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ISOTHERMAL MASS EXCHANGE IN INHOMOGENEOUS POROUS ADSORBENT GRANULES WITH A SEQUENTIAL MACRO- AND MICRODIFFUSION TRANSFER MECHANISM

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In the 1-D format, the problem of nonstationary isothermal local distribution of a diffusing single-species substance in successively located axisymmetric spherical regions of a granule with different permeabilities of macro- and micropores is formulated. The initial-boundary value problem for a system of differential equations of parabolic type with a boundary condition of the first kind on the outer boundary of a granule and of the fourth kind on the boundary of conjugation of the domains is integrated numerically. A computational experiment has demonstrated the influence of the regions permeability and the dislocation of the boundary between them on the kinetics of material transport.

Keywords: mass transfer; adsorbent granules; heterogeneity; diffusion.

Introduction

The analysis of the adsorption kinetics on the scale of an adsorbent granule, as a rule, is based on the assumption that its internal structure is pseudo-uniform [1]. However, this approach negates the possibility of assessing effect of different-permeable regions dislocation on the absorption rate of adsorbents by the intragranular space [2]. This circumstance is taken into account by the pre-selected topology of the granule regions arrangement: sequential, parallel, mixed, randomly distributed [3]. In general, this problem is solved so far only with the help of an experimental approach [4]. The topology of the sequential arrangement of differently permeable regions is considered under the condition of additional assumptions, the main ones of which are [5]: granules sphericity and arrangement axisymmetry of bidisperse inhomogeneities associated with diffusion transfer mechanisms in macro- and micropores; spatial one-dimensionality; constancy of physical and chemical parameters; isometric; perfect contact at the border of the mating areas. A simplified mathematical formulation is represented as a system of parabolic equations in a 1-D spherical coordinate system [6]:

$$\frac{\partial c_m(r,\tau)}{\partial \tau} = \frac{1}{r^2}\frac{\partial}{\partial r}\left[D_m r^2 \frac{\partial c_m(r,\tau)}{\partial r}\right], 0 \le r < r_m; \tag{1}$$

$$\frac{\partial c_M(r,\tau)}{\partial \tau} = \frac{1}{r^2}\frac{\partial}{\partial r}\left[D_M r^2 \frac{\partial c_M(r,\tau)}{\partial r}\right], r_m \le r \le r_M \tag{2}$$

with initial boundary condition

$$c_m(r,0) = c_M(r,0) = c_0 \tag{3}$$

of the first kind on the surface of the granule

$$c_M(r_M,\tau) = c_s \tag{4}$$

boundary conditions of the fourth kind, reflecting the perfect contact between regions of different permeability

$$c_m(r_m,\tau) = c_M(r_m,\tau); \tag{5}$$

$$D_m \frac{\partial c_m(r_m,\tau)}{\partial r} = D_M \frac{\partial c_M(r_m,\tau)}{\partial r}; \tag{6}$$

with the additional condition of boundedness at the point of symmetry

$$c_m(0,\tau) \neq \infty, \tag{7}$$

where τ is time; r – current radial coordinate; c_M, c_m – local concentrations of adsorbate in areas of different permeability $0 \le r < r_m$ and $r_m \le r \le r_M$, accordingly; $c_0 = const$ – the concentration of the adsorbent on the granule surface; , D_M, D_m – diffusion coefficients in areas $0 \le r < r_m$ and $r_m \le r \le r_M$; r_m; r_m – radius of the contact surface of the regions; r_M is the granule radius.

1. Numerical Scheme

System (1)–(7), represented in dimensionless form using relative variables

$$\theta = \tau D_m / r_m^2; R = r/r_m; D = D_M/D_m;$$

$$C_{m,M}(R,\theta) = \left[c_{m,M}(r,\tau) - c_0\right] / (c_s - c_0); \eta = r_M/r_m;$$

$$\frac{\partial\left[RC_m(R,\theta)\right]}{\partial\theta} = \frac{\partial^2\left[RC_m(R,\theta)\right]}{\partial R^2}, 0 \le R < 1; \tag{8}$$

$$\frac{\partial\left[RC_M(R,\theta)\right]}{\partial\theta} = D\frac{\partial^2\left[RC_M(R,\theta)\right]}{\partial R^2}, 1 \le R \le \eta; \tag{9}$$

$$C_m(R,0) = C_M(R,0) = 0; \tag{10}$$

$$C_M(\eta,\theta) = 1; \tag{11}$$

$$C_m(1,\theta) = C_M(1,\theta); \tag{12}$$

$$\frac{\partial C_m(1,\theta)}{\partial R} = D\frac{\partial C_M(1,\theta)}{\partial R}; \tag{13}$$

$$C_m(0,\theta) \neq \infty \tag{14}$$

is integrated numerically on a uniform grid of the definition domain according to the +-shaped template (Fig. 1).

