

STUDY AND NUMERICAL SOLUTION OF A GENERALIZED MATHEMATICAL MODEL OF ISOTHERMAL ADSORPTION

Yu. A. Komissarov, V. N. Vetokhin*
V. A. Tsenev, and E. L. Gordeeva

UDC 541.183.5.001.57:518.61

A generalized mathematical model of isothermal adsorption that takes into account mass transfer on the surface of a particle, diffusion in micro- and macropores, and dispersion along the length of the apparatus is considered. The parameters λ and φ^2 determine the dominating effect of any of the mass transfer mechanisms of the adsorption process. A numerical algorithm for solving the generalized adsorption model is suggested.

In a number of works [1-3] various aspects of physical and chemical phenomena occurring both in the interior of a porous particle of adsorbent and in the phase external to the particle are elucidated. However, many problems in the theory and practice of the process of adsorption have not received sufficient study, and there is a lack of generalizing criteria for choosing the form of a mathematical model.

In the present work we consider a generalized mathematical model of isothermal adsorption and propose an algorithm for its solution.

As is known [4], the quantity of adsorbate per unit cross section of adsorbent can be written as the sum of the flux in the free space of a pore and the flux at the phase interface:

$$J = - \left[D_p \frac{\partial C}{\partial r} + \rho_p D_s \frac{\partial q}{\partial r} \right]. \quad (1)$$

The material balances of the change in the concentration in the interior of a particle and on its surface will be respectively written in the form

$$\varepsilon_p \frac{\partial C}{\partial t} = r^{-n} \frac{\partial}{\partial r} \left(r^n D_p \frac{\partial C}{\partial r} \right) - \rho_p G(C, q), \quad (2)$$

$$\frac{\partial q}{\partial t} = r^{-n} \frac{\partial}{\partial r} \left(r^n D_s \frac{\partial C}{\partial r} \right) + G(C, q). \quad (3)$$

In describing the initial and boundary conditions for Eqs. (2) and (3) we assume that the particle is free of adsorbate, i.e., that the voids are filled with a "liquid" having inert components:

$$t = 0; \quad C = q = 0, \quad (4)$$

with the boundary conditions for the external and internal phases being prescribed separately because of the different nature of the surface mass transfer and diffusion in the pores:

* Deceased.

$$r = 0; \quad \frac{\partial C}{\partial r} = \frac{\partial q}{\partial r} = 0, \quad (5)$$

$$r = R; \quad k_m (C_b - C|_R) = D_p \left. \frac{\partial C}{\partial r} \right|_R + \rho_p D_s \left. \frac{\partial q}{\partial r} \right|_R. \quad (6)$$

In addition, the rate of change of the concentration of the adsorbable components on the particle surface is balanced by the "net" rate of adsorption [5], i.e.,

$$r = R; \quad \left. \frac{\partial q}{\partial t} \right|_R = G(C, q). \quad (7)$$

In order to develop a complete formulation of a mathematical model of isothermal adsorption, it must be supplemented with the equations of hydrodynamics in the adsorber:

$$V \frac{dC_b}{dt} = - \left(\frac{m_p}{\rho_p} \right) \left(\frac{S_{\text{ads. } p}}{V_{\text{ads. } p}} \right) \left[D_p \frac{\partial C}{\partial r} + \rho_p D_s \frac{\partial q}{\partial r} \right]_R \quad (8a)$$

(a batch-operated adsorber with ideal mixing),

$$V \frac{dC_b}{dt} = F(C_0 - C_b) - \left(\frac{m_p}{\rho_p} \right) \left(\frac{S_{\text{ads. } p}}{V_{\text{ads. } p}} \right) \left[D_p \frac{\partial C}{\partial r} + \rho_p D_s \frac{\partial q}{\partial r} \right]_R \quad (8b)$$

(a continuous-action adsorber with a fluidized bed),

$$\begin{aligned} \varepsilon_b \frac{dC_b}{dt} = E_A \frac{\partial^2 C_b}{\partial z^2} - \varepsilon_b U \frac{\partial C_b}{\partial z} - \\ - \left(\frac{S_{\text{ads. } p}}{V_{\text{ads. } p}} \right) (1 - \varepsilon_b) \left[D_p \frac{\partial C}{\partial r} + \rho_p D_s \frac{\partial q}{\partial r} \right]_R \end{aligned} \quad (8c)$$

(a continuous-action adsorber with a fixed bed).

