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Simulation of Molecular Distillation Process for Lactic Acid

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Abstract: In this work, a procedure to simulate the MD (molecular distillation) process for lactic acid purification was developed. The simulation was carried out with the aid of the Aspen Plus® Process Simulator. Flash vessel was used to represent the MD process since the software does not present this unit operation. The simulation results with efficiency factors were in agreement with previously reported experimental data.

Key words: Simulation, lactic acid, molecular distillation, separation process.

1. Introduction

Lactic acid is a naturally occurring organic acid which has a wide variety of applications such as cosmetics, pharmaceutical products, chemistry, food and more recently in the medical area [1]. It can be made by fermentation of sugars obtained from renewable resources; therefore, it is an eco-friendly product which has attracted much attention in recent years. In 2010, the US Department of Energy issued a report which listed the lactic acid as potential building block for the future. Exploitation of its full potential, however, depends largely on how cost-effectively it can be produced with high levels of purity. The major technology barrier in cost-effective production of high purity lactic acid is its DSP (downstream processing) [2].

MD (Molecular distillation) or short path distillation has been used to recovery lactic acid with purity up to 95-96% [3-5]. MD is a non-conventional unit operation of diffusional mass transfer indicated for separation of homogeneous liquid mixtures with low volatility, thermally sensitive and high molecular mass. The process is distinguished by the following features: short residence time in the zone of the molecular evaporator exposed to heat; low operating temperature due to vacuum in the space of distillation; a characteristic mechanism of mass transfer in the gap between the evaporating and condensing surfaces [6].

Previous experiments [7, 8] showed the viability of the MD process for lactic acid purification. Nevertheless, a deep knowledge of the process is required in order to obtain the desired product streams: small process variations may result in product streams with completely different characteristics [9]. Furthermore, experimental works are expensive and time consuming. In this context, it is interesting to develop a simulation tool based on commercial simulator since components data bank and facilities to integrate with other unit operation are available [10]. In this work, Aspen Plus® will be used in the simulations. As the software does not have a specific tool that simulates the MD process, it is necessary to choose one among the unit operation available to reproduce the main MD features. Flash vessel was used to the MD simulations, since it is easier to start the procedure development with flash operation than use straight way the mass transfer models, as a rate base system [10].

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Bearing all this in mind, the objective of this paper was to evaluate the simulation of the MD process for the lactic acid purification and compare with experimental results.

2. Molecular Distillation

Molecular distillation apparatus have two basic configurations: centrifugal and falling film. In both models, the separation principle is the vacuum, enabling molecules to evaporate from the evaporator to the condenser, and the formation of a thin liquid film which promotes effective heat and mass transfers [11]. In centrifugal distiller, the centrifugal force allows for the formation of a thin liquid film that passes through the heated disk and makes contact with the condenser surface [12]. Falling film distiller uses gravity force to promote a thin film on the evaporating cylinder, usually with a wiping element that mixes and distributes the liquid over the whole evaporator surface [13].

Experimental results were obtained in previous work [7] using a molecular distiller, Model Pope 2 Wiped Film Still, manufactured by Pope Scientific Inc. (Saukville, WI, USA) associated with an external condenser, as shown in Fig. 1 (Falling Film distiller with wiping element). Because of the addition of the external condenser, the system was named HSPE (hybrid short path evaporation). The details of the equipment and experimental procedures can be seen in Ref. [7].

3. Simulation Approach

The simulation of the HSPE process was conducted in Aspen Plus® using Flash vessel, as shown in Fig. 2, for the binary system lactic acid and water. Flash vessel was selected to represent the HSPE operation because Aspen Plus® does not possess a molecular distillation operation tool in its database.