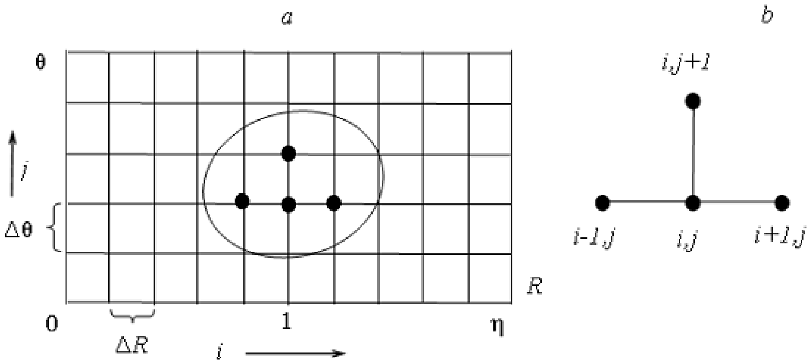

Fig. 1. Discretization of the integration domain (a) and a template for constructing a finite-difference scheme (b)

The finite-difference analogue (8)–(14) is represented by an explicit scheme for the exact function $C_{m,M}^{i,j} = C_{m,M}\left(i\Delta R, j\Delta\theta\right)$:

$$C_m^{i,j+1} = A_m^i C_m^{i+1,j} + B_m C_m^{i,j} + C_m^i C_m^{i-1,j}; \tag{15}$$

$$C_M^{i,j+1} = A_M^i C_M^{i+1,j} + B_M C_M^{i,j} + C_M^i C_M^{i-1,j}; \tag{16}$$

$$C_m^{i,0} = 0, i = \overline{1, M1}; C_M^{i,0} = 0, i = \overline{M1+1, M}; \tag{17}$$

$$C_M^{M+1,j} = 0; j = \overline{0, N}; \tag{18}$$

$$C_m^{M1,j} = C_M^{M1,j}; j = \overline{0, N}; \tag{19}$$

$$C_m^{M1,j} = -\left(4C_M^{M1+1,j} - C_M^{M1+2,j} + 4C_m^{M1-1,j-1} - C_m^{M1-2,j-1}\right) \Big/ \left[3\left(D+1\right)\right], j = \overline{0, N}; \tag{20}$$

$$C_m^{1,j} = -\left(4C_m^{2,j} - C_m^{3,j}\right)/3, j = \overline{0, N}, \tag{21}$$

where

$$A_m^i = \Delta\theta\left(1 + i^{-1}\right)/\Delta R^2;\ B_m = 1 - 2\Delta\theta/\Delta R^2;\ C_m^i = \Delta\theta\left(1 - i^{-1}\right)/\Delta R^2;$$

$$A_M^i = DA_m^i; B_M = 1 - 2D\Delta\theta/\Delta R^2; C_M^i = DC_m^i;$$

$\Delta R = \eta/M$ (M – the segments number of the region partition R); $\Delta\theta = \varepsilon\Delta R$ ($\varepsilon \ll 1$, is selected $\varepsilon = 0,01$); $M1$ – node number in R corresponding to coordinate R=1; N – finite value of the steps number in dimensionless time.

2. Computational Experiment

The calculation results (Fig. 2) show that at $D > 1$, the matter transfer is more intense than at $D < 1$ (i.e., the permeability of the granule core limits the kinetics). If the granule dislocation between the regions is shifted towards the granule center, then the absorption kinetics also tends to decrease.

Conclusion

A toolkit has been developed for assessing the kinetics of intragranular adsorbate absorption taking into account the adsorbent structure with a sequential arrangement of regions of different permeability in the isothermal regime.

