Numerical-analytical method for determining the barodiffusion coefficient of technological process of ion-exchange suspension filtration

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Abstract. A method for determining an experimental parameter of the barodiffusion coefficient for conducting computational experiments in technological process of filtering liquid ionized solutions is given in the paper. The developed mathematical model allows obtaining calculated data for the study of other parameters of the unit, taking into account the physicomechanical properties of fluid when cleaning solutions in an ion-exchange column. An analytical solution to the systems of linear equations of diffusion and mass transfer with a constant flow velocity and a variable pressure gradient is obtained. Using these data we can verify the adequacy of the developed mathematical models of the mass transfer process in porous media.

1. Introduction

Currently, there arises a problem of a wider use of modern methods of research of technological processes using computer systems that make it possible to predict these processes in conditions as close as possible to the object of study. The combination of these methods with the methods of computer and chemical technology is the basis of the methodology for a systems approach in modern chemical and food technology.

In the process of ionized solution motion through the ion exchange filter, the resin beads swell and the filter porosity and permeability change, so, its resistance changes as well. A mathematical model that takes this phenomenon into account contains a new parameter, the so-called “barodiffusion coefficient” \( bD \), which is an experimental parameter. In each case it is determined by experimental observations. As a rule, these experiments are very labor-consuming. However, by combining the numerical-analytical solution with simple experimental observation, it is possible to obtain the value of the barodiffusion coefficient \( bD \) with a fairly high accuracy. The present work is devoted to the determination of the barodiffusion coefficient \( bD \).

Many scientists are involved in this problem study and significant scientific results have been obtained. In particular, in [1], inverse problems were studied in the form of nonlinear heat equations...
with varying convection and diffusion coefficients. A method to solve the problem based on Crank-Nicholson studies was given. To improve the error order, the Tikhonov regularization method was used. The problems were solved by software package MATLAB. The resulting inverse problems were transformed into non-linear minimization problems and were solved using the lsqnonlin subroutine from MATLAB tool.

The authors in [2] have constructed analytical models that successfully predict the values of the filter permeability coefficient. A computational experiment was carried out in MATLAB.

In [3], study established three-dimensionally random structures of fiber filters with fiber diameters in the range of 10 to 20 μm and solid volume fractions in the range of 12 to 19%, in order to study the infiltration process inside the fiber filters three-dimensional random structures with fibrous filters were studied by the method of fluid dynamics and discrete elements. The results obtained were from 10 to 20 μm and volume fractions - in the range from 12 to 19%. The filtering efficiency and pressure drop of the filters were calculated, analyzed and compared using a solution of semi-analytical models.

A nonlinear mathematical model in the form of a differential equation in partial derivatives of gas filtration in porous media, taking into account the changes in hydrodynamic parameters of the object under study, was developed in [4]. The authors applied locally one-dimensional schemes and longitudinal-transverse direction schemes; several methods for constructing an iterative process were also tested.

The authors in [5] have proposed a mathematical model and an efficient numerical algorithm based on a finite-difference scheme with second-order errors in the process of water filtering from oil in a porous medium. They conducted computational experiments and analyzed the problems of displacement of one fluid by another in a porous medium.

In [6], a mathematical model was developed for multiple ion-exchange filtering of suspensions with a multilayer filter and as well as a computational algorithm for conducting computational experiments. In other study of these authors the process of water and salt transport in soil was considered. There was proposed a mathematical model for carrying out a comprehensive study taking into account the clogging of soil pores with fine particles over time. The authors implemented a numerical algorithm based on the Samarsky-Fryazinov vector difference scheme with a second-order error approximation.

2. Statement of the problem

To find the sought for distribution functions of substances in a sorbing medium at any stage of the process, a system of differential equations is derived that quantitatively describes the process of dynamic sorption. Differential equations describing the processes of sorption dynamics in the most general form are partial differential equations of the first and second order. The systems of differential equations of sorption dynamics are difficult to solve in a complete analytical form. Only in partial cases and under simplifying assumptions, is it possible to obtain a complete analytical solution. In those cases when the methods of mathematical physics do not allow solving the problems of sorption dynamics, numerical integration of differential equations is done, i.e. they are solved using the methods of finite differences.

Let us consider the derivation of equations of sorbed substances balance in the process of their motion through a porous medium. Let the flow of a mixture of sorbed substances move in a certain direction inside the porous medium (figure 1).