System of equations (2)-(8) describes all the dynamic changes in the concentration of the adsorbate in the external phase and in the interior and on the surface of an adsorbent particle.

To investigate and solve the dynamic equations it is worthwhile to reduce them to a dimensionless form. To characterize the concentration in the pores we use the initial concentration of the adsorbate in the volumetric phase. Suppose the concentration on the surface of the adsorbed component q_0 for any prescribed value of C_0 can be determined from the equation

$$G(C_0, q_0) = 0, \quad (9)$$

then, introducing the dimensionless variables

$$A = C/C_0; \quad A_s = q/q_0; \quad A_b = C_b/C_0; \quad x = r/R; \quad h(A, A_s) = \frac{G(C, q)}{G(C_0, 0)};$$

$$\xi = z/h; \quad \lambda = \frac{\rho_p D_s q_0}{D_p C_0}; \quad \varphi^2 = \frac{\rho_p R^2 G(C_0, 0)}{C_0 D_p};$$

$$\psi = \frac{\varepsilon_p C_0 (-\partial h / \partial A_s)}{\rho_p q_0 (\partial h / \partial A)} \Big|_{A=1, h(A, A_s)=0} ; \quad \tau = \frac{\psi}{1 + \psi} \frac{D_p t}{R^2 \varepsilon_p} ; \quad \text{Bi}_p = \frac{k_m R}{D_p} ; \quad (10)$$

(for a continuous-action adsorber with a fixed bed);

$$N = \begin{cases} \frac{\varepsilon_p (m_p / \rho_p)}{V} \frac{1 + \psi}{\psi} ; \\ \frac{\varepsilon_p (1 - \varepsilon_b)}{\varepsilon_b} \frac{1 + \psi}{\psi} \end{cases}$$

(for a continuous-action adsorber with a fixed bed), we will write the system of equations (2)-(8) in dimensionless form for $n = 2$:

$$\alpha = \begin{cases} \frac{(1 + \psi) R^2 \varepsilon_p / \psi D_p}{V/F} \\ \frac{(1 + \psi) R^2 \varepsilon_p / \psi D_p}{h/U} \end{cases}$$

$$\frac{\psi}{1 + \psi} \frac{\partial A}{\partial \tau} = \nabla^2 A - \varphi^2 h(A; A_s); \quad (11a)$$

$$\frac{1}{1 + \psi} \frac{\partial A_s}{\partial \tau} = \lambda \nabla^2 A_s + \varphi^2 h(A; A_s); \quad (11b)$$

$$x = 0; \quad \partial A / \partial x = \partial A_s / \partial x = 0; \quad (11c)$$

$$x = 1, \quad \frac{1}{1 + \psi} \frac{\partial A_s}{\partial \tau} \Big|_1 = \varphi^2 h(A; A_s) \Big|_1; \quad (11d)$$

$$x = 1, \quad (A_b - A) = \frac{1}{\text{Bi}} \left[\frac{\partial A}{\partial x} + \lambda \frac{\partial A_s}{\partial x} \right]; \quad (11e)$$

$$\frac{dA_b}{d\tau} = -3N \left[\frac{\partial A}{\partial x} + \lambda \frac{\partial A_s}{\partial x} \right]_1 \quad (11f)$$

(a batch-operated adsorber);

$$\frac{dA_b}{d\tau} = \alpha (1 - A_b) - 3N \left[\frac{\partial A}{\partial x} + \lambda \frac{\partial A_s}{\partial x} \right]_1 \quad (11g)$$

(a continuous-action adsorber with a fluidized bed);

$$\frac{dA_b}{d\tau} = \alpha \left[\frac{1}{\text{Pe}} \frac{\partial^2 A_b}{\partial \xi^2} - \frac{\partial A_b}{\partial \xi} \right] - 3N \left[\frac{\partial A}{\partial x} + \lambda \frac{\partial A_s}{\partial x} \right]_1 \quad (11h)$$