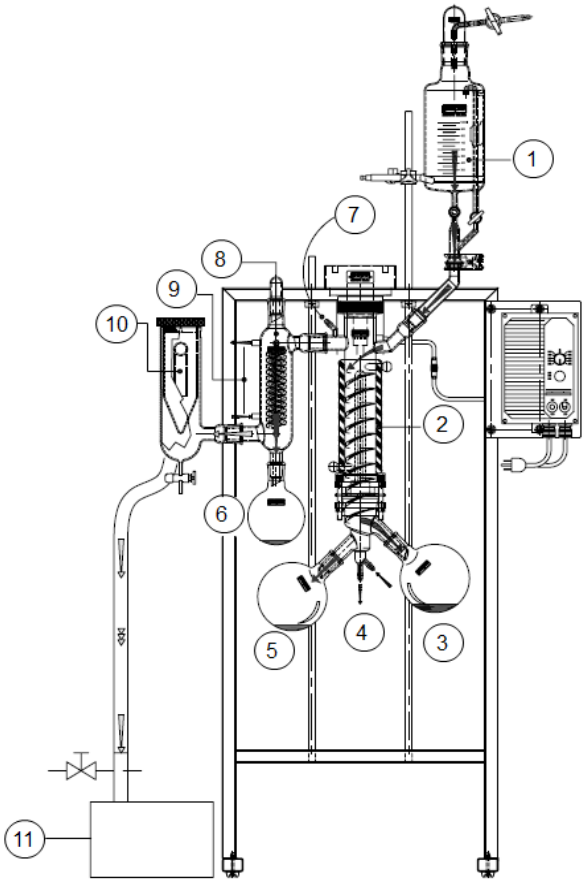

Fig. 1 Hybrid short path evaporation system. (1) feed, (2) electric jacket, (3) residue, (4) coolant, (5) internal condenser distillate, (6) external condenser distillate, (7) vacuum gauge, (8) external condenser, (9) coolant, (10) cold trap, (11) vacuum pump. By permission of Pope Scientific, Inc., Saukville, WI, USA.

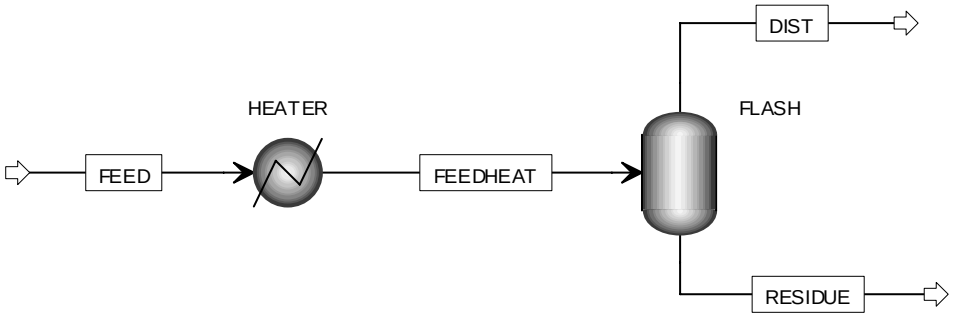

Fig. 2 Flash vessel for molecular distillation simulation in Aspen Plus® environment.

Table 1 Simulation conditions used in Aspen Plus®.

Stream/Block	Temperature (K)	Pressure (kPa)	Total flow (kg/hr)	Lactic acid mass-frac
Feed	298.15	101.3	100	0.3
Feedheat	303-343	101.3	100	0.3
Heater	303-343	1	-	-
Flash	303-343	1	-	-

The simulation conditions of the streams and blocks are shown in Table 1. Lactic acid mass-frac used in feed stream (30 wt. %) agreed with that used in previous studies [7]. Although lactic acid produced by fermentation is a mixture more complex (salts, residual sugars, biomass, nutrients, and other organic acids) than binary system, it was used due to its simplicity and experimental data available.

Mass percentage of residue (% R) and lactic acid purity at residue (% PR) were used for comparison among simulation and experimental data. The operation temperature was the analyzed parameter, since it is the limiting factor for the great majority of MD applications [13]. The flash temperature was varied in order to evaluate in which operation temperature a residue mass percentage was equal to the obtained using a real molecular distillation process.

4. Thermodynamic Model

The selection of a thermodynamic model to determine the activity coefficient is important to the prediction of phase equilibrium. Experimental data available in the literature for the binary system lactic acid and water [14] were compared with data generated by the thermodynamic models NRTL (Non-Randow, Two-Liquid) and UNIFAC (Universal Functional Activity Coefficient) in Aspen Plus®. The selected thermodynamic model was the one which presented the better agreement with experimental data.

5. Results and Discussion

Experimental data for the binary system lactic acid and water obtained by Ref. [14] were compared with thermodynamic models NRTL and UNIFAC using Aspen Plus® for mole fraction of water in liquid and vapor phase. The sum of absolute percentage error was calculated using each thermodynamic model. NRTL was the method which best fit the experimental data. Fig. 3 shows the vapor-liquid equilibrium curves comparing thermodynamic model and experimental data. Hayden O'Connell equation-of-state was used for the calculation of thermodynamic properties in vapor phase. This model accounts for strong association and solvation effects, including those found in systems containing organic acids, such as lactic acid. So, the model NRTL-HOC was used in the simulation in Aspen Plus®.

