Simulation of the process of rectification with the account of longitudinal diffusion

A B Golovanchikov, N A Prokhorenko, N V Shhibitova, M D Romanenko and O A Zalipayeva

Volgograd State Technical University, pr. Lenina, 28 Lenina Street, Volgograd 400005, Russian Federation

1E-mail: natasha292009@yandex.ru

Abstract. Based on the differential equations of material balance and mass transfer, taking into account the longitudinal mixing of the boiling solution, the formulas of the working lines of the reinforcing and exhaustive parts of the packed distillation column, the concentration profiles along the nozzle height, and the algorithm for calculating the height of the nozzle are proposed. The equations of the working lines of the reinforcing and exhaustive parts of the distillation column are analytically derived, taking into account the longitudinal diffusion, which, when the longitudinal diffusion number or the longitudinal diffusion coefficient, is transformed into the known equations of the working lines for the flow patterns of ideal displacement in both phases. Analytically, on the basis of the differential equations of material balance, the equations of working lines and mass transfer in a rectifying column for binary mixtures with allowance for longitudinal diffusion are derived. It is shown that in its absence, when the flow structure for both phases corresponds to an ideal displacement, that is, the Peclet number of longitudinal diffusion, and the longitudinal diffusion coefficient itself, the resulting equations of working lines and mass transfer become known equations for the reinforcing and exhaustive parts of the column. Comparative examples of calculations for typical structures of the ideal displacement flow and for derived equations that take into account longitudinal diffusion for the binary mixture "ethyl alcohol-ethyl alcohol" are given.

1. Introduction

Since the last century, in the description of the flow structure of chemical reactors, various other models began to take into account deviations from ideality: cell-based, combined, combining in series and parallel connection of zones of ideal displacement and mixing. But the most accurate description of the real flow structure is given by the model with diffusion flow structure or flow with reverse mixing. Gradually, this model was also used in heat and mass transfer processes (heat exchangers, absorbers, adsorbers and ion exchange columns with a fixed and moving sorbent layer, extractors, drum dryers and fluidized beds, ultrafiltration and reverse osmosis machines and others. In modern studies, the authors will calculate the rectification process without taking into account the longitudinal diffusion [1-3]. For the first time, they began to use diffusion in the calculations of the absorption process; the calculation algorithm is presented in the textbooks [4].

However, in practice, this model is practically not used when describing rectification processes, where heat and mass transfer processes occur simultaneously.
The known typical models of the flow pattern in the packed columns are based on the ideal displacement of both phases along the entire height of the column [5-6]. Corresponding to this physical model, analytical equations of the working lines of the strengthening and exhaustive parts of the column are deduced on the basis of the material balance, which are linear dependences of the concentration of the readily volatile component in the vapor and liquid phases, which are the basis for calculating the minimum reflux ratio, the number of theoretical plates, the optimum reflux ratio and geometric dimensions of packed and tray rectification columns.

The purpose of the article is an analytical conclusion based on the material balance of the equations of the working lines of the strengthening and exhaustive parts of a distillation column, taking into account the longitudinal diffusion of the vapor and liquid phases, and analyzing these equations for the minimum reflux number, the number of theoretical plates, the optimum reflux number and the geometric dimensions of the distillation column.

2. Methodology

To eliminate these deviations of the real structure of the flows from ideal displacement, one can take into account the efficiency of the plate, the kinetic curves that take into account the degree of use of the local driving force, the empirical dependences associated with the height of the theoretical plate (HEP) or the height of the transfer unit (HTU) [6].

The aim of the article is an analytical conclusion based on the material balance of the working-line equations of the strengthening and exhaustive parts of the distillation column, taking into account the longitudinal diffusion of the vapor and liquid phases, and analysis of these equations by the minimum reflux ratio, the number of theoretical plates, the optimum reflux ratio and the geometric dimensions of the distillation column.

We derive the equation of the working line for the exhaustive part of the column, taking into account the longitudinal diffusion in the vapor phase.

We select the section I-I from the bottom of the column at a distance z from the support grid of the nozzle (where the steam enters the nozzle) (figure 1).