TABLE 1. Parametric Regions of Admissibility of Various Adsorption Models

1	Diffusion in pores and equilibrium model of adsorption $\lambda \ll 1, \varphi \gg 1$	Combined diffusion model and equilibrium model of adsorption $\varphi \gg 1$	Model of surface diffusion and equilibrium model of adsorption $\lambda \gg 1, \varphi^2/\lambda \gg 1$
$\frac{\varphi}{1+\varphi}$	Model of diffusion in pores and kinetic model of adsorption $\lambda \ll 1$	Combined diffusion model and kinetic model of adsorption	Model of surface diffusion and kinetic model of adsorption $\lambda \gg 1$
	Kinetic model of adsorption $\varphi \ll 1$		
0	$\frac{\lambda}{1+\lambda}$		

(a continuous-action adsorber with a fixed bed);

$$\xi = 0, \quad 1 = A_b - \frac{1}{Pe} \frac{\partial^2 A_b}{\partial \xi^2}; \tag{12a}$$

$$\xi = 1, \quad \frac{\partial A_b}{\partial \xi} = 0. \tag{12b}$$

Two parameters, λ and φ^2 , determine the predominant effect of any of the mass transfer mechanisms occurring in the adsorber [6]. The parameter

$$\lambda = \frac{\rho_p D_s q_0}{D_p C_0} \tag{13}$$

is the ratio of the greatest possible rates of diffusion on the surface and in the pores. The parameter φ^2 characterizes the relationship between the rates of adsorption and diffusion in the pores.

The magnitude of these parameters and the relationship between them determine the predominance of a particular mechanism of mass transfer in the process of isothermal adsorption and may serve as criteria for the selection of a simplified mathematical model. The parametric regions of admissibility of various adsorption models are given in Table 1.

The resulting system of differential equations (11), (12) was solved by the finite-difference method following the Crank–Nicolson scheme.

Introducing the step along the radius of the particle Δx for the current instant of time, it is possible to rewrite Eqs. (11a), (11b) in the following form with the internal variable I ($I = \overline{1, N}$):

$$\begin{aligned} & A_{I-1}^{n+1} \left(\frac{S_2}{I} - S_2 \right) + A_I^{n+1} (S_1 + 2S_2) + A_{I+1}^{n+1} \left(-S_2 - \frac{S_2}{I} \right) = \\ & = S_1 A_I^n + S_2 (A_{I+1}^n - 2A_I^n + A_{I-1}^n) + \frac{S_2}{I} (A_{I+1}^n - A_{I-1}^n) - S_3 (h_I^{n+1} + h_I^n); \end{aligned} \tag{13a}$$

$$\begin{aligned} & A_{sI-1}^{n+1} \left(\frac{S_5}{I} - S_5 \right) + A_{sI}^{n+1} (S_4 + 2S_5) + A_{sI+1}^{n+1} \left(-S_5 - \frac{S_5}{I} \right) = \\ & = S_4 A_{sI}^n + S_5 (A_{sI+1}^n - 2A_{sI}^n + A_{sI-1}^n) + \frac{S_5}{I} (A_{sI+1}^n - A_{sI-1}^n) + S_3 (h_I^{n+1} + h_I^n). \end{aligned} \tag{13b}$$

Boundary conditions (11c)-(11e) will be written in the form

$$x = 0, \quad A_I^{n+1} \left(S_1 + \frac{2S_2}{I} \right) + A_{I+1}^{n+1} \left(\frac{-2S_2}{I} \right) = S_1 A_I^n + 2 \frac{S_2}{I} (A_{I+1}^n - A_I^n) - S_3 (h_I^{n+1} + h_I^n); \quad (13c)$$

$$A_{s_I}^{n+1} \left(S_4 + \frac{2S_5}{I} \right) + A_{s_{I+1}}^{n+1} \left(\frac{-2S_5}{I} \right) = S_4 A_{s_I}^n + \frac{2S_5}{I} (A_{s_{I+1}}^n - A_{s_I}^n) - S_3 (h_I^{n+1} + h_I^n); \quad (13d)$$

