



Separation Science and Engineering

Performance Prediction of Structured Packing Column for Cryogenic Air Separation with Hybrid Model[☆]

Xiaobin Zhang, Jiakai Zhu, Zhao Wu, Wei Xiong, Xuejun Zhang, Limin Qiu^{*}

Institute of Refrigeration and Cryogenics, Zhejiang University, Hangzhou 310027, China

ARTICLE INFO

Article history:

Received 29 May 2013

Received in revised form 24 July 2013

Accepted 10 December 2013

Available online 17 June 2014

Keywords:

Distillation

Cryogenic air separation

Structured packings

Hybrid model

Aspen

ABSTRACT

A detailed investigation of a thermodynamic process in a structured packing distillation column is of great importance in prediction of process efficiency. In order to keep the simplicity of an equilibrium stage model and the accuracy of a non-equilibrium stage model, a hybrid model is developed to predict the structured packing column in cryogenic air separation. A general solution process for the equilibrium stage model is developed to solve the set of equations of the hybrid model, in which a separation efficiency function is introduced to obtain the resulting tri-diagonal matrix and its solution by the Thomas algorithm. As an example, the algorithm is applied to analyze an upper column of a cryogenic air separation plant with the capacity of 17000 m³ h⁻¹. Rigorous simulations are conducted using Aspen RATEFRAC module to validate the approach. The temperature and composition distributions are in a good agreement with the two methods. The effects of inlet/outlet position and flow rate on the temperature and composition distributions in the column are analyzed. The results demonstrate that the hybrid model and the solution algorithms are effective in analyzing the distillation process for a cryogenic structured packing column.

© 2014 The Chemical Industry and Engineering Society of China, and Chemical Industry Press. All rights reserved.

1. Introduction

Cryogenic air separation is now the most economical approach to separate oxygen (O₂) and nitrogen (N₂) from the air on a large scale, which can provide customized products of different purity by changing the process [1]. Column is a key unit for the cryogenic air separation with high power consumption. Compared with traditional random-packing columns, structured-packing column (SPC) has the merits of greater capacity, smaller pressure drop and higher separation efficiency [2,3]. In order to improve the efficiency of structured packings and reduce the initial investment, the design of the distillation process needs to be optimized.

Two strategies are usually used to model the distillation in a column, equilibrium-stage (EQ) model and non-equilibrium stage (NEQ) model [4,5]. The EQ model is widely used, which assumes thermodynamic equilibrium between bulk phases, with an empirical efficiency correlation, such as the Murphree efficiency, to offset the difference between calculations and practical conditions. The accuracy of the correlations for different stages under different thermodynamic conditions is questionable [6]. Comparably, the NEQ model is more accurate since it treats the separation process as a mass-transfer-rate-governed one that it really is [7]. Instead of the assumption of thermodynamic equilibrium between bulk phases, the thermodynamic equilibrium is only assumed in a thin interfacial zone. The heat and mass transfer between a bulk phase

and interfacial zone is determined by empirical correlations [8,9]. Seader and Henley have pointed out that the NEQ model and its solution lead to a new era in separation equipment design and simulation [10]. However, since the NEQ model has much more non-linear equations, it is difficult to obtain converged solutions. As a result, its application to large-scale industrial distillation processes is limited. Additionally, calculations of empirical heat and mass transfer coefficients significantly increase the uncertainty of the solution. Good initialization is necessary to obtain final converged solutions [11,12]. In fact, the turbulence-intensified heat exchange between phases is much faster than the mass transfer, so it is reasonable to neglect the thermal non-equilibrium in the NEQ model. The reduced NEQ model is called hybrid model [12,13]. Tang and Wu [12] have evaluated the hybrid model by modeling a separation process for methanol/ethanol/*n*-propanol ternary mixture in SPC. The application of the model to cryogenic SPC for air separation has not been reported.