To simplify the recording, we assume that the costs of the initial mixture \(G_f\), reflux \(G_f\) and distillate \(G_d\) 

\[
\left(G_f + G_f\right) \cdot x + \left(G_f + G_d\right) \cdot y_0 + \frac{V_{d_s} \cdot S \cdot \rho_d}{M_d} = \left(G_f + G_f\right) \cdot x_k + \left(G_f + G_d\right) \cdot y + \frac{V_{d_s} \cdot S \cdot \rho_d}{M_d},
\]

where \(G_f\) is amount of initial mixture; \(G_f\) - amount of reflux in the column; \(G_d\) - amount of selected distillate in the form of the finished product; \(x\) - fluid concentration; \(y\) - concentration in gas; \(x_k\) - reflux concentration; \(S\) - rectification area; \(V_{d_s}\) - initial velocity of longitudinal vapour diffusion; \(M_d\) - molecular diffusion.

Here, on the left side of the material balance, the arrival of the volatile component in the allocated volume between the sections O-O and I-I, in the right-hand side is its consumption. The longitudinal diffusion rate along the vapor phase can be written in the form of a modified Fick law

\[
V_{d_s} = -D_l \cdot \frac{dy}{dz},
\]

where \(D_l\) - is coefficient of longitudinal diffusion in the vapor phase.

Then the connection between \(y\) and \(x\) can be represented after the algebraic transformations by the equation:

\[
y = y_0 + \left[\frac{G_f + G_f}{G_f + G_d}\right] \cdot (x - x_k) - \frac{S \cdot \rho_d \cdot \left(\frac{dy}{dz}\right)_0 - \left(\frac{dy}{dz}\right)}{M_d \cdot (G_f + G_d)} \cdot D_l.
\]
We divide the expression in the square brackets of the second term on $G_d$ and having in mind the third term for the continuity equation, from which the expression for the fictitious vapor velocity follows:

$$V_y = \frac{(G_r + G_d) \cdot M_d}{\rho_d \cdot S},$$

and also passing to the dimensionless height coordinate $h = \frac{z}{H}$, we get:

$$y = y_0 + \left(\frac{F + R}{R + 1}\right) (x - x_K) - \frac{[g_0 - g]}{Pe},$$

where $g = \frac{dy}{dx}$ and $g_0 = \left(\frac{dy}{dz}\right)_{z=0}$, $Pe = \frac{V_v \cdot H}{D_l}$ - Peclet number in the vapor phase.

**Figure 1.** The rectification scheme in the exhaustive part of a column with material flows and concentrations of an easily volatile component in the vapor and liquid phases, taking into account the longitudinal diffusion along the vapor phase.

For $h = 1$, that is, at $z = Hu$ at the input of the initial solution to the exhausting part of the column $x = x_F$, $y = y_F$, $g = g_F$:

$$y_F = y_0 + \left(\frac{F + R}{R + 1}\right) (x_F - x_K) - \frac{(g_0 - g_F)}{Pe}.$$
From the known boundary condition at the input for the diffusion model it follows:

\[ h = 0 \quad y_K = y_0 - \frac{g_0}{Pe}. \]  

(2)

Then, substituting the value of \( y_0 \) in the equation of material balance, we get:

\[ y_F = y_K + \left( \frac{F + R}{R + 1} \right) \cdot (x_F - x_K) + \frac{g_F}{Pe}. \]

But from the material balance of the entire exhausting part of the column:

\[ (R+1) \cdot (y_F - y_K) = (F + R) \cdot (x_F - x_K), \]  

i.e., the gradient \( g_F = \left( \frac{dy}{dh} \right)_{h=1} = 0 \).

The final equation of the working line of the exhaustive part of the packed distillation column taking into account the longitudinal diffusion along the vapor phase takes the form:

\[ y = y_K = \left( \frac{F + R}{R + 1} \right) \cdot (x - x_K) + \frac{g}{Pe} \]

(3)

with boundary conditions:

\[ h = 0, \quad y_0 = y_K + \frac{g_0}{Pe}; \]

\[ h = 1, \quad g_F = 0, \]  

(4)

As can be seen, equation (3) in the general case is nonlinear and goes over into the typical linear equation of the working line of the exhaustive part of the distillation column corresponding to ideal displacement in both phases, with \( Pe \to \infty \) or \( D_j \to \infty \).

