

Peculiarities of calculating the longitudinal mixing of adsorbent in a fixed layer with account of surface friction

O R Karataev¹ and E S Karataeva²

¹Federal State Budget Educational Institution of Higher Education «Kazan National Research Technological University», Kazan city, Karl Marx street, bld.68, Russia

²Kazan (Privolzhsky) Federal University, engineering institute, Kazan city, S.Saidashev street, bld.12, Russia

e.s.karataeva@mail.ru

Abstract. The paper presents a theoretical one-dimensional model of the dynamics of adsorption in a fixed layer, taking into account the first-order chemical reaction. The general case is considered when the resistance to mass transfer is concentrated both in the external and internal phases.

1. Equilibrium in sorption processing

Sorption treatment of wastewater is most rational if they contain predominantly aromatic compounds, nonelectrolytes or weak electrolytes, dyes, unsaturated compounds or hydrophobic (for example, containing chlorine or nitro groups) aliphatic compounds. If only inorganic compounds are contained in water, as well as lower monohydric alcohols, this method is not applicable.

Between the amounts of the substance adsorbed by the sorbent and remaining in the solution, in dilute solutions a equilibrium occurs, that obeys the law of distribution, according to which both longitudinal mixing and the flow of substance are simultaneously taken into account due to a chemical reaction (a negative source of substance) [1, 2].

$$\frac{\partial C(x, \tau)}{\partial \tau} + \delta \frac{\partial C_a(x, \tau)}{\partial \tau} + W \frac{\partial C(x, \tau)}{\partial x} = D_L \frac{\partial^2 C(x, \tau)}{\partial x^2} - K_c C(x, \tau), \quad (1)$$

$$C_a(x, \tau) = AC^*(C_a) - B. \quad (2)$$

Here A and B are constants, $C_a(x, \tau)$ is a concentration of the adsorbed substance in the sorbent in the cross section x at a particular time τ ; $C(x, \tau)$ is a concentration of adsorbent in the flow at a distance x at a particular time τ ; W is a flow rate; K is a mass transfer coefficient; K_c is a reaction rate constant; $\delta = \frac{(1-\varepsilon)}{\varepsilon}$ is a coefficient; ε is a fraction of the free section of the adsorbent (a volume-constant porosity of the fixed layer); C^* is a concentration of the target component in the equilibrium flow with an average content of the adsorbent C_a in the layer; D_L is a coefficient of the longitudinal diffusion (mixing).

The first two terms on the left-hand side of equation (1) are the rate of change in the mass of the target component in the gaps between the particles and inside the particles, respectively. The third term corresponds to the increment in the mass of the target component due to convective transport



with the flow. The first and second terms on the right-hand side (1) take into account the change in the mass of the target component due to molecular diffusion (longitudinal mixing) and the behavior of the chemical reaction, respectively.

In the initial section of the fixed layer at an arbitrary moment of time τ the concentration of the target component is constant and equal to C_0 , since in (1) the second derivative of the concentration in time is presented, owing to the account of longitudinal mixing [3].

The driving force of the processes under consideration is the difference between the working (excess) pressure over the initial solution and the osmotic pressure of the solution. The most promising are reverse osmosis and ultrafiltration in local wastewater treatment systems with their small expenditures for concentrating and isolating the relatively valuable components and water purification. For example, purification of wastewater, generated during metalworking, etching, painting, plating from toxic substances such as cyanides, chromium, nickel, copper, zinc and others, which can also be regenerated [4].

2. Calculation of longitudinal mixing of adsorbent in a fixed layer with account of surface friction

Transformations (2) with due account allow to write down the following:

$$\frac{\partial C(x, \tau)}{\partial \tau} + W \frac{\partial C(x, \tau)}{\partial x} = D_L \frac{\partial^2 C(x, \tau)}{\partial x^2} - \delta K \left[C(x, \tau) - \frac{C_a(x, \tau)}{A} - \frac{B}{A} \right] - K C(x, \tau),$$

$$0 \leq x < \infty, 0 < \tau < \infty, \quad (3)$$

$$\frac{\partial C_a(x, \tau)}{\partial \tau} = K \left[C(x, \tau) - \frac{C_a(x, \tau)}{A} - \frac{B}{A} \right], \quad 0 \leq x \leq \infty, 0 \leq \tau \leq \infty. \quad (4)$$

Unlike microfiltration and ultrafiltration, impurities trapped in the reverse osmosis process have dimensions at the level of molecules, associates, ions, acid residues.

The value of the flow passing through the reverse osmosis membrane is just as important as its selectivity with respect to various types of dissolved substance. One of the reasons for the formation of the surface layer is the special nature of material loading under friction. The main distinguishing feature of the friction process is the discrete, stochastic character of the frictional contact interaction [5]. This type of interaction for surfaces that come into contact for the first time is due to an initially imperfect surface relief. In the case of interaction of the used surfaces it is due to the presence of a microrelief (equilibrium roughness), formed on the surfaces in the process of friction [3]. In the proposed model, the material is represented by a set of N elements representing power centers and having the ability of translational motion. The viscous force of interaction between two elements (the concentration of substance C from the time of separation) is determined by the relative speed of motion of the elements and is directed opposite to the vector of this velocity [4].

$$F(x, s) \bullet \circ C(x, \tau) = \left[C_0 F(\tau) - B \delta \gamma \int_0^\tau F(t) F_1(\tau - t) dt \right] e^{\frac{Wx}{2a^2}} +$$

$$+ B \delta \gamma \begin{cases} \frac{1}{\sqrt{a_2}} e^{-\frac{a_1 \tau}{2}} \sin \sqrt{a_2} \tau \text{ when } a_2 > 0, \\ \frac{1}{\sqrt{-a_2}} e^{-\frac{a_1 \tau}{2}} sh \sqrt{-a_2} \tau \text{ when } a_2 < 0. \end{cases}, \quad (5)$$

$$\begin{aligned}
 \dots\dots\dots \Phi(x,s) \longrightarrow C_a(x,\tau) = & \left\{ k C_0 \int_0^\tau e^{-\gamma(\tau-t)} F(t) dt - k B \delta \gamma \times \right. \\
 & \left. \int_0^\tau e^{-\gamma \xi} \left[\int_0^{\tau-\xi} F(t) F_1(\tau-t) dt \right] d\xi \right\} e^{\frac{W x}{2a^2}} + \frac{k B \delta \gamma e^{-\gamma \tau}}{(\gamma^2 - a_1 \gamma + a_0)} \times
 \end{aligned} \quad (6)$$

For each material layer, you can define properties different from those of the other layers, so different pairs of layers can have different characteristics. This approach allows you to design a microelevation from several materials with different properties, thereby modeling the material with coatings.

The result of solving the temperature problem and, consequently, the behavior of the friction system as a whole is strongly influenced by the choice of the boundary conditions [5].

References

- [1] Karataev O R and Ananikov S V 2013 Dynamics of adsorption taking into account the chemical reaction during cleaning of swimming pool drains Herald of Kazan Technological University **14** (Kazan: Kazan Technological University Press), pp 59-65
- [2] Doetsch G 1958 Guide to practical application of Laplace transform (Moscow: GIFML) p 208
- [3] Panteleev A V and Yakimova A S 2001 *Theory of functions of complex variable and operational calculus in examples and problems* (Moscow: High school) p 445
- [4] Dwight T B 1964 Tables of integrals and other mathematical formulas (Moscow: Science) p 228
- [5] Rubtsov V E 2004 Modeling of deformation and thermal processes in surface layer of elastoplastic material in friction: Candidate of physical and mathematical sciences Diss. (Tomsk) p 145