![Figure 1. Schematic view of suspension flow inside the filter unit: D1-flow medium; D2-porous medium; D3-purified flow medium.](image)

Assume that the average porosity and sorption properties of the medium at all points are the same, and introduce the following notation: x, y, z — rectangular coordinates in which the motion of sorbed
substances is considered; \( t \) is the time of the process; \( u \) is the linear flow velocity inside the porous medium – the vector quantity \( (\vec{u}) \); \( j \) is the number of components of the substance mixture; \( i \) is the ordinal number of components of the substance mixture; \( n_i \) is the volume concentration of the \( i \)-th component in the composition of the mobile phase per unit volume of the porous medium; \( N_i \) is the volume concentration of the \( i \)-th component in the composition of stationary phase - the sorbent, per unit volume of the porous medium.

Now summarize the overall balance of substance in the elementary layer:

\[
-[\text{div}(n_i \vec{u})] dxdydz + \frac{\partial n_i}{\partial t} dxdydz dt = 0. \tag{1}
\]

If, in addition to the mechanical flow, an additional transport of substances occurs as a result of molecular diffusion and convection, then an additional term must be introduced into equation (1), which takes into account substance transport processes.

Diffusion-convection transport can be taken into account according to the theory of diffusion using the following equation [7]

\[
\frac{\partial n_i}{\partial t} + \frac{\partial N_i}{\partial t} + \text{div}(n_i \vec{u}) = D_{m,i} (\Delta n_i + \lambda_i \Delta T) \tag{2}
\]

For the process of sorption dynamics of substance mixture, we obtain a system \( N \) of such balance equations \( (1 \leq i \leq N) \).

When solving the sorption problems (separation of components) in equation (2), the term \( \Delta T \) is usually neglected.

Given the change in the pressure gradient in the ion exchanger column, the equation of substance balance (2) is written as

\[
\frac{\partial n_i}{\partial t} + \frac{\partial N_i}{\partial t} + \text{div}(n_i \vec{u}) = D_{m,i} \Delta n_i + \frac{D_b}{P} \frac{\partial P}{\partial x}, \tag{3}
\]

where \( D_b \) - is the barodiffusion coefficient, being positive and negative value; \( P \) – is the pressure in the column of filter unit.

To determine the barodiffusion coefficient, we write the general equation for the sorption dynamics of one substance with a linear Henry sorption isotherm in the form [7]:

\[
m \frac{\partial n}{\partial t} + W \frac{\partial n}{\partial x} + \frac{\partial N}{\partial t} + \frac{\partial^2 n}{\partial x^2} + \frac{D_b}{P} \frac{\partial P}{\partial x} = D \frac{\partial^2 n}{\partial x^2}, \tag{4}
\]

\[
\frac{\partial N}{\partial t} = \beta (n - \Gamma N), \tag{5}
\]

\[
m \frac{\partial P}{\partial t} = \frac{\partial}{\partial x} \left( k \frac{\partial P}{\partial x} \right), \tag{6}
\]

where \( \Gamma \) - is the Henry coefficient.

Boundary conditions are written in the form

\[
\begin{align*}
n_{01} &= n, \quad N = N_0, \quad P = f(x), \quad (t = 0) \\
n &= n_0, \quad k \frac{\partial P}{\partial x} + \gamma P = P_0, \quad (x = 0) \\
n &= n_{02}, \quad \partial P / \partial x = 0, \quad (x = \infty)
\end{align*} \tag{7}
\]
where $\gamma, f(x)$ are the set values; $n, N$ – nonequilibrium concentrations in solution and sorbent; $W$ – the velocity of solution flow in the ion exchange column; $D, D_b$ – the diffusion and barodiffusion coefficients; $P$ – pressure; $\beta$ - effective constant of exchanging ions; $m, k$ – the porosity and permeability coefficients of ion exchanger; $n_0, N_0$ – initial concentrations of ions in solution and ion exchanger; $P_0$ – initial pressure in the column.

For the sorption problem $n_{01} = 0, n_{02} = n_0$, for the desorption problem $n_{01} = n_0, N_0 = 0, n_{02} = 0$.

3. Numerical-analytical method for solving the problem
The task is to combine the analytical solution of system (4) - (7) with experimental data and to obtain an explicit analytical form of the barodiffusion coefficient.

