

NONSTATIONARY MASS TRANSFER AND CONTROLLING THE PROCESS DURING THE LAMINAR MOTION OF A LIQUID IN PACKED-COLUMN APPARATUSES

D. V. Elizarov, R. R. Shavaleev, and V. V. Elizarov

UDC 66.011

Approximate solutions have been obtained for the equations of nonstationary mass transfer in packed-column apparatuses, and a method has been proposed to calculate them under the conditions of laminar motion of a liquid phase and displacement of a gas. On the basis of the nonstationary-mass-transfer equations, a problem of control of packed-column apparatuses has been solved. The solutions of the equations have been obtained in the form of an expansion of functions in a trigonometric series; formulas to determine the values of terms in the series have been presented. Initial conditions for the equations of nonstationary mass transfer are equations of a stationary process. Exact and approximate solutions for the stationary-mass-transfer equations have been obtained based on which an algorithm has been proposed for designing packed-column apparatuses. A calculation of the process of absorption of an acetone vapor from air by water has been carried out. Plots of the control and of the concentration change in controlling and with different perturbations have been presented.

Keywords: mass transfer, mathematical model, designing, control of the process, packed-type column, packing, absorption.

Introduction. Packed-column apparatuses with regular and irregular packings figure prominently among commercial mass-exchange apparatuses [1]. In recent times, active development of high-efficiency packings and bringing them into commercial practice have been carried out [2–5].

Packed-column apparatuses for mass-exchange processes between a gas and a liquid operate most frequently in a film regime. Owing to the intense interaction between a thin liquid film and a gas flow, their use allows obtaining quality products. This accounts for the wide use of film (wetted-wall) apparatuses to conduct heat- and mass-transfer processes of absorption, condensation, rectification, extraction, heating, and cooling.

In rectifying, distilling, evaporating, and condensing, we observe the first and second laminar regimes of flow ($12 \leq Re_{\text{film}} \leq 1200 \pm 200$), and in absorption processes, the second wave laminar and turbulent regimes; at $Re_{\text{film}} \geq 2500$, the laminar regime becomes turbulent [2].

Technological designing of an apparatus involves determining the basic dimensions and the flow rate of a separating agent. The separating-agent's flow rate is found from the material-balance equation containing the flow rate of the starting material and the concentrations of the component at the inlet and outlet of the flow [5, 7]. At an assigned inlet concentration of the gas and liquid phases, the concentrations of the phases at the apparatus outlet remain unknown and for them to be determined, it is necessary to calculate the concentration distribution over the height of the packing layer [8, 9].

In the system of automated control of packed-column apparatuses, mathematical models of nonstationary processes represent a system of partial differential equations. For solution of such equations, use is usually made of numerical methods [10–12], which are laborious and require great volumes of random-access memory and much computer time. They give no way of making an engineering analysis of the entire process in general form. In this work, it is proposed that a system of control of the process of absorption in packed columns be constructed on the basis of the approximate analytical solution of such equations.

Mathematical Modeling of Nonstationary Mass Transfer in a Packed-Column Apparatus during the Laminar Flow of a Liquid and the Displacement of a Gas. At the mean values of the liquid and gas velocity over the height of the packing layer, the equations of nonstationary mass transfer take the form [7, 10, 13]

Kazan National Research Technological University, 47 Stroitelei Ave., Nizhnekamsk, 423570, Republic of Tatarstan, Russia; email: rif.shav@gmail.com, atpp.nchti@mail.ru. Translated from *Inzhenerno-Fizicheskii Zhurnal*, Vol. 92, No. 4, pp. 906–916, July–August, 2019. Original article submitted December 13, 2017.

$$\frac{\partial x}{\partial t} + u \frac{\partial x}{\partial \xi} = -k_x a_V (x^* - x), \quad (1)$$

$$\frac{\partial y}{\partial t} + v \frac{\partial y}{\partial \xi} = -k_y a_V (y - y^*), \quad (2)$$

with initial and boundary conditions

$$x = x(\xi), \quad y = y(\xi) \quad \text{at } t = 0, \quad x = x_0(t) \quad \text{at } \xi = 1, \quad y = y_0(t) \quad \text{at } \xi = 0, \quad (3)$$

where $k_x a_V$ and $k_y a_V$ are the volume mass-transfer coefficients expressed in the concentrations of the liquid and gas phases, $x_0(t)$ and $y_0(t)$ are the inlet concentrations of the liquid and the gas, $\xi = \frac{\bar{\xi}}{H}$ is the dimensionless concentration over the apparatus's height, $\xi = 0$ and $\xi = 1$ are the coordinates of entry of the gas and the liquid into the packing layer for the phase counterflow, $u = \frac{L_0 + L_f}{2S}$ and $v = \frac{G_0 + G_f}{2S}$, L_0 and L_f are the flow rates of the liquid at entry into the packing layer at $\xi = 1$ and at exit from the packing layer at $\xi = 0$, and G_0 and G_f are the flow rates of the gas at entry into the packing layer at $\xi = 0$ and exit from the packing layer at $\xi = 1$. We assume that the volume mass-transfer coefficients over the height of the packing layer are constant.

A solution to the system of partial equations (1) and (2) with initial and boundary conditions (3) will be obtained in the form of series expansions in trigonometric functions.