$$x = 1, \quad A_{I+1}^{n+1} (-S_6) + A_{s_{I-1}}^{n+1} S_7 + A_I^{n+1} (1 + S_6) + S_7 A_{s_I}^{n+1} = A_{I-1}^n S_6 + \\ + A_{s_{I-1}}^n S_7 + A_I^n (-1 - S_6) + A_{s_I}^n (-S_7) + A_{b_I}^{n+1} + A_{b_I}^n; \quad (13e)$$

$$S_4 A_{s_I}^{n+1} = S_3 (h_I^{n+1} + h_I^n) + S_4 A_{s_I}^n; \quad (13f)$$

The resulting system of equations can be written in matrix form:

$$S_1 = \frac{\psi}{1 + \psi}; \quad S_2 = \frac{\Delta\tau}{2\Delta x^2}; \quad S_3 = \frac{\varphi^2 \Delta\tau}{2}; \quad S_4 = \frac{1}{1 + \psi};$$

$$S_5 = \lambda S_2; \quad S_6 = \frac{1}{\text{Bi} \Delta x}; \quad S_7 = \lambda S_6.$$

$$\begin{bmatrix} S_1 + 2S_2 & 0 & -2S_2 & 0 & 0 & 0 & \cdot & \cdot & \cdot & \cdot \\ 0 & S_4 + 2S_5 & 0 & -2S_5 & 0 & 0 & \cdot & \cdot & \cdot & \cdot \\ -\frac{1}{2}S_2 & 0 & S_1 + 2S_2 & 0 & -\frac{3}{2}S_2 & 0 & \cdot & \cdot & \cdot & \cdot \\ 0 & -\frac{1}{2}S_5 & 0 & S_4 + 2S_5 & 0 & -\frac{3}{2}S_5 & 0 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & \cdot & \cdot & 0 & -S_6 & S_7 & 1 + S_6 & S_7 \\ 0 & 0 & \cdot & \cdot & \cdot & 0 & 0 & 0 & 0 & S_4 \end{bmatrix} \times$$

$$\times \begin{bmatrix} A_1^{n+1} \\ A_{s_1}^{n+1} \\ A_2^{n+1} \\ A_{s_2}^{n+1} \\ \cdot \\ \cdot \\ A_N^{n+1} \\ A_{s_N}^{n+1} \end{bmatrix} = \begin{bmatrix} Z_1 \\ \bar{Z}_1 \\ Z_2 \\ \bar{Z}_2 \\ \cdot \\ \cdot \\ Z_N \\ \bar{Z}_N \end{bmatrix} \quad (14)$$

The first and second rows of the matrix are the left-hand sides of Eqs. (13c) and (13d). Rows 3, ..., $N-2$ are the left-hand sides of Eqs. (13a) and (13b). Rows $N-1$ and N are the left-hand sides of Eqs. (13e) and (13f), respectively; $Z_1, \bar{Z}_1, \dots, Z_N, \bar{Z}_N$ are the right-hand sides of equations corresponding to the left-hand sides of the matrix.

Knowing $Z_1, \bar{Z}_1, \dots, Z_N, \bar{Z}_N$, it is possible to find A and A_s for the next instant of time, taking $h_I^{n+1} = h_I^n$ as a first approximation, with its subsequent iteration refinement.

After similar transformations and introduction of a step along the length of the apparatus $\Delta\xi$, Eq. (13h) will be written in the form of the following system of nonlinear equations with the internal variable J ($J = \overline{1, M}$):

$$\begin{aligned} A_{b_{J-1}}^{n+1} (-S_8 - S_9) + A_{b_J}^{n+1} (1 + 2S_8) + A_{b_{J+1}}^{n+1} (S_9 - S_8) = A_{b_J}^n + S_8 (A_{b_{J+1}}^n - \\ - 2A_{b_J}^n + A_{b_{J-1}}^n - S_9 (A_{b_{J+1}}^n - A_{b_{J-1}}^n) - S_{10} [(A_I^{n+1} + A_I^n - A_{I-1}^{n+1} - A_{I-1}^n) + \\ + \lambda (A_{s_{I+1}}^{n+1} + A_{s_I}^n - A_{s_{I-1}}^{n+1} - A_{s_{I-1}}^n)] l_1, \end{aligned} \quad (15)$$