Similarly, the equations of the working line for the vapor phase for the strengthening part of the column are derived (figure 2).

In this case, the equation of the working line of the reinforcing part of the distillation column with longitudinal diffusion along the pair becomes [7]:

\[ y = y_F + \frac{R}{R + 1} \cdot (x - x_F) + \frac{1}{Pe} \cdot g \]

(5)

with boundary conditions:

\[ h = 0, \quad y_F = y_H - \frac{1}{Pe} \cdot g_d; \]

\[ h = 1, \quad g_d = 0, \]  

(6)

Figure 3 shows the graphs of the working line equations for the exhaustive and reinforcing parts of the distillation column: typical 2a and 2b, which do not take into account longitudinal diffusion, that is, corresponding to ideal displacement in both phases at \( Pe \to \infty \) or \( D_j \to 0 \), and 3a and 3b, taking into account the longitudinal diffusion along the vapor phase and corresponding to the above derived working line equations for the exhaustive part of the column (3) with the boundary conditions (4) and for the reinforcing part of the column with the equation of the working line (5) with the boundary conditions (6).

3. Results and Discussions

From the graphs of the working-line equations (3) and (5), it can be seen that longitudinal diffusion first leads to a jump in the concentrations at the steam inlet into the exhausting and strengthening parts of the column, that is, \( y_0 > y_K \), and \( y_F > y_F \) (figure 3), and secondly the working lines themselves are not straight, but are described by convex curves. Both differences can significantly reduce local and average driving forces, which leads to an increase in the number of theoretical plates, the number of
transfer units, the minimum and optimal reflux numbers, and with them the diameters and heights of each part of the column.

Figure 2. The rectification scheme in the reinforcing part of the column with material flows and concentrations of the volatile component in the vapor and liquid phases, taking into account the longitudinal diffusion along the vapor phase.

Figure 3. Equilibrium (1) and working lines: typical without longitudinal diffusion for exhaustive (2a) and reinforcing (2b) parts of the column; taking into account the longitudinal diffusion for the vapor phase for the exhaustive (3a) and reinforcing (3b) parts of the column.
Similar mathematical calculations were made by the authors for the column, taking into account the longitudinal diffusion over the liquid phase in the paper [3].

In the general case, when longitudinal diffusion takes place both over the vapor and liquid phases, we obtain the equations of the working lines, taking into account the corresponding concentration gradients and Peclet numbers of longitudinal diffusion along both phases in both parts of the column.

For the exhaustive part:

$$ y = y_k + \left( \frac{F + R}{R + 1} \right) \left( x - x_k \right) - \frac{F + R}{R + 1} \cdot \left( \frac{g}{Pe_x} \right) + \left( \frac{g}{Pe_y} \right) $$

(7)

For the strengthening part of the column:

$$ y = \left( \frac{x_d + R \cdot x}{R + 1} \right) - \frac{R}{R + 1} \cdot \left( \frac{g}{Pe_x} \right) + \left( \frac{g}{Pe_y} \right) $$

(8)

Graphs of the equations of the working lines of the reinforcing and exhaustive parts of the column, taking into account the longitudinal diffusion in both phases, are shown in figure 4 (lines 3a and 3b).

Figure 4. Equilibrium (1) and working lines: typical without longitudinal diffusion for the exhaustive (2a) and reinforcing (2b) parts of the column; taking into account the longitudinal diffusion in both phases for the exhaustive (3a) and reinforcing (3b) parts of the column.

4. Conclusion
Longitudinal diffusion reduces the local and medium motivational forces of the mass transfer processes in both parts of the distillation column due to a jump in the concentrations at the inlet through the vapor and liquid phases, and also leads to a transition from linear equations of the working lines to nonlinear ones. At critical values of Peclet numbers on the steam $Pe_x$ the phases K, F and D of the working lines (Figure 4) fall on the equilibrium line 1, that is, the working lines 3a and 3b cross the equilibrium line, which theoretically increases the height of the column to infinity. In the general case, allowance for longitudinal diffusion may require an increase in the reflux ratio as compared to a typical calculation and lead to an increase in the diameter and height of both parts of the distillation column.
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