We represent the solution of Eqs. (1) and (3) in the form of the series

$$x(\xi, t) = x_0(t) + \sum_{k=1}^{\infty} x_k(t) \cos \frac{k\pi}{2} \xi, \quad (4)$$

$$y(\xi, t) = y_0(t) + \sum_{k=1}^{\infty} y_k(t) \left(1 - \cos \frac{k\pi}{2} \xi\right), \quad k = 1, 3, 5, \dots \quad (5)$$

We substitute solutions (4) and (5) into Eqs. (1) and (2) respectively, multiply them by $\cos \frac{m\pi}{2} \xi$ ($m = 1, 3, 5, \dots$), and integrate with respect to ξ between the limits from zero to unity

$$\begin{aligned} & \frac{dx_0}{dt} \int_0^1 \cos \frac{m\pi}{2} \xi d\xi + \frac{dx_k}{dt} \int_0^1 \sum_{k=1}^{\infty} \cos \frac{k\pi}{2} \xi \cos \frac{m\pi}{2} \xi d\xi \\ & - \frac{u}{H} \int_0^1 \sum_{k=1}^{\infty} \frac{k\pi}{2} x_k \sin \frac{k\pi}{2} \xi \cos \frac{m\pi}{2} \xi d\xi \\ & = -\frac{k_x a_V}{m_0} \left[y_0(t) \int_0^1 \cos \frac{m\pi}{2} \xi d\xi + \int_0^1 y_k \cos \frac{m\pi}{2} \xi d\xi - \int_0^1 y_k \cos \frac{k\pi}{2} \xi \cos \frac{m\pi}{2} \xi d\xi \right] \\ & + k_x a_V \left[x_0(t) \int_0^1 \cos \frac{m\pi}{2} \xi d\xi + \int_0^1 x_k \cos \frac{k\pi}{2} \xi \cos \frac{m\pi}{2} \xi d\xi \right], \end{aligned}$$

$$\begin{aligned}
& \frac{dy_0}{dt} \int_0^1 \cos \frac{m\pi}{2} \xi d\xi + \frac{dy_k}{dt} \int_0^1 \cos \frac{m\pi}{2} \xi d\xi - \frac{dy_k}{dt} \int_0^1 \cos \frac{k\pi}{2} \xi \cos \frac{m\pi}{2} \xi d\xi \\
& \quad + \frac{v}{H} \frac{k\pi}{2} y_k \int_0^1 \sin \frac{k\pi}{2} \xi \cos \frac{m\pi}{2} \xi d\xi \\
& = -k_y a_V \left[y_0(t) \int_0^1 \cos \frac{m\pi}{2} \xi d\xi + y_k \int_0^1 \cos \frac{m\pi}{2} \xi d\xi - y_k \int_0^1 \cos \frac{k\pi}{2} \xi \cos \frac{m\pi}{2} \xi d\xi \right] \\
& + k_y a_V m_0 \left[x_0(t) \int_0^1 \cos \frac{m\pi}{2} \xi d\xi + x_k \int_0^1 \cos \frac{k\pi}{2} \xi \cos \frac{m\pi}{2} \xi d\xi \right] (k=1, 3, 5, \dots; \quad m=1, 3, 5, \dots).
\end{aligned}$$

As a result of rearrangements, we arrive at a system of ordinary differential equations for the unknown $x_m(t)$ and $y_m(t)$ ($m=1, 3, 5, \dots$):

$$\frac{dx_m}{dt} - c_{1m}x_m(t) + q_{1m}y_m(t) = e_{1m}(t), \quad (6)$$

$$\frac{dy_m}{dt} + c_{2m}y_m(t) - q_{2m}x_m(t) = e_{2m}(t), \quad (7)$$

where

$$e_{1m} = \frac{4}{m\pi} \left(-\frac{k_x a_V}{m_0} y_0(t) + k_x a_V x_0(t) - \frac{dx_0(t)}{dt} \right) \sin \frac{m\pi}{2},$$

$$c_{1m} = \frac{u}{H} + k_x a_V, \quad q_{1m} = \frac{k_x a_V}{m_0} \left(\frac{4}{m\pi} \sin \left(\frac{m\pi}{2} \right) - 1 \right),$$

$$e_{2m} = \frac{4 \sin \frac{m\pi}{2}}{4 \sin \frac{m\pi}{2} - m\pi} \left(2k_y a_V m_0 x_0(t) - 2k_y a_V y_0(t) - \frac{dy_0(t)}{dt} \right),$$

$$c_{2m} = \frac{v}{H} \frac{m\pi}{4 \sin \frac{m\pi}{2} - m\pi} + k_y a_V, \quad q_{2m} = m_0 k_y a_V \frac{m\pi}{4 \sin \frac{m\pi}{2} - m\pi}, \quad m=1, 3, 5, \dots$$

First, we differentiate Eq. (6) with respect to t

$$\frac{d^2 x_m}{dt^2} - c_{1m} \frac{dx_m}{dt} + q_{1m} \frac{dy_m}{dt} = e'_{1m}(t), \quad (8)$$

where $e'_{1m}(t) = \frac{de_{1m}(t)}{dt}$. We resolve Eq. (6) for $y_m(t)$

$$y_m(t) = \frac{1}{q_{1m}} \left(e_{1m}(t) - \frac{dx_m(t)}{dt} + c_{1m}x_m(t) \right), \quad (9)$$

and Eq. (7) for $\frac{dy_m}{dt}$:

$$\frac{dy_m}{dt} = e_{2m}(t) - c_{2m}y_m(t) + q_{2m}x_m(t) . \quad (10)$$

Substituting these values into Eq. (8), we obtain the system of second-order equations linear for $x_m(t)$

$$\begin{aligned} \frac{d^2x_m}{dt^2} + (c_{2m} - c_{1m}) \frac{dx_m}{dt} + (q_{1m}q_{2m} - c_{1m}c_{2m})x_m(t) \\ = e'_{1m}(t) - q_{1m}e_{2m}(t) + c_{2m}e_{1m}(t) , \quad m = 1, 3, 5, \dots , \end{aligned}$$

whose solution for each m (dropping the subscripts $m = 1, 3, 5, \dots$) takes the following form:

$$x(t) = \frac{e'_1 - q_1e_2 + c_2e_1}{(r_2 - r_1)r_1r_2} (r_2 - r_2e^{\eta t} + r_1e^{r_2t} - r_1) + g_{10}e^{\eta t} + g_{20}e^{r_2t} . \quad (11)$$