and boundary conditions (12) will be reduced to the form

$$\xi = 0; \quad A_{b_J}^{n+1} (1 + S_{10}) + A_{b_{J+1}}^{n+1} (-S_{10}) = A_{b_J}^{n+1} (-1 - S_{10}) + A_{b_{J+1}}^n S_{10} + 2; \quad (16a)$$

$$\xi = 1; \quad A_{b_{J-1}}^{n+1} (-1) + A_{b_J}^{n+1} = A_{b_{J-1}}^n - A_{b_J}^n; \quad (16b)$$

$$S_8 = \frac{\alpha\Delta\tau}{\text{Pe } 2\Delta\xi^2}; \quad S_9 = \frac{\alpha\Delta\tau}{4\Delta\xi}; \quad S_{10} = \frac{\alpha 3N\Delta\tau}{2\Delta x}; \quad S_{11} = \frac{1}{\text{Pe } \Delta\xi}.$$

Similarly to the system of equations (13), the system of linear algebraic equations (SLAE) (15) will be written in matrix form:

$$\begin{bmatrix} 1 + S_{10} & -S_{10} & 0 & 0 & 0 & 0 & \cdot & \cdot & \cdot \\ -S_8 - S_9 & 2S_8 + 1 & -S_8 + S_9 & 0 & 0 & 0 & \cdot & \cdot & \cdot \\ 0 & -S_8 - S_9 & 2S_8 + 1 & -S_8 + S_9 & 0 & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 0 & -1 & 1 \end{bmatrix} \times \begin{bmatrix} A_{b_1}^{n+1} \\ A_{b_2}^{n+1} \\ A_{b_3}^{n+1} \\ \cdot \\ A_{b_M}^{n+1} \end{bmatrix} = \begin{bmatrix} Q_1 \\ Q_2 \\ Q_3 \\ \cdot \\ Q_M \end{bmatrix} \quad (17)$$

Based on studies of the generalized mathematical model and its numerical solution, we wrote the program ADSS, whose operating algorithm is given in Fig. 1 and consists in:

1. Input of initial data (the physical characteristics and properties of the adsorbent, hydrodynamic conditions in the apparatus, the technical parameters of the apparatus, calculation accuracy).