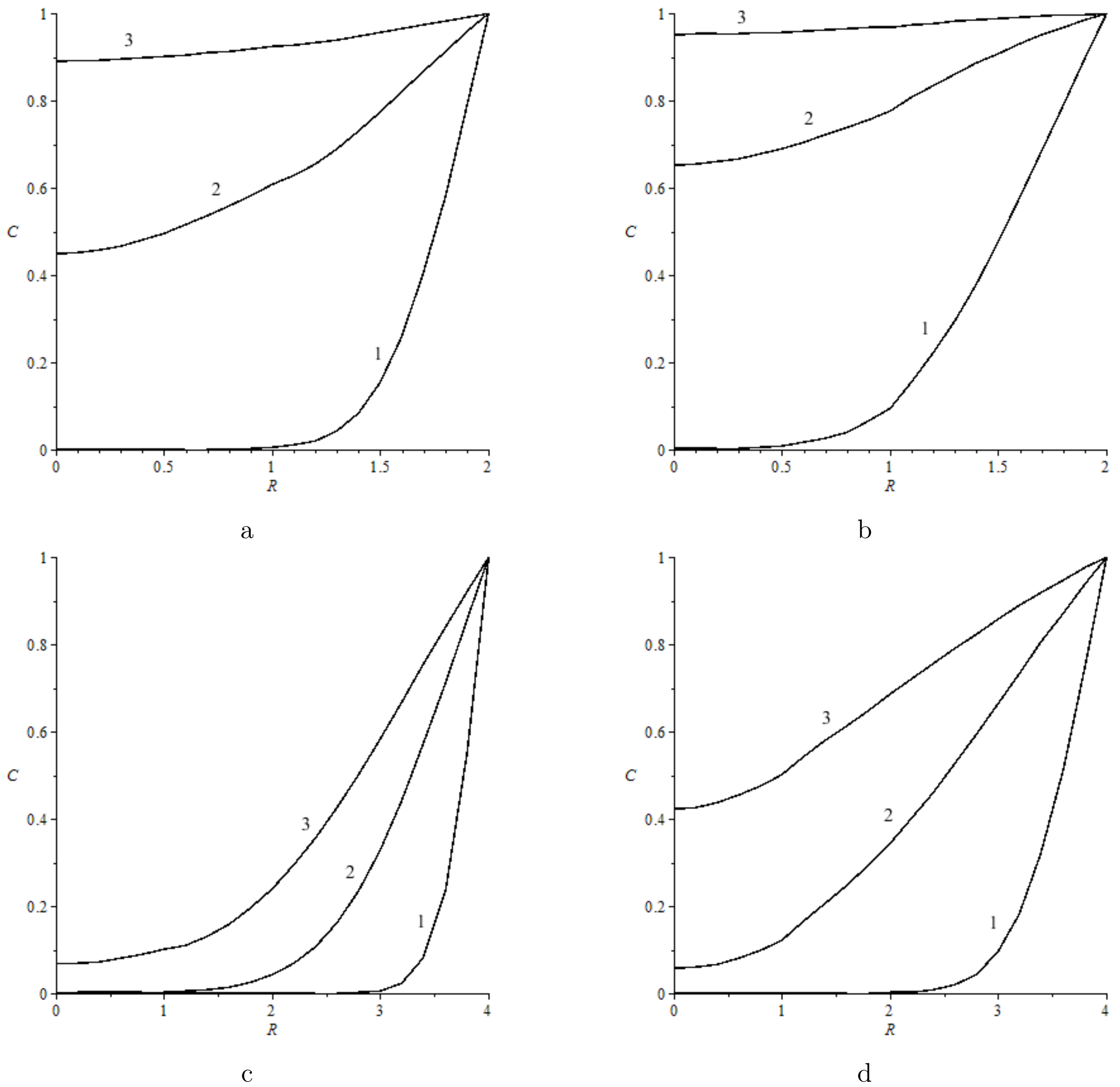

Fig. 2. Local concentration fields at: a – $D = 0.5$; $\eta = 2$; b – $D = 1.5$; $\eta = 2$; c – $D = 0.5$; $\eta = 4$; d – $D = 1.5$; $\eta = 4$ at various moments of dimensionless time θ: 1 – 0.1; 2 – 0.75; 3 – 1.7

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ИЗОТЕРМИЧЕСКИЙ МАССООБМЕН В ГРАНУЛАХ НЕОДНОРОДНО-ПОРИСТОГО АДСОРБЕНТА С ПОСЛЕДОВАТЕЛЬНЫМ МАКРО- И МИКРОДИФФУЗИОННЫМ МЕХАНИЗМОМ ПЕРЕНОСА

А. В. Ряжских, А. В. Келлер, А. В. Хорват, А. С. Викулин, В. И. Ряжских

В формате 1-D сформулирована задача нестационарного изотермического локального распределения диффундирующего одновидового вещества в последовательно расположенных осесимметричных сферических областях гранулы с разной проницаемостью макро-и микропор. Начально-краевая задача для системы дифференциальных уравнений параболического типа с граничным условием первого рода на внешней границе гранулы и четвертого рода на границе сопряжения областей проинтегрирована численно. Вычислительный эксперимент продемонстрировал влияние проницаемости областей и дислокации границы между ними на кинетику транспортирования вещества.

Ключевые слова: массообмен; гранулы адсорбента; неоднородность; диффузия.

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