The integration constant g_{10} will be found from the initial condition: $x = x(\xi)$ at $t = 0$, $g_{10} = x(\xi) - g_{20}$. We differentiate Eq. (11) with respect to t :

$$\frac{dx}{dt} = \frac{e'_1 - q_1e_2 + c_2e_1}{r_2 - r_1} (e^{r_2t} - e^{\eta t}) + (x(\xi) - g_{20})r_1e^{\eta t} + g_{20}r_2e^{r_2t} . \quad (12)$$

Substituting the resulting values of $\frac{dx}{dt}$ and $x(t)$ from Eqs. (11) and (12) into Eq. (9), we obtain

$$y(t) = \frac{1}{q_1} \left(e_1 - \frac{e'_1 - q_1e_2 + c_2e_1}{r_2 - r_1} \left(e^{r_2t} - e^{\eta t} - \frac{c_1}{r_1} (1 - e^{\eta t}) - \frac{c_1}{r_2} (e^{r_2t} - 1) \right) + \right. \\ \left. + (x(\xi) - g_{20})e^{\eta t}(c_1 - r_1) + g_{20}e^{r_2t}(c_1 - r_2) \right) . \quad (13)$$

From initial condition (3) ($y = y(\xi)$ at $t = 0$), we find

$$g_{20} = \frac{y(\xi)q_1 - x(\xi)(c_1 - r_1) - e_1}{r_1 - r_2}$$

for each $\xi \in [0, 1]$ and $m = 1, 3, 5, \dots$. The initial values of the functions $x(t)$ and $y(t)$ at $t = 0 - x(\xi)$ and $y(\xi)$ are determined from the equations of stationary mass transfer in the packing layer.

Mathematical Modeling of Stationary Mass Transfer in a Packed-Column Apparatus during the Laminar Motion of a Liquid and the Displacement of a Gas. The material-balance equations for the liquid and gas phases in the packing layer are of the form [8, 9, 10, 14]

$$u \frac{dx}{d\xi} = -k_x a_V (x^* - x) , \quad v \frac{dy}{d\xi} = -k_y a_V (y - y^*) \quad (14)$$

with conditions at the boundaries $y = y_0$ at $\xi = 0$ at entry of the gas and $x = x_0$ at $\xi = 1$ at entry of the liquid, where $x(\xi)$ and $y(\xi)$ are the concentration of the extracted component in the liquid and gas phases. We introduce the notation

$$\frac{k_x a_V H}{u} = a , \quad \frac{k_y a_V H}{v} = b .$$

In dimensionless quantities, Eqs. (14) will be written as follows:

$$\frac{dx}{d\xi} = -\frac{a}{m_0} y + ax , \quad (15)$$

$$\frac{dy}{d\xi} = -by + bm_0 x . \quad (16)$$

We differentiate Eq. (15) with respect to ξ

$$\frac{d^2x}{d\xi^2} = -\frac{a}{m_0} \frac{dy}{d\xi} + a \frac{dx}{d\xi}. \quad (17)$$

We substitute into (17), instead of $\frac{dy}{d\xi}$, the value from Eq. (16)

$$\frac{d^2x}{d\xi^2} = a \frac{dx}{d\xi} - \frac{a}{m_0} (-by + bm_0x), \quad (18)$$

and obtain the value of y in Eq. (18) from Eq. (15)

$$y(\xi) = -\frac{m_0}{a} \left(\frac{dx}{d\xi} - ax \right). \quad (19)$$

Then Eq. (18) will be written as

$$\frac{d^2x}{d\xi^2} + (b-a) \frac{dx}{d\xi} = 0,$$

and its solution will take the form

$$x(\xi) = c_1 + c_2 e^{(a-b)\xi}. \quad (20)$$

The integration constant c_1 is determined from the inlet condition: $x = x_0$ at $\xi = 1$

$$c_1 = x_0 - c_2 e^{(a-b)}.$$

The solution (20) is written as follows:

$$x(\xi) = x_0 + c_2 (e^{(a-b)\xi} - e^{(a-b)}). \quad (21)$$

We differentiate Eq. (20) with respect to ξ

$$\frac{dx}{d\xi} = c_2 e^{(a-b)\xi} (a-b). \quad (22)$$

We substitute the value of the derivative of (22) and the value of the function $x(\xi)$ (21) into Eq. (19) and find the integration constant c_2 from the condition $y = y_0$ at $\xi = 0$. We obtain the exact solution of Eqs. (14)

$$x(\xi) = \frac{y_0}{m_0} + \frac{x_0 m_0 - y_0}{m_0 \left(\frac{a}{b} e^{a-b} - 1 \right)} \left(\frac{a}{b} e^{(a-b)\xi} - 1 \right), \quad (23)$$

$$y(\xi) = m_0 x_0 + \frac{y_0 - m_0 x_0}{\left(\frac{b}{a} - e^{(a-b)} \right)} \left(\frac{b}{a} e^{(a-b)\xi} - e^{(a-b)} \right). \quad (24)$$

In Eqs. (23) and (24), x_0 and y_0 are assigned values of the concentrations of the liquid and the gas at the apparatus inlet. To determine the initial values of the variables $x(\xi)$ and $y(\xi)$ at $t = 0$ in Eqs. (11) and (13) at $m = 1, 3, 5, \dots$, we obtain the approximate solution of Eqs. (14). For this purpose, we represent the concentration distributions in the form of series expansions

$$x(\xi) = x_0 + \sum_{m=1}^{\infty} x_m \cos \frac{m\pi}{2} \xi, \quad (25)$$

$$y(\xi) = y_0 + \sum_{m=1}^{\infty} y_m \left(1 - \cos \frac{m\pi}{2} \xi \right), \quad m = 1, 3, 5, \dots, \quad (26)$$

where x_m and y_m ($m = 1, 3, 5, \dots$) are the unknown quantities.