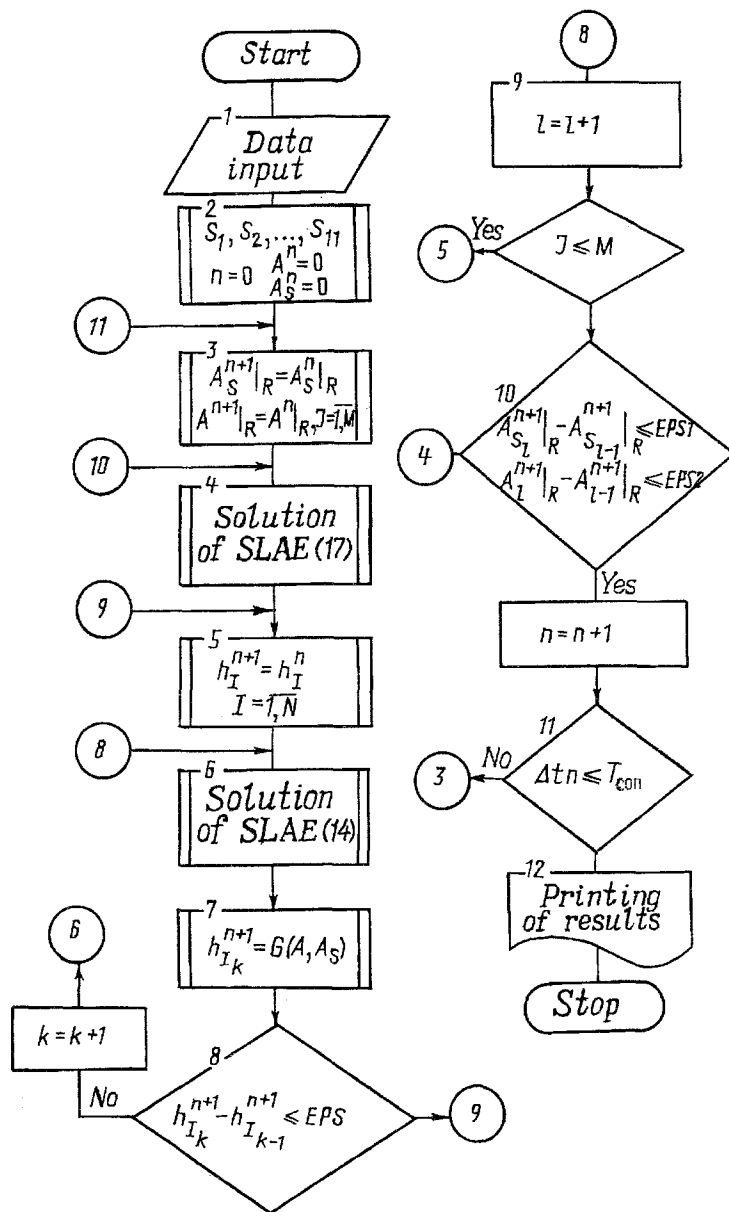


Fig. 1. Block diagram of the calculation of the adsorption process.

2. Specification of the initial distribution of concentrations. The formation of a matrix of the left-hand sides of Eqs. (14), (17), which approximate the distribution of concentrations along the length of the apparatus and the radius of a particle.

3. The following assumption for all the partition points along the apparatus length:

$$A_s^{n+1}|_R = A_s^n|_R; \quad A^{n+1}|_R = A^n|_R.$$

4. Formation of the vector of the right-hand sides of system (17) along the length of the apparatus. Solution of the system of equations (17) by the method of matrix fitting.

5. For the current point along the length of the apparatus the vector of the right-hand sides of system (14) is constructed along the particle radius with the assumption that $h_I^{n+1} = h_I^n$ ($I = \overline{1, N}$).

6. Formation of the vector of the right-hand sides of the system of equations (14) for partition along the particle radius. Determination of the profile for the concentrations A_I^{n+1}, A_{sI}^{n+1} .

7. Refinement of the value of $h_{I,k}^{n+1} = G(A, A_s)$, where k is the number of the iteration refinement cycle.

8. If the condition $|h_{I,k}^{n+1} - h_{I,k-1}^{n+1}| \leq EPS$ is not satisfied, then we pass to item 6.

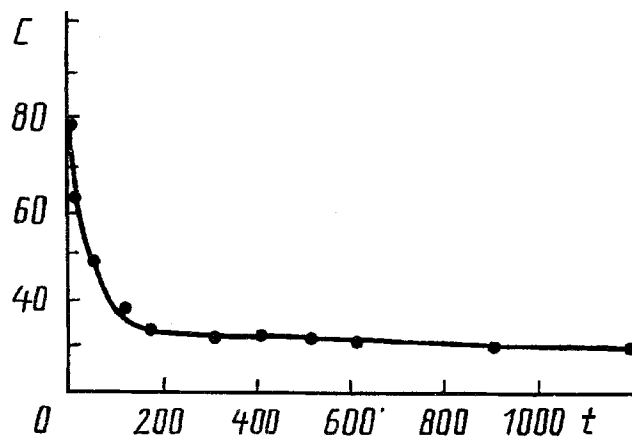
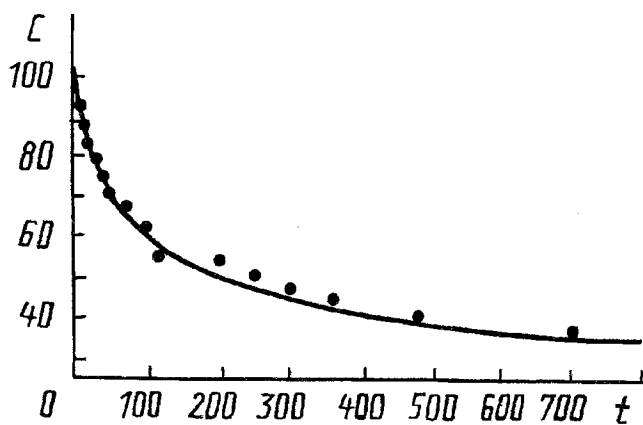


