \tag{5}$$

The permeability coefficient is a characteristic parameter that is often described as an intrinsic parameter that is easily available from simple permeation experiments with membranes with a known thickness (t).

In this study, a hollow fiber module was used as the membrane module. Comparing with other membrane modules, the hollow fiber module is widely used in the industrial applications because of its many advantages such as lower energy requirement, chemical-free operation, compacteness, and high-efficiency [26,27]. The mathematical equation for overall mass transfer coefficient that is related to the membrane area required in its process conditions was obtained from a previous study [27]. Fig. 2 presents a schematic of hollow fiber membrane separation. The model considered the specific bundle area. The packing density of hollow fiber membrane module is defined as the fraction of the cross section area of all fibers over the cross section area of the module. The bundle of fibers is sealed at one end while the other end of the fiber bundle is retained open to allow the flow of vapors. The fiber bundle is stored as a tube in the middle of a shell. The feed vapor enters the system from the shell side that flows radially inward perpendicular to the fibers toward the middle side. The permeate

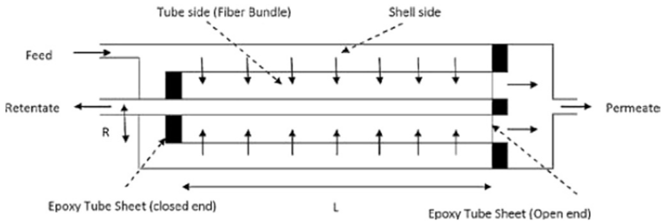

Fig. 2. Schematic diagram of hollow fiber membrane separation [26,27].