The solutions of (25) and (26) satisfy specified conditions at $\xi = 0$ and $\xi = 1$. Assuming that the series converge to the exact solutions (24), we set expressions (23) and (25) equal to (24) and (26). We obtain

$$x_0 + \sum_{m=1}^{\infty} x_m \cos \frac{m\pi}{2} \xi = \frac{y_0}{m_0} + \frac{x_0 m_0 - y_0}{m_0 \left(\frac{a}{b} e^{a-b} - 1 \right)} \left(\frac{a}{b} e^{(a-b)\xi} - 1 \right), \quad (27)$$

$$y_0 + \sum_{m=1}^{\infty} y_m \left(1 - \cos \frac{m\pi}{2} \xi \right) = m_0 x_0 + \frac{y_0 - m_0 x_0}{\frac{b}{a} - e^{(a-b)}} \left(\frac{b}{a} e^{(a-b)\xi} - e^{(a-b)} \right), \quad m = 1, 3, 5, \dots \quad (28)$$

Since the number of unknown parameters x_m and y_m ($m = 1, 3, 5, \dots$) in Eqs. (27) and (28) is larger than the number of equations, we take the coefficients with $m = 3, 5, \dots$ equal to zero and determine the coefficients x_1 and y_1 from Eqs. (27) and (28). Then Eqs. (27) and (28) take the form

$$x_0 + x_1 \cos \frac{\pi}{2} \xi = \frac{y_0}{m_0} + \frac{x_0 m_0 - y_0}{m_0 \left(\frac{a}{b} e^{a-b} - 1 \right)} \left(\frac{a}{b} e^{(a-b)\xi} - 1 \right), \quad x_3 = x_5 = \dots = 0,$$

$$y_0 + y_1 \left(1 - \cos \frac{\pi}{2} \xi \right) = m_0 x_0 + \frac{y_0 - m_0 x_0}{\frac{b}{a} - e^{(a-b)}} \left(\frac{b}{a} e^{(a-b)\xi} - e^{(a-b)} \right), \quad y_3 = y_5 = \dots = 0.$$

The unknown coefficients x_1 and y_1 will be found from the outlet conditions of the flows: at $\xi = 0$, we find x_1 , and at $\xi = 1$, the value of y_1 :

$$x_1 = x_{f,c} = \left(x_0 - \frac{y_0}{m_0} \right) \left(\frac{a-b}{ae^{a-b} - b} - 1 \right), \quad y_1 = y_{f,c} = (y_0 - m_0 x_0) \left(\frac{be^{(a-b)} - ae^{(a-b)}}{b - ae^{(a-b)}} - 1 \right). \quad (29)$$

The solutions of the stationary-mass-transfer equations are of the form

$$x(\xi) = x_0 + \left(x_0 - \frac{y_0}{m_0} \right) \left(\frac{a-b}{ae^{a-b} - b} - 1 \right) \cos \frac{\pi}{2} \xi,$$

$$y(\xi) = y_0 + (y_0 - m_0 x_0) \left(\frac{be^{(a-b)} - ae^{(a-b)}}{b - ae^{(a-b)}} - 1 \right) \left(1 - \cos \frac{\pi}{2} \xi \right). \quad (30)$$

Algorithm for Designing Packed-Column Apparatuses. Based on the obtained solutions (23) and (24) or (30), the apparatus is designed, and the flow rate of the absorbent is determined, in the following order. The amount of the component extracted from the gas (vapor) phase by a liquid absorbent in the phase counterflow is assigned by the degree of extraction $\varphi = \frac{G_0 y_0 - G_f y_f}{G_0 y_0}$, where G_0 , G_f , y_0 , and y_f are the flow rates and concentrations of the component in the gas phase at the apparatus inlet and outlet. Then the amount of the component absorbed by the liquid absorber will be equal to

$$W_A = \varphi G_0 y_0,$$

and the amount of the escaping gas, to

$$G_f = G_0 - W_A.$$

The concentration of the component in the gas phase at exit from the apparatus y_f is expressed by the degree of extraction φ and the concentration y_0 at entry into the apparatus:

$$y_f = \frac{y_0(1 - \varphi)}{1 - \varphi y_0} \quad (31)$$

From the equation of total material balance, we determine the concentration of the component in the liquid phase at exit from the apparatus

$$G_0 y_0 - G_f y_f = L_f x_f - L_0 x_0$$

It follows that

$$x_{f,b} = \frac{\varphi G_0 y_0 + L_0 x_0}{L_f} \quad (32)$$

Here L_0 and L_f are the flow rates of the absorbent at entry into the apparatus and at exit from it respectively.

In the next step we assign the flow rate of the absorbent as a first approximation $L_0^{(1)}$, compute the mean values of flow rates of the gas $\bar{G} = (G_0 + G_f)/2$ and of the liquid $\bar{L} = (L_0^{(1)} + L_f^{(1)})/2$, select a packing, and calculate the mean values of the liquid and gas velocities, the dimensions of the apparatus, the kinetic parameters of mass transfer, and the height of the packing layer H .

From Eqs. (29), we obtain the values of the concentrations of the liquid $x_{f,c}$ and the gas $y_{f,c}$ at exit from the apparatus, which are compared with the values obtained from the equations of total material balance (31) and (32):

$$x_{f,b} - x_{f,c} = 0, \quad y_{f,b} - y_{f,c} = 0 \quad (33)$$

If the conditions are observed, the dimension of the apparatus and the flow rate of the absorbent $L_0^{(1)}$ satisfy the material-balance equations and the requirements of the assignment. Otherwise, we select the approximation $L_0^{(2)} = L_0^{(1)} + \Delta L$ and repeat the calculation until condition (33) is observed.