Fig. 2. Adsorption of blue dye on chitin, $m_p = 1$ g, $R = 0.0302$ cm, $V = 1700$ cm³, $k_m = 2.5 \cdot 10^{-3}$ cm/sec, $D_s = 1.0 \cdot 10^{-8}$ cm²/sec, $C_{b0} = 100$ mg/dm³, $\rho_p = 450$ g/dm³, $T_{\max} = 800$ min, $D_p = 1.0 \cdot 10^{-4}$ 1/sec, constants of the Freundlich isotherm: $AF = 33.9$, $BF = 0.339$; points, experiment; curve, calculation. C , mg/dm³; t , min.

Fig. 3. Adsorption of phenol on activated carbon, $m_p = 0.990$ g, $R = 0.0452$ cm, $V = 1700$ cm³, $k_m = 1.33 \cdot 10^{-2}$ cm/sec, $D_s = 7.78 \cdot 10^{-8}$ cm²/sec, $C_{b0} = 96.3$ mg/dm³, $T_{\max} = 1200$ min, $\rho_p = 1300$ g/dm³, $D_p = 1.44 \cdot 10^{-6}$ 1/sec, $AF = 78.1$, $BF = 0.212$.

9. Transition to the next step of calculation along the length of the apparatus and to the refinement of the concentration profile along the particle radius, i.e., passage to item 6.

10. If the conditions $|A_{s_l}^{n+1}|_R - A_{s_{l-1}}^{n+1}|_R| \leq \text{EPS1}$ and $|A_l^{n+1}|_R - A_{l-1}^{n+1}|_R| \leq \text{EPS2}$ (l is the number of the iteration refinement cycle along the length of the apparatus) are not satisfied, then we pass to item 4.

11. Transition to the next time step.

12. Printout of the concentration profile in time at the exit from the apparatus.

The basic difference between this algorithm and those proposed earlier lies in the fact that by using one of Eq. (8) to describe the hydrodynamic situation in the apparatus and changing the number of partitions along the length of the apparatus in step 3, it is possible to perform calculations of the adsorption process in both batch-operated and continuous-action apparatuses.

The efficiency of the mathematical model was verified by comparing the experimental data with the calculated results for the adsorption of steam on aluminum oxide in a continuous-action apparatus containing a fixed bed, as well as with data given in [7].

Experimental data for the adsorption of steam on aluminum oxide were obtained on a setup of the All-Union Research Institute of Chemical Reagents and Especially Pure Chemical Substances (Moscow).

Results of calculations and experimental data are presented in Figs. 2-4.

The studies performed permit the following conclusions to be drawn.

1. Since the model is based on surface diffusion and the concentrations of the external volumetric phase are calculated using values of concentrations of the solid phase, the concentration profiles depend strongly on the kind of mathematical description used for the shape of the isotherm.

2. The model has a set of constants whose calculation or experimental determination is difficult and very laborous. Therefore, to obtain the initial estimates of certain parameters it is possible to use simplified models for calculating mass transfer coefficients [8], the diffusion coefficient [9], and the surface diffusion coefficient [10].

3. The computer time depends on the number of partition intervals, the magnitude of the time step, and the calculation accuracy; it can be fairly large.

4. The program can be used for predicting the concentration profile with a high degree of accuracy over a very large time interval.