This study develops a hybrid model to obtain the solution of the distillation process in SPC for cryogenic air separation. We consider the pressure drop and mass transfer resistance in the liquid phase. The model equations are turned into a tri-diagonal matrix by introducing a separation efficiency function and solved by the Thomas algorithm, instead of the complex Newton iteration method used in [12], so that the calculations of partial derivatives of thermodynamic functions are not needed. A cryogenic upper column of an air separation plant with the capacity of 17000 m³ h⁻¹ is considered, with O₂ and N₂ components only in the air mixture. The model is validated by the temperature and component distributions with the rigorous simulations using the Aspen RATEFRAC module. Finally, the effects of inlet/outlet positions and flow rates on the distillation process are analyzed.

[☆] Supported by the Major State Basic Research Development Program of China (2011CB706501) and the National Natural Science Foundation of China (51276157).

^{*} Corresponding author.

E-mail address: limin.qiu@zju.edu.cn (L. Qiu).

2. Model and Algorithm

Commercially available SPCs are comprised of identical n layers of structured packing. Each packing layer is rotated 90° with respect to the previous one. Each layer is an ensemble of a large number of corrugated sheets as shown in Fig. 1, forming a triangular flow channel with dimensions of height (h), side (s), and base (b), as well as the corrugation angle α with respect to the horizontal. Two adjacent corrugated sheets are superimposed so that the opposite corrugations form a cross-type pattern with the crests of the corrugations nearly in contact.

Each layer can be considered as one stage as in traditional plate columns, where the bulk phases are homogeneous. The column has n stages. On each stage, it is assumed that $T_j^L = T_j^I = T_j^V$, where T is the temperature, superscripts L, I, and V represent the liquid phase, interface and vapor phase, respectively, and subscript j stands for the j th stage of total n . The following assumptions are also made for the calculations: (a) pressure in equilibrium, $P_j^L = P_j^I = P_j^V$; (b) no component and temperature gradient in the radial direction; and (c) phase equilibrium only in the gas/liquid interfacial zone. Fig. 2 shows the model on the j th stage, which involves gas-phase feed rate F_j^V , liquid-phase feed rate F_j^L , molar flow rate L , molar fractions of component i in the liquid phase x_i and in the gas phase y_i , specific enthalpy h per mole, temperature T , exhausting gas S_j^V and liquid S_j^L , mass flux $N_{i,j}$ and heat flux $e_{i,j}$ between phases, here $e_{i,j} = 0$ for our calculations.

Based on the above assumptions, the set of control equations is exactly the same as that of the conventional NEQ model [10] without the heat transfer equations.

Material balance equations for the component:

$$M_{i,j}^V \equiv (V_j + S_j^V)y_{i,j} - V_{j-1}y_{i,j-1} - F_j^V z_{i,j}^V + N_{i,j}^V = 0, \quad i = 1, 2, \dots, c \quad (1)$$

$$M_{i,j}^L \equiv (L_j + S_j^L)x_{i,j} - L_{j+1}x_{i,j+1} - F_j^L z_{i,j}^L - N_{i,j}^L = 0, \quad i = 1, 2, \dots, c. \quad (2)$$

Material balance equation at the phase interface:

$$M_{i,j}^I \equiv N_{i,j}^V - N_{i,j}^L = 0, \quad i = 1, 2, \dots, c. \quad (3)$$

Energy balance equations without the heat lost:

$$E_j^V \equiv (V_j + S_j^V)H_j^V - V_{j-1}H_{j-1}^V - F_j^V H_{F,j}^V = 0 \quad (4)$$

$$E_j^L \equiv (L_j + S_j^L)H_j^L - L_{j+1}H_{j+1}^L - F_j^L H_{F,j}^L = 0. \quad (5)$$

The equations for the molar-fraction summation for each phase are applied at the vapor–liquid interphase:

$$\sum_{i=1}^c x_{i,j}^I - 1 = 0, \quad \sum_{i=1}^c y_{i,j}^I - 1 = 0. \quad (6)$$

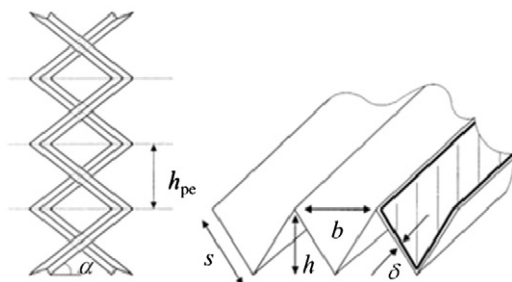


Fig. 1. Basic geometry of the packing.

