Equations of working lines in packed columns with regard to longitudinal diffusion

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Abstract. The analysis of differential equations of material balance with mass transfer taking into account longitudinal diffusion on both phases in a packed absorber and a distillation column is carried out. It is proposed according to the known algorithms for the calculation of absorption processes to calculate the working lines separately for two cases: 1) solid phase moves in the mode with longitudinal diffusion and dispersion in the ideal displacement mode; 2) continuous phase moves in the ideal displacement mode and dispersion mode with longitudinal diffusion, and then by summing the ordinates of the resulting working lines, to its overall significance to him and the equilibrium line on a standard methodology to calculate the height and diameter of the column.

1. Introduction

Methods for calculating mass transfer processes (absorption, rectification, extraction) in packing columns taking into account longitudinal diffusion, when one of the phases, solid or dispersed, moves in the mode of ideal displacement, and the second - with longitudinal diffusion, are known and used in the design of mass transfer packing columns [1-4].

In the textbook [1], the conclusions of the formulas of the working lines of mass transfer processes are given taking into account longitudinal diffusion along the continuous phase, and its influence is taken into account by the correction parameter introduced into the mass transfer equation, which reduces the mass transfer rate. Also, the conclusions of the equations of the working lines are given [2], but already specifically for the absorption process. The article [3] discusses the features of mass transfer processes of ion exchange taking into account longitudinal diffusion over the continuous phase, but the method of calculating the height of the nozzle or layer of ion exchanger is carried out through the number of transfer units without switching to the mass transfer coefficient. Papers [5-9] consider the features of mass transfer processes of rectification, absorption, ultrafiltration and ion exchange taking into account longitudinal diffusion over the continuous phase, but the method for calculating the height of the nozzle or ion exchanger layers is given through the number of transfer units without going to the mass transfer coefficient.

Known methods for calculating plate-shaped distillation columns are based on a model of ideal vapor phase displacement and perfect mixing in a boiling solution, and packed ones on ideal displacement in both phases. In a number of works on absorption, extraction, adsorption and ion exchange, longitudinal mixing is taken into account, which is based on the diffusion model of the continuous phase flow structure, however, this calculation is based on the correction coefficient introduced into the formula for
the dependence of mass transfer coefficient on mass transfer coefficients or on the Peclet number of longitudinal diffusion also introduced into the mass transfer equation, but not taking into account the influence of longitudinal diffusion on the equations of the working lines. The problem of the claimed topic is that the influence of longitudinal diffusion on the equations of the working lines is not taken into account in standard calculations that correspond to ideal displacement.

The development of new technical complexes based on the obtained experimental data will help to upgrade existing industrial designs, which will have higher productivity and energy efficiency. It will be possible to develop new promising solutions in heat and mass transfer processes.

From the middle of the last century, in describing the structure of the flow of chemical reactors, deviations from ideality began to be taken into account by various other models: cellular, 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 the diffusion structure of the flow or back-mixing flow. Gradually, this model began to be used in heat and mass transfer processes (heat exchangers, absorbers, adsorbers and ion-exchange columns with a fixed and moving sorbent bed, extractors, drum and fluidized bed dryers, ultrafiltration apparatuses and reverse osmosis apparatuses and others). However, in practice, this model is practically not used in the description of rectification processes, where heat and mass transfer processes occur simultaneously.

The aim of the work is to simulate the working lines in mass transfer processes, taking into account longitudinal diffusion simultaneously in the continuous and dispersed phases, as well as to assess their influence on the technological parameters and geometric dimensions of the columns.

2. Methodology

The complexity arises in the case when the motion of both phases (solid and dispersed) is described by a one-parameter diffusion model with different modes, the Peclet numbers: for solid $Pe_c$ and dispersed phases $Pe_d$. In this case, the structure of the dispersed phase flow is usually closer to the ideal displacement, so:

$$Pe_d > Pe_c.$$

Graphical interpolation of material flows is shown in figure 1. The equation of the working line on the gas phase for the absorption process taking into account the longitudinal diffusion is written as [10] (the left part of the figure1):

$$y = y_n + \frac{L}{G} (x - x_k) + \frac{1}{Pe_y} \frac{dy}{dh}$$

(1)

with boundary conditions of Danckwerts [11]:

$$h = 0, \quad y = y_o - \frac{1}{Pe_y} \xi_o$$

$$h = 1, \quad \xi = 0$$

(2)

where, $y, y_n, y_0$ – current, initial and input concentrations of the extracted component in the gas (taking into account the concentration jump at the inlet of the absorbent to the apparatus); $x, x_k$ – current and final concentrations of the extracted component in the absorbent; $G, L$ – expenses of inert part of gas and absorbent; $Pe_y$ – the Peclet number longitudinal diffusion gas; $\xi, \xi_0$ – gradients of concentrations of the extracted component in the gas at dimensionless height:

$$h = \frac{Z}{H}$$

in arbitrary section (current value):
Figure 1. Scheme of absorption process: on the left – with the diffusion structure of the flow in the gas phase and the ideal displacement in the liquid phase; on the right – with an ideal displacement in the gas phase and the diffusion structure of the flow in the liquid phase.