Calculation of the process of absorption of an acetone vapor from air by water. The calculation is carried out on the basis of the data given in [14]. The flow rate of the gas mixture is $G_0 = 62.5$ kmole/h and the concentration of acetone in the mixture is $y_0 = 0.0639$ mole fractions. The degree of extraction is $\varphi = 98\%$. The specific surface of the packing is $a_V = 204$ m²/m³, the equivalent diameter is $d_e = 0.0145$ m, the free volume of the packing is $\varepsilon_{fr} = 0.74$, the distribution coefficient is $m_0 = 1.68$, the coefficient of diffusion of acetone in water is $D_{liq} = 1.03 \cdot 10^{-9}$ m and of acetone in air is $D_g = 0.082 \cdot 10^{-4}$ m²/s, and the amount of acetone going from the gas phase into the liquid phase is $\varphi G_0 y_0 = G_0 y_0 - G_f y_f = 3.91$ kmole/h, $G_f = G_0 - 3.91 = 58.6$ kmole/h.

As a first approximation, we take, for the calculation, the data obtained in [14]. The diameter of the apparatus is $D^{(1)} = 0.675$ m, the cross section is $S^{(1)} = 0.358$ m², the height of the layer is $H^{(1)} = 16.8$ m, and $L_0^{(1)} = 166.7$ kmole/h. The flow rate of water at exit from the apparatus is $L_f^{(1)} = L_0^{(1)} + \varphi G_0 y_0 = 170.6$ kmole/h, and the average flow rate is $L_{av} = 168.7$ kmole/h. The regime of motion of the liquid film is laminar: $Re_{film} = \frac{4u_{av}d_e}{\nu_{liq}} = 694$.

The coefficients of mass transfer in the liquid film β_x and in the gas phase β_y are determined on the basis of hydrodynamic analogy [15, 16]. In the liquid film, we take a parabolic velocity profile to determine the film thickness. In the gas phase, we determine the rate of dissipation of the energy ε_{g-liq} of the gas flow to calculate the dynamic velocity at the phase boundary. We obtain

$$\beta_x = 1.93 \sqrt{\frac{M_{liq} \bar{L} D_{liq}}{3600 \cdot 1000 S \varepsilon_{liq,d} \pi d_e}} \quad (34)$$

$$\beta_y = 0.013 \frac{\left(\frac{\varepsilon_{g-liq} V_g}{\rho_g} \right)^{0.25}}{Sc_g^{2/3} Q^{0.4}} \quad (35)$$

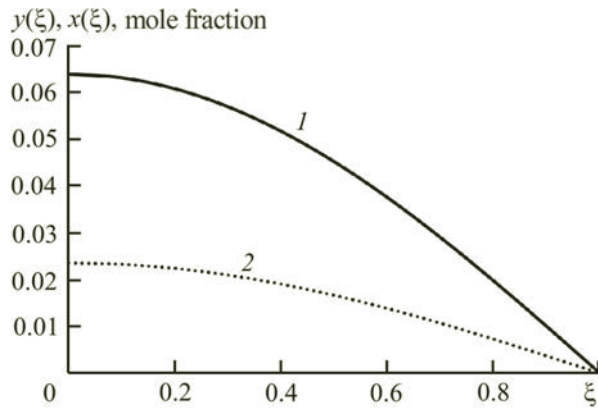


Fig. 1. Concentration distribution of acetone in the gas (1) and liquid (2) phases over the height of the packing layer at the flow rate of the absorbent $L = 3000$ kg/h.

where $\varepsilon_{g-liq} = \frac{\Delta P_{g-liq} v}{(\varepsilon_{fr} - \varepsilon_{liq})H} = 2353.15$ W/m³ is the energy dissipation, $Sc_g = v_g/D_g = 1.84$ is the Schmidt number for the gas phase, $\nu_g = 15.06 \cdot 10^{-6}$ m²/s is the kinematic viscosity of the gas, $v = \frac{M_g G_0}{3600 \rho_g S} = 1.17$ m/s is the velocity of the gas flow in the apparatus, $\Delta P_{g-liq} = \Delta P_{irr} = \Delta P_{dr}(1 - \psi)$, $\Delta P_{irr} = \Delta P_{dr} \cdot 10^{bQ}$ is the hydraulic resistance of the irrigated packing ($b = 0.051$ [7]), $\Delta P_{dr} = \xi_{dr} \frac{H \rho_g v^2}{2d_e \varepsilon_{fr}}$ is the hydraulic resistance of a dry packing ($\Delta P_{g-liq} = \Delta P_{irr}$ at the wettability coefficient of the liquid $\psi = 1$), Pa, $\varepsilon_{liq} = \varepsilon_{liq,d}$ is the amount of the retained liquid, Q is the liquid spray rate, m³/(m²·s), and M_{liq} and M_g are the molar masses of the liquid and gas mixtures. The calculated values of mass-exchange coefficients are equal to

$$\beta_x = 3.2 \cdot 10^{-5} \text{ m/s}, \quad \beta_y = 4 \cdot 10^{-2} \text{ m/s}.$$

The calculated values of mass-transfer coefficients are equal to

$$K_x = 2.8 \cdot 10^{-5} \text{ m/s}, \quad K_y = 4.4 \cdot 10^{-3} \text{ m/s}.$$

The coefficients in Eqs. (30) are as follows:

$$a = \frac{k_x a_V H}{u} = \frac{5.712 \cdot 10^{-3} H}{0.012}; \quad b = \frac{k_y a_V H}{v} = \frac{8.976 \cdot 10^{-1} H}{1.17}.$$

Substituting the coefficients a and b into Eq. (30), we obtain the concentration profiles of acetone in the liquid and gas phases over the height of the packing layer (Fig. 1) and the concentration of the saturated absorbent $x_f = 2.35 \cdot 10^{-2}$ mole fractions and of the escaping gas $y_f = 0.00143$ mole fractions.

The new height of the packing layer will be calculated from the equation

$$H = \frac{\varphi G_0 y_0}{3600 \rho_g K_y a_V S \Delta y_{av}} = 17.2 \text{ m},$$

where $\Delta y_{av} = 4.4 \cdot 10^{-3}$ is the mean logarithmic motive force of mass transfer and $\rho_g = 1.295$ kg/m³ is the density of the gas mixture. The height H satisfactorily, with an error of 2.4%, agrees with that taken as a first approximation [14].