To do so, first solve equation (4) with the corresponding boundary conditions (7). In general, porosity $m$ and permeability $k$ are functions of $x$ and $t$. To obtain an analytical solution to the problem, assume that $k = const, m = const$ and instead of equation (6) we get the following one:

$$\frac{\partial p}{\partial t} = a \frac{\partial^2 p}{\partial x^2}$$

under initial condition

$$t = 0, P = P_0 = const,$$

and boundary conditions

$$x = 0, \frac{\partial P}{\partial x} + \gamma P = f(t),$$

$$x = \infty, \frac{\partial P}{\partial x} = 0,$$

where $a = k/m$.

The problem is solved by the operational method. If we apply the Laplace transform to differential equation (8), then the image equation with initial condition has the form

$$P''_L(x, s) - \frac{s'}{a} P'_L(x, s) + \frac{P_0}{a} = 0.$$

Boundary conditions for the image equation are

$$P'_L + \gamma P_L = F(s), \quad x = 0;$$

$$P'_L = 0.$$

Solution to equation (12) in a general form is written as:

$$P_L - \frac{P_0}{s} = Ae^{\frac{s}{a} x} + Be^{-\frac{s}{a} x},$$

$$P' = \sqrt{\frac{s}{a}} \left[ Ae^{\frac{s}{a} x} - Be^{-\frac{s}{a} x} \right].$$
\[ x = 0, \quad \sqrt{\frac{s}{a}} \left( Ae^{\frac{x}{\sqrt{a}}} - Be^{-\frac{x}{\sqrt{a}}} \right) + \gamma (A + B) = F, \quad \sqrt{\frac{s}{a}} (A - B) + \gamma (A + B) = F(s), \]

from condition (7) we get \( A = 0 \). Constant \( B \) is determined from boundary conditions (7):

\[ -B \sqrt{\frac{s}{a}} + \gamma B = F(s), \quad B(\gamma - \sqrt{\frac{s}{a}}) = F, \]

hence

\[ B = F(s) / \gamma - \sqrt{\frac{s}{a}}, \quad (16) \]

Then the solution to the image equation is:

\[ P_L(x, s) = \frac{F(s)}{(\gamma - \sqrt{\frac{s}{a}})} e^{-\frac{x}{\sqrt{a}}} + P_0 \quad (17) \]

To find the original one, the image table is used, from which we find

\[ P(x, t) = H \left\{ \frac{1}{(-b)^3} e^{b_1 x + b_2 t} \cdot \text{erfc} \left( \frac{k}{2} \right) \cdot \frac{1}{b_1 + b_2} \cdot \sum_{m=0}^{\infty} (-2b_1 t)^m \cdot i^m \cdot \text{erfc} \left( \frac{k}{2} \right) \right\} + P_0 \]

where

\[ b = \gamma \sqrt{a}, \quad k = x / \sqrt{a}, \quad H = \sqrt{a} \cdot c^n. \]

I. \[ \sum_{m=0}^{\infty} (-2b_1 t)^m \cdot i^m \cdot \text{erfc} \left( \frac{k}{2} \right) = \text{erfc} \left( \frac{k}{2} \right) \left[ 1 - 4b_1^2 t \right] - 2b_1 t \cdot i \cdot \text{erfc} \left( \frac{k}{2} \right). \]

II. \[ i \cdot \text{erfc} \left( \frac{k}{2} \right) = \frac{1}{\sqrt{\pi}} e^{-\frac{k}{2} t} - \frac{k}{2} \text{erfc} \left( \frac{k}{2} \right) ; \quad \sum_{m=0}^{\infty} (1 - 4b_1^2 t) \cdot \text{erfc} \left( \frac{k}{2} \right) - \frac{2b_1 t}{\sqrt{\pi}} e^{-\frac{k}{4} t} = 2b_1 t \cdot \text{erfc} \left( \frac{k}{2} \right) - \frac{k}{2} \text{erfc} \left( \frac{k}{2} \right). \]