Figure 1 shows the flows: $g, g_0, g_k$ – concentration gradients of the extracted component in the liquid; $\upsilon_D, \upsilon_{D0}, \upsilon_{Dk}$ – speed of mass transfer by the modified Fick’s first law taking into account the longitudinal diffusion gas; $U_D, U_{D0}, U_{Dk}$ – speed of mass transfer by the modified Fick’s first law taking into account the longitudinal diffusion in the liquid; $D_l$ and $Pe_l$ – the ratio of the longitudinal diffusion and the Peclet number longitudinal diffusion gas; $D_k$ and $Pe_k$ – the ratio of the longitudinal diffusion and the Peclet number longitudinal diffusion in the liquid.

The equation of the working line, when the gas moves in the mode of ideal displacement, and the absorbent, taking into account the longitudinal diffusion, has the form [12] (the right part of figure 1):

$$y = y_k + \frac{L}{G} (x - x_n) + \frac{L}{GPe_x} g$$

(3)
with boundary conditions of Danckwerts:

\[ h = 0, g_k = 0 \]  \hspace{1cm} (4)

\[ h = 1, x_n = x_o - \frac{1}{Pe_x} g_o \]

where, \( x_o \) – input concentrations of the extracted component in the absorbent.

Figure 2 shows the graphs of the equilibrium line 1 working line 2 for a typical calculation method, when liquid phase (absorbent) and gas phase on the structure of the flow correspond to the ideal displacement mode; graphics working line 3 mode longitudinal diffusion in the gas phase and ideal displacement for the liquid phase, the working line 4 to the ideal displacement mode in the gas phase, and longitudinal diffusion in the liquid phase; the working line 5 for the longitudinal mode of diffusion in both phases.

The equation of the working line 5 has the form:

\[ y = y_a + \frac{L}{G} (x - x_k) + \frac{1}{Pe_y} \xi - \frac{L}{G} \frac{1}{Pe_x} g \]  \hspace{1cm} (5)

with boundary conditions of Danckwerts:

\[ h = 0, \quad y_n = y_o - \frac{1}{Pe_y} \xi_o, \quad g_k = 0 \]

\[ h = 1, \xi_k = 0, \quad x_n = x_o - \frac{1}{Pe_x} g_o \] \hspace{1cm} (6)

3. Results and discussions

From the graphs (figure 2) it can be seen that the longitudinal diffusion in both phases: first, reduces the concentration of the extracted substance in the gas at the inlet from \( y_0 \) to \( y_n \) and increases this concentration at the inlet of the liquid from \( x_0 \) to \( x_n \), which reduces the driving force at the inlet. Secondly, the concavity of both working lines 3 and 4 in the height of the absorbent further reduces the driving force. Bringing the working line to equilibrium.

Now the need to increase the height of the nozzle is mainly due to the small time of phase contact in the volume of the nozzle, equivalent to the theoretical plate, when the transition is not achieved and the so-called kinetic curve is built to the left and above the equilibrium line, and the working line remains the same. Simultaneous consideration of the longitudinal diffusion of the gas and liquid phases, leads to an even greater reduction of local driving forces in the absorption process, compared with the longitudinal diffusion of only one phase (liquid – absorbent or gas). In calculations, this leads to an increase in the height of the packing column. In addition, a jump in the concentration at the inlet of the gas phase can lead to its value \( y_0 \), less than the equilibrium concentration (point III on the graph becomes lower than point IV, figure 2), which will require an increase in the flow rate of the absorbent and the diameter of the column to move point III to the left.

An increase in the concentration at the inlet of the absorbent from \( x_n \) to \( x_0 \) can lead to its value greater than \( x_k \) the intersection of the working line 5 of the equilibrium line 1 (figure 2). This will require either a decrease in the concentration of \( x_n \), a deeper purification of the absorbent during desorption in the column, or an increase in pressure to bring the equilibrium line closer to the abscissa axis.
Figure 2. Equilibrium (1) and absorption process working lines: 2 – with the flow structure of ideal displacement in the liquid and gas phases; 3 – ideal displacement in the liquid phase and longitudinal diffusion in the gas phase; 4 – ideal displacement in the gas phase and longitudinal diffusion in the liquid phase; 5 – longitudinal diffusion simultaneously in the gas and liquid phases.

It is clearly seen that the number of theoretical plates increases from 2.7 to 4.6 that is 1.7 times, which can be explained by a decrease in the efficiency of the plate due to longitudinal diffusion:

\[ \eta = \frac{2.7}{4.6} = 0.587. \]  \hspace{1cm} (7)

This leads to the need to increase the height of the nozzle in the column by 70% compared to the typical calculation, when both phases are moving in the mode of ideal displacement. Similar results can be obtained by calculating the number of transfer units by the formula (8):

\[ \text{number of transfer units} = \frac{\Delta y}{y - y^*} \]  \hspace{1cm} (8)

Conclusion
The developed mathematical model, taking into account longitudinal diffusion, for the adsorption and rectification process, more accurately describes the behaviour of the flow structure in the mass transfer column. Work lines were constructed in the processes of mass transfer taking into account longitudinal diffusion simultaneously in the continuous and dispersed phases, and their influence on the technological parameters and geometric dimensions of the columns was evaluated.

Longitudinal diffusion reduces the local and average driving forces of mass transfer processes in both parts of the mass transfer column due to a jump in concentrations at the inlet along the vapour and liquid phases, and also leads to a transition from linear equations of working lines to nonlinear.

All of the above shows that a deviation from the ideal displacement, both in the liquid and in the gas phases, leads to: increase the consumption of absorbent, sputum and also leads increase the height and diameter of the absorber and distillation column.

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