Figure 1 gives the concentration distribution of acetone in the liquid and gas phases at the calculated values of technological and structural parameters of the apparatus. Figure 2 gives the concentration profiles of acetone in the liquid phase at different initial concentrations y_0 and the flow rate of the absorbent $L_0 = 2957$ kg/h (curves 2 and 3) and different flow rates of the absorbent and the initial concentration $y_0 = 0.0639$ mole fractions (curves 4 and 5).

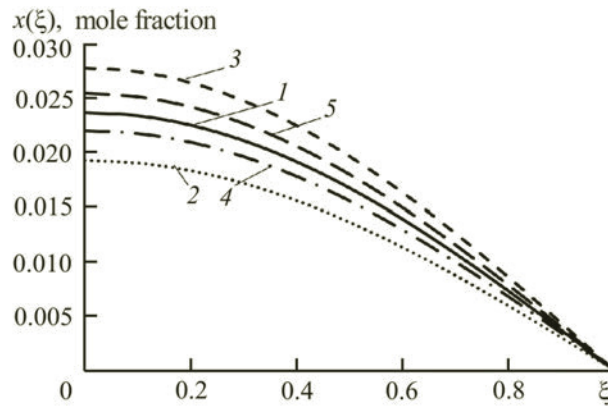


Fig. 2. Concentration distribution of acetone in the liquid phase over the height of the packing layer at different initial concentrations in the gas phase: 1) $y_0 = 0.0639$, 2) 0.052 , and 3) 0.071 mole fractions, and also at $y_0 = 0.639$ mole fractions and different flow rates of the absorbent: 1) $L_0 = 2957$, 4) 2500 , and 5) 3500 kg/h.

Controlling the Process of Absorption of Acetone by Water. The flow rate of the gas mixture, the pressure and temperature in the apparatus are considered constant, whereas the composition of the gas mixture varies. The parameters of the process's steady state are determined from the stationary-mass-transfer equations considered in the previous items: the concentration of acetone in the original gas mixture is y_0 and at the apparatus outlet, y_f , the concentration of acetone in the liquid at entry of the absorbent into the apparatus is x_0 and in the saturation absorbent at the apparatus outlet, x_{f0} , and the rate of the absorbent in the steady state is L_0 .

The concentration distribution of acetone over the height of the apparatus in the liquid phase $x(\xi)$ and in the gas phase $y(\xi)$ is shown in Fig. 1.

The variation in the composition of the gas mixture or the liquid is determined by the departure of the parameters $e_{1m}(t)$ and $e_{2m}(t)$ on the right-hand side of Eqs. (6) and (7) from a steady state. The values of the concentration of the gas mixture and the liquid, and also the rate of their growth at the apparatus inlet at the instant of time $t = t_0$, change by the value of Δy_0 or Δx_0 : $y_0 = y_0 \pm \Delta y_0$, $x_0 = x_0 \pm \Delta x_0$, dy_0/dt , and dx_0/dt .

The solutions of Eqs. (11) and (13), once the perturbations Δy_0 and Δx_0 have been introduced, show the changes in the acetone concentrations with time at any cross section of the apparatus ξ . At exit of the gas mixture from the apparatus at $\xi = 1$, the concentration of acetone is equal to $y_f(t)$ and at the exit of the absorbent from the apparatus at $\xi = 0$, the concentration of acetone is equal to $x_f(t)$; these values differ from the stationary values y_{f0} and x_{f0} obtained at y_0 and x_0 .

It is necessary to find the control of the process, i.e., the flow rate of the absorbent $L(t)$ at which the departure of the concentration of acetone in the gas phase at exit from the apparatus $y_f(t)$ or in the liquid $x_f(t)$ from the stationary values y_{f0} and x_{f0} will be minimum, e.g.,

$$R = (y_f(t) - y_{f0})^2 \rightarrow \min . \quad (36)$$

The dependence of the concentrations $y_f(t)$ and $x_f(t)$, according to Eqs. (11) and (13), on the flow rate of the absorbent $L(t)$ is complex and implicit in character. The expression to determine the extremum of the function R has a cumbersome form.

To determine the control $L(t)$, it is proposed that a numerical method be used. At each time interval $\Delta t = t_{i+1} - t_i$ ($i = 0, 1, 2, \dots, n$) $n = T/\Delta t$, the flow rate of the absorbent will be assumed constant:

$$L_{i+1} = L_i + \Delta L_i \text{ sign } (y_f(t_i) - y_{f0}) , \quad (37)$$

where the symbol "sign" is the function of sign, $y_f(t_i)$ is the value of the concentration at the instant of time t_i , and ΔL_i is the change in the absorbent's flow rate at the time interval Δt_i .

With a positive departure of the concentration $y_f(t_i)$ at the instant of time t_i from the stationary value y_{f0} , the flow rate of the absorbent increases by the value of ΔL_i and with a negative departure, decreases by ΔL_i :