After some transforms of equation (8) with conditions (9) - (11) we obtain the sought for function

\[ P = He^{b_1 t} \cdot e^{b_2 \sqrt{a}} \cdot \left[ 1 - \text{erfc} \left( \frac{x}{2 \sqrt{at}} + b_1 \sqrt{t} \right) \right] - \frac{H}{(-b)^3} (1 - 4b_1^2 t) \times \]

\[ x \left[ 1 - \text{erfc} \left( \frac{x}{2 \sqrt{at}} \right) \right] + \frac{Hb}{(-b)^3} \sqrt{a} x \left( 1 - \text{erfc} \left( \frac{x}{2 \sqrt{at}} + b_2 \sqrt{t} \right) \right) + \frac{H \cdot 2b_1 \sqrt{t}}{(-b)^3} e^{-x^2/4at}; \]

\[ \frac{\partial P}{\partial x} = He^{b_1 t} \cdot e^{b_2 \sqrt{a}} \cdot b \sqrt{a} \left[ 1 - \text{erfc} \left( \frac{x}{2 \sqrt{at}} + b_1 \sqrt{t} \right) \right] + \frac{He^{b_1 t}}{(-b)^3} e^{b_2 \sqrt{a}} \times \]

\[ \times \left\{ -\frac{2}{\sqrt{\pi}} e^{-\left( \frac{x}{2 \sqrt{at}} + b_2 \sqrt{t} \right)^2} \cdot \frac{1}{2 \sqrt{at}} + \frac{H}{(-b)^3} (1 - 4b_1^2 t) \cdot \frac{1}{2 \sqrt{at}} + \frac{H}{(-b)^3} e^{-x^2/4at} \times \right\} \]
\[ \times \left(1 - \operatorname{erfc} \frac{x}{2 \sqrt{at}} \right) + \frac{H}{(b)^2 \sqrt{a}} x \left( - \frac{2}{\sqrt{\pi}} e^{\left(\frac{x}{2 \sqrt{at}}\right)^2} \cdot \frac{1}{2 \sqrt{at}} \right) + \frac{H \cdot 2 \sqrt{t}}{(b)^2 \sqrt{\pi}} e^{-x^2/4at} \cdot \left( - \frac{x}{2at} \right). \]

Thus, the sought for function is obtained to determine the pressure inside the filter.

If the value of \( n \) is known at some point that is not a point on the boundaries, then the formula for determining the barodiffusion coefficient can be written as follows

\[ D_b = \frac{n(x_k, t) - q_1(x_k, t)}{q_2(x_k, t)}, \]

where \( x_k \) – is any point inside the considered domain,

\[ q_2(x, t) = e^{(k_2 + k_3)x} \cdot \left( \frac{D_m}{m} \right)^{k_2 + k_3} \cdot \left( \frac{D_m}{m} \right)^{k_2 + k_3} \cdot \operatorname{erfc} \left( \frac{x}{2 \sqrt{D_m t}} \right) + e^{D_m (k_2 + k_3)} \cdot \operatorname{erfc} \left( \frac{x}{2 \sqrt{D_m t}} \right) + \frac{n_{01} x}{2 \sqrt{m \pi t^3}} e^{-(k_2 + k_3)x} \cdot e^{-D_m x^2/4mt} + \frac{D_b}{D} \int_{0}^{\infty} \Phi_0(\tau) \operatorname{erfc} \left( \frac{x}{2 \sqrt{C_0 (t - \tau)}} \right) d\tau. \]

So, based on the obtained formula, computational experiments were conducted under the following initial data:

\[ \beta = 0.00248; \quad \gamma = 0.705; \quad M = 0.4; \quad n_{01} = 51; \quad DT = 0.010; \quad D = 0.00000029; \]

\[ W = 0.0025; \quad H_1 = 0.050; \quad n_1 = 0.02800; \quad n_2 = 0.02500; \quad N_x = 21.0; \quad N_t = 10. \]

4. Conclusion

An analytical solution to the systems of linear equations of diffusion and mass transfer with a constant flow velocity and a variable pressure gradient is obtained. Using these data we can verify the adequacy of the developed mathematical models of the mass transfer process in porous media.

At insufficient experimental data, the barodiffusion coefficient was determined from the obtained solutions, being one of the key parameters of technological processes of ion-exchange filtering of ionic solutions. As follows from numerical calculations to determine the barodiffusion coefficient, a change in its value obeys the logarithmic law. From the calculated values of the barodiffusion coefficient, we can obtain a functional dependence for calculating the barodiffusion coefficient

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