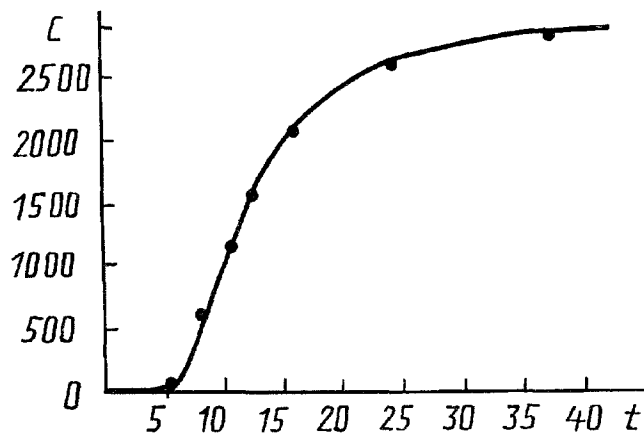


Fig. 4. Adsorption of steam on aluminum oxide, $m_p = 0.22$ g, $R = 0.025$ cm, $k_m = 1.5 \cdot 10^{-3}$ cm/sec, $D_s = 6.6 \cdot 10^{-6}$ cm²/sec, $D_p = 2.0 \cdot 10^{-6}$ 1/sec, $C_0 = 3555$ mg/dm³, $\rho_p = 435$ g/dm³, $\varepsilon_b = 0.48$, $u = 8.15 \cdot 10^{-5}$ m/sec, $E_a = 1.15 \cdot 10^{-7}$ m²/sec, $V = 8.83 \cdot 10^{-3}$ m³, $AF = 0.705$, $BF = 0.424$.

NOTATION

C , concentration of free adsorbate in pores; C_{ext} , adsorbate concentration in external phase; D_p , coefficient of diffusion in adsorbent pores; D_s , coefficient of surface diffusion; E_a , coefficient of axial dispersion along the apparatus length; F , volumetric rate of flow; $G(C, q)$, "net" rate of adsorption, defined as the ratio of the quantity of absorbed moles or mass of adsorbate per unit mass of adsorbent per unit time (for example, for the Langmuir isotherm the "net" rate of adsorption will be written in the form $G(C, q) = k_a C(q_\infty - q) - k_d q$); k_a , rate constant of the adsorption process; k_d , rate constant of the desorption process; k_m , coefficient of mass transfer; L , length of the adsorber; m_p , total mass of adsorbent in the apparatus; N , number of partitions along the particle radius; n , coefficient of the geometrical shape of a particle ($n = 0$, plate; 1, cylinder; 2, sphere determined for formulas (2)-(13); M , number of partitions along the apparatus length; Pe , Peclet number, $Pe = (\varepsilon_b \mu L) / E_a$; q , concentration of adsorbed component; q_∞ , the largest possible concentration of adsorbate on the particle surface; r , space variable of differentiation with respect to the adsorbent particle; R , adsorbent particle radius; $S_{\text{ads},p}$, surface area of the adsorbent particle; t , time; V , volume of the apparatus excluding the volume of particles and their internal voids; $V_{\text{ads},p}$, adsorbent particle volume; Z , variable of differentiation with respect to the apparatus length; α , λ , φ , parameters defined in Eq. (9); ε_b , coefficient of the free volume in the apparatus; ε_p , adsorbent particle porosity; ρ_p , adsorbent particle density.

REFERENCES

1. A. N. Planovskii and P. I. Nikolaev, Processes and Apparatuses of Chemical and Petrochemical Technology [in Russian], Moscow (1987).
2. S. J. Gregg and K. W. Sing, Adsorption, Specific Surface, and Porosity [Russian translation], Moscow (1984).
3. G. Peel Russell, A. Benedek, and C. M. Crowe, AIChE J., 27, No. 1, 26-32 (1981).
4. R. Aris, Ind. Eng. Chem. Fundam., 22, No. 1, 150-151 (1983).
5. G. McKay, S. McKee, and H. R. J. Walters, Chem. Eng. Sci., 42, No. 5, 1145-1151 (1987).
6. D. M. Smith and I. F. Keller, Ind. Eng. Chem. Fundam., 24, 497-499 (1985).
7. D. D. Do and R. G. Rice, Chem. Eng. Sci., 42, No. 10, 2269-2284 (1987).
8. H. Spahn and E. U. Schlunder, Chem. Eng. Sci., 30, No. 4, 529-537 (1975).
9. G. McKay, Chem. Eng. Res. Des., 62, No. 2, 235-246 (1984).
10. G. McKay, AIChE J., 30, No. 4, 692-697 (1984).