$$\Delta L_i = \frac{y_f(t_i) - y_{f0}}{K} ,$$

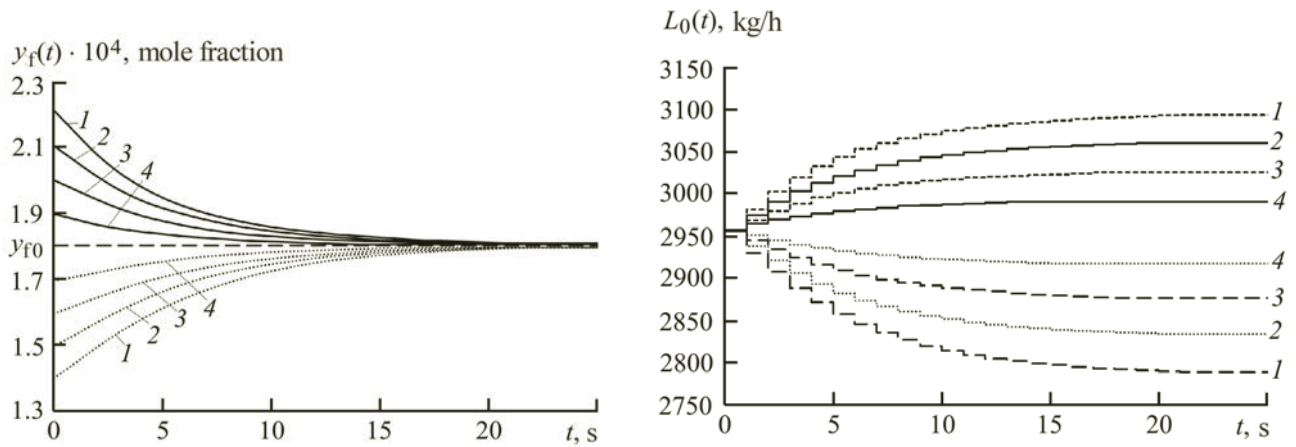


Fig. 3. Time change in the concentration of acetone in the gas phase at the apparatus outlet with the control and stepwise perturbation of the composition of acetone in the original gas mixture: 1) ± 20 , 2) ± 15 , 3) ± 10 , and 4) ± 5 wt.%.

Fig. 4. Control of the process of absorption of acetone (flow rate of the absorbent) L (kg/h) with stepwise perturbation of the composition of acetone in the original gas mixture: 1) ± 20 , 2) ± 15 , 3) ± 10 , and 4) ± 5 wt.%.

where K is the gas concentration–absorbent flow rate channel gain. To determine the gain K , we calculate the steady state of mass transfer at $y = y_0$ and $x = x_0$ and at $y_0 = y_0 \pm \Delta y_0$, and $x_0 = x_0 \pm \Delta x_0$

$$K = \left| \frac{y_{f,n} - y_{f0}}{L_{0n} - L_0} \right|,$$

where $y_{f,n}$ and L_{0n} are the new steady-state values of the concentration y_f and of the flow rate of the absorbent L_0 . The gain is dependent on perturbations arriving from other channels: the pressure in the apparatus, the concentration of the arriving absorbent, and the absorbent's flow rate.

The time of the transient process T is determined from Eqs. (5) and (13) with the condition adopted in control theory [17]: the departure of the concentration at exit from the apparatus $y_f(T)$ at $\xi = 1$ from the stationary value y_{f0} is no higher than 5%: $y_f(T) - y_{f0} = 0.05y_{f0}$. For example, writing Eq. (5) with account of expression (13) with the given condition, we obtain the equation to determine the time T

$$y(1, T) = y_f(T) = y_0$$

$$+ \frac{1}{q_1} \left[e_1 - \frac{e'_1 - q_1 e_2 + c_2 e_1}{(r_2 - r_1)} \left(e^{r_2 T} - e^{r_1 T} - \frac{c_1}{r_1} (1 - e^{r_1 T}) - \frac{c_1}{r_2} (e^{r_2 T} - 1) \right) + \right. \\ \left. + (x(\xi) - g_{20}) e^{r_1 T} (c_1 - r_1) + g_{20} e^{r_2 T} (c_1 - r_2) \right] - y_{f0} = 0.05 y_{f0}. \quad (38)$$

At each instant of time, by changing the flow rate of the absorbent, it is necessary to reduce the value of the concentration of acetone in the escaping gas y_f to the stationary value y_{f0} . Figure 3 plots y_f versus t for the control and different perturbations of the composition of the original mixture, and Fig. 4 gives the plots of the control (flow rate of water) at $K = 1.6 \cdot 10^{-6}$. Figures 5 and 6 give the plots of the concentration change for the control and different perturbations with gain $K = 0.3 \cdot 10^{-6}$ and the plots of the control (flow rate of water).

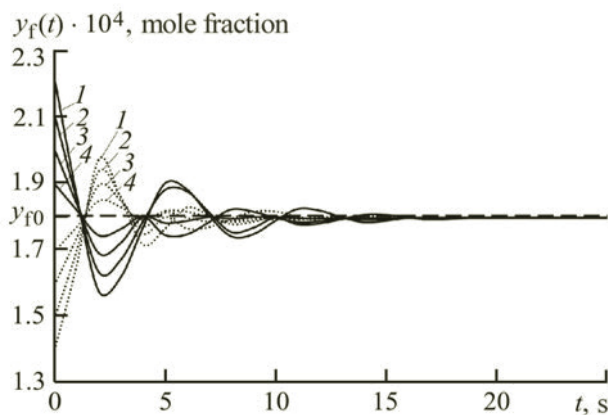


Fig. 5. Time change in the concentration of acetone in the gas phase at the apparatus outlet with the control and stepwise perturbation of the composition of acetone in the original gas mixture: 1) ± 20 , 2) ± 15 , 3) ± 10 , and 4) ± 5 wt. %.

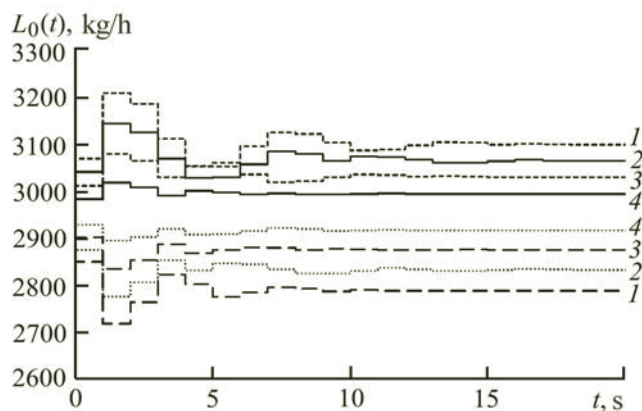


Fig. 6. Control of the process of absorption of acetone (flow rate of the absorbent) L (kg/h) with stepwise perturbation of the composition of acetone in the original gas mixture: 1) ± 20 , 2) ± 15 , 3) ± 10 , and 4) ± 5 wt. %.