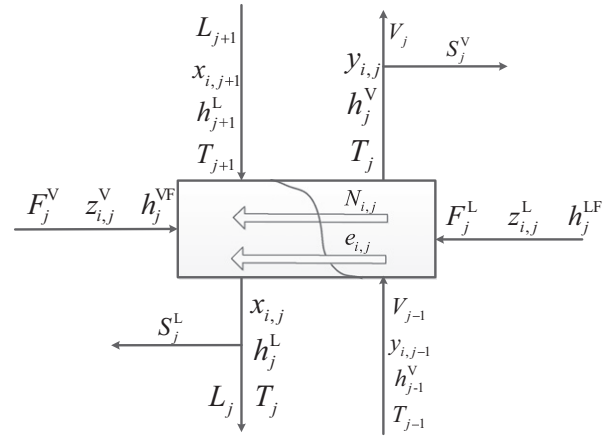


Fig. 2. Schematic diagram of stage j .

The hydraulic equation for stage pressure drop is given by

$$P_{j+1} - P_j - \Delta P_j = 0 \quad (7)$$

where ΔP_j is the pressure drop at stage j .

Phase equilibrium for each component is assumed to exist only at the interphase:

$$y_{i,j}^I - K_{i,j}x_{i,j}^I = 0 \quad (8)$$

where $K_{i,j}$ is the phase equilibrium constant. The general forms for mass-transfer rates of component i across vapor and liquid films on a stage are as follows

$$N_{i,j}^V \equiv k_{i,j}^V a_j v_j (y_{i,j} - y_{i,j}^I) + y_{i,j} N_{t,j} \quad (9)$$

$$N_{i,j}^L \equiv k_{i,j}^L a_j v_j (x_{i,j}^I - x_{i,j}) + x_{i,j} N_{t,j} \quad (10)$$

where $k_{i,j}^V$ and $k_{i,j}^L$ are the mass transfer coefficients ($\text{mol} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$), a_j is the effective mass transfer area at stage j ($\text{m}^2 \cdot \text{m}^{-3}$), and v_j is the volume of stage j (m^3).

Combining Eqs. (8) and (3) with Eqs. (9) and (10), we have

$$x_{i,j}^I = \frac{k_{i,j}^L a_j x_{i,j} + k_{i,j}^V a_j y_{i,j} + (y_{i,j} - x_{i,j}) \sum_{i=1}^c N_{i,j}^V}{k_{i,j}^L a_j + k_{i,j}^V a_j K_{i,j}}. \quad (11)$$

Substituting Eq. (11) into Eqs. (8) and (9), and relating it with Eq. (1), the ‘separation efficiency function’, which shows the relationship between vapor and liquid compositions, we have

$$x_{i,j} = \alpha_{i,j} y_{i,j} - \beta_{i,j} y_{i,j+1} - \gamma_{i,j} \quad (12)$$

$$\alpha_{i,j} = \frac{k_{i,j}^L k_{i,j}^V a_j + k_{i,j}^L \sum_{i=1}^c N_{i,j}^V + (k_{i,j}^V K_{i,j} + k_{i,j}^L) (V_j + S_j^V)}{k_{i,j}^L k_{i,j}^V a_j K_{i,j} - k_{i,j}^V K_{i,j} \sum_{i=1}^c N_{i,j}^V} \quad (13)$$

$$\beta_{i,j} = \frac{(k_{i,j}^V K_{i,j} + k_{i,j}^L) V_{j+1}}{k_{i,j}^L k_{i,j}^V a_j K_{i,j} - k_{i,j}^V K_{i,j} \sum_{i=1}^c N_{i,j}^V} \quad (14)$$

Download English Version:

<https://daneshyari.com/en/article/167393>

Download Persian Version:

<https://daneshyari.com/article/167393>

[Daneshyari.com](https://daneshyari.com)