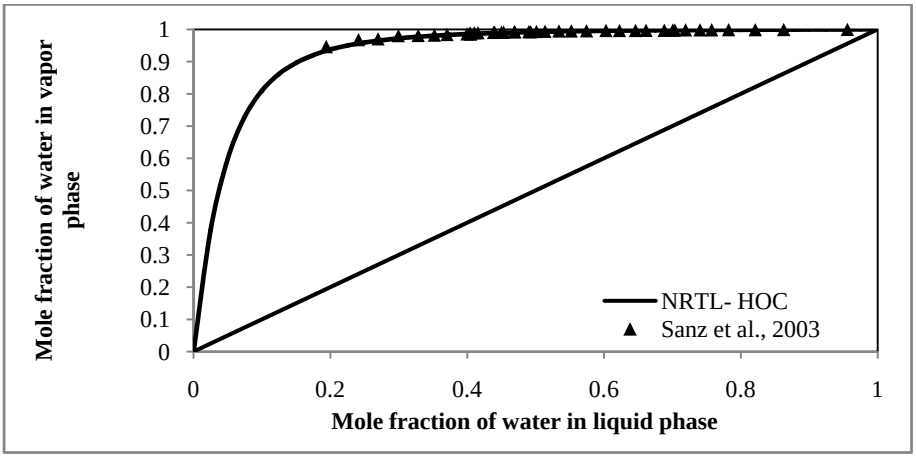

Fig. 3 Vapor-liquid equilibrium curves for water and lactic acid at 1 atm.

Table 2 Experimental and simulation data.

Experimental (HSPE)			Simulation (Flash)		
Temperature (K)	% R	% PR	Temperature (K)	% R	% PR
403	33.90	74.53	303	31.64	94.13
413	27.10	69.33	325.6	27.34	98.46
423	25.59	69.48	329.9	25.62	98.77
433	22.26	70.05	335.5	22.12	99.09
443	15.42	80.89	342.6	14.61	99.36

HSPE = hybrid short path evaporation; % R = mass percentage of residue; % PR = lactic acid purity at residue.

Table 2 shows the experimental data reported by Ref. [7] and simulation results obtained in Aspen Plus® using Flash vessel for mass percentage of residue (% R) and lactic acid purity at residue (% PR).

According to Table 2, for similar mass percentage of residue using simulation approach and experimental data, different operation temperatures were required. It was observed that higher temperature is required using HSPE than using flash vessel. This occurred since HSPE is governed by mass transfer limitations. On the other hand, Flash vessel is an equilibrium operation with and efficiency of 100%. This behavior is in accordance with results obtained by Ref. [10] for the binary system of dibuthyl phthalate and dibutyl sebacate. Similarly, lactic acid purity at residue using Flash is higher than using HSPE. To compare the performance of flash and HSPE, factor of efficiency can be calculated according to Eq. (1).

$$E = \frac{T_{Flash}}{T_{HSPE}} \quad (1)$$

in which T_{Flash} is the temperature using Flash vessel (K) and T_{HSPE} is the temperature using hybrid short path evaporation (K).

Table 3 Experimental and simulation data corrected with efficiency factor.

Experimental (HSPE)	Simulation (Flash)	
% PR	E	% PR corrected
74.53	0.75	70.77
69.33	0.79	77.62
69.48	0.78	77.03
70.05	0.77	76.78
80.89	0.77	76.84

HSPE = hybrid short path evaporation; E = the efficiency factor calculated by Eq. (1); % PR = lactic acid purity at residue.

Values of lactic acid purity at residue were adjusted multiplying the efficiency factor E calculated by Eq. (1) to the % PR of Flash simulation. Table 3 shows the experimental results and % PR corrected with efficiency factor as well as efficiency factors.

Observing Table 3, the values of % PR corrected were in accordance with experimental data. From these results, it can be concluded that Flash vessel is adequate to represent the HSPE data after adjusting by the efficiency factor. The advantage of this approach is simulating a complex unit operation like hybrid short path distillation using a simple unit operation like Flash.

6. Conclusions

In this work was proposed the use of Flash vessel to predict the response of short path evaporation (HSPE) through Aspen Plus® Process Simulator. The results obtained by simulations with efficiency factors showed good agreement in the separation of the mixture lactic acid and water when compared with experimental data. In addition, it was observed that the operating temperatures for the Flash were below to the temperatures adopted for the HSPE. This occurs because Flash is an equilibrium operation and HSPE is rate base system. Based on the results obtained in this work, it can be concluded that the simulation approach using Flash is suitable as a preliminary approach to model the HSPE.

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