CONCLUSIONS

1. Iterative calculation of packed-column apparatuses on the basis of stationary-mass-transfer equations ensures substantiated selection of technological and structural parameters of an apparatus.

2. The approximate solution of nonstationary-mass-transfer equations allows constructing a system of control of the quality of the obtained products.

NOTATION

a_V , specific surface of the packing, m^2/m^3 ; D_{liq} , diffusion coefficient, m^2/s ; $e_1, c_1, q_1, e_2, c_2, q_2, a$, and b , coefficients of the equations; G , flow rate of the gas, $kmole/h$; g_{10} and g_{20} , integration constants; g , free-fall acceleration, m/s^2 ; H , height of the packing layer, m ; K , gain; k_x , mass-transfer coefficient expressed in the concentration of the liquid phase, m/s ; k_y , mass-transfer coefficient expressed in the concentration of the gas phase, m/s ; L , flow rate of the absorbent, $kmole/h$; m_0 , distribution coefficient; Re , Reynolds number; r_1 and r_2 , roots of the characteristic equation; S , cross-sectional area of the apparatus, m^2 ; T , time of the transient process, s ; t , time, s ; u , mean value of the liquid velocity in the apparatus, m/s ; v , mean value of the gas velocity in the apparatus, m/s ; W , amount of the component absorbed by a liquid absorbent, $kmole/h$; x , concentration of the extracted component in the liquid phase, mole fractions; $x^* = y/m_0$, equilibrium concentration of the component in the liquid phase, mole fractions; y , concentration of the extracted component in the gas phase, mole fractions; $y^* = m_0x$, equilibrium concentration of the component in the gas phase, mole fractions; β_x , mass-exchange coefficient, m/s ; ϵ , free volume of the packing; $\epsilon_{liq,d}$, dynamic component of the retainment of the liquid; ν_{liq} , coefficient of kinematic viscosity of the liquid, m^2/s ; ξ , dimensionless coordinate over the height of the apparatus; φ , degree of extraction of the component from the gas. Subscripts: 0, zero value (at entry into the apparatus); A, absorbent; f, final value (at exit from the apparatus); k and m , numbers of terms of the Fourier series; f.b, final balance value; f.c, final calculated value; liq, liquid phase; d, dynamic component; film, film flow; f.n, final new value; 0n, initial new value; fr, free; g, gas; av, average, mean; g-liq, at the phase boundary; irr, irrigated; dr, dry.

REFERENCES

1. V. M. Olevskii, *Film Heat- and Mass-Transfer Equipment* [in Russian], Khimiya, Moscow (1988).
2. M. I. Farakhov, A. G. Laptev, and M. M. Basharov, Modernizing mass-exchange apparatuses by new packings in chemical engineering, *Teor. Osn. Khim. Tekhnol.*, **49**, No. 3, 247–252 (2015).

3. A. M. Kagan, L. A. Yudina, and A. S. Pushnov, Active surface of elements of irregular heat- and mass-transfer packings, *Teor. Osn. Khim. Tekhnol.*, **46**, No. 2, 199–206 (2012).
4. L. S. Gordeev, A. I. Kozlov, M. B. Glebov, and N. V. Khitrov, Investigation of the use of high-porosity cellular materials in packed rectification columns, *Teor. Osn. Khim. Tekhnol.*, **43**, No. 5, 567–574 (2009).
5. S. V. Alekseenko, D. M. Markovich, A. R. Evseev, A. V. Bobylev, B. V. Tarasov, and V. M. Karsten, Experimental investigation of the distribution of a liquid in a column with structural packings, *Teor. Osn. Khim. Tekhnol.*, **41**, No. 4, 442–448 (2007).
6. A. G. Kasatkin, *Basic Processes and Apparatuses of Chemical Technology* [in Russian], Khimiya, Moscow (1973).
7. V. M. Ramm, *Absorption of Gases* [in Russian], Khimiya, Moscow (1976).
8. V. I. Elizarov, R. R. Shavaleev, E. S. Titova, and A. R. Safarov, Mathematical model of mass transfer in packed columns, *Vestn. Kazansk. Tekhnol. Univ.*, **18**, No. 22, 134–136 (2015).
9. R. R. Shavaleev, V. V. Elizarov, and V. D. Elizarov, Mathematical modeling of stationary mass transfer in packed-column apparatuses, *Vestn. Kazansk. Tekhnol. Univ.*, **20**, No. 5, 109–113 (2017).
10. B. V. Devyatov, N. D. Demidenko, and V. A. Okhorzin, *The Dynamics of Distributed Processes in Technological Apparatuses, Distributed Monitoring, and Control* [in Russian], Krasnoyarskoe Knizhnoe Izd., Krasnoyarsk (1976).
11. A. N. Tikhonov and A. A. Samarskii, *Equations of Mathematical Physics* [in Russian], Nauka, Moscow (1972).
12. A. A. Samarskii and E. S. Nikolaev, *Methods for Solving Grid Equations* [in Russian], Nauka, Moscow (1978).
13. V. V. Kafarov, *Principles of Mass Transfer* [in Russian], Vysshaya Shkola, Moscow (1972).
14. K. F. Pavlov, P. G. Romankov, and A. A. Noskov, *Examples and Problems on the Course of Processes and Apparatuses of Chemical Technology: A Manual for Graduate Students* [in Russian], Khimiya, Leningrad (1987).
15. S. G. D'yakonov, V. I. Elizarov, and A. G. Laptev, *Theoretical Foundations and Modeling of the Processes of Separation of Substances* [in Russian], Izd. Kazansk. Univ., Kazan (1993).
16. S. G. D'yakonov, V. V. Elizarov, and V. I. Elizarov, *Theoretical Foundations of Designing Chemical-Technology Apparatuses on the Basis of Conjugate Physical and Mathematical Modeling* [in Russian], KGTU, Kazan (2009).
17. L. D. Pevzner, *The Theory of Control Systems* [in Russian], Lan', St. Petersburg (2013).