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CHAPTER 12

MATHEMATICAL MODELING OF MASS TRANSFER IN BAROMEMBRANE PROCESSES

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Abstract. *To determine the optimal modes of rational exploitation of membranes the phenomena of concentration polarization was researched. To simulate the real processes of separation, we used geometric, physical and mass-exchange characteristics of real membrane systems. Depending on the pressure, membrane characteristics and flow turbulence, the concentration polarization may exceed the value of 10, which must be taken into account in order to prevent the formation of sediment on the surface of the membrane.*

Keywords: *membrane, modeling, separation, concentration polarization, mas transfer.*

Introduction. The problem of the use of membrane technology is complicated by membrane contamination, since the operation modes are sometimes far from optimal. As a result, the concentration of solutes at the membrane surface increases significantly (the phenomenon of concentration polarization). When the solution concentration i high, some components may form insoluble compounds, gel-like sediment etc. When the concentration in the layer near the membrane surface becomes higher comparing with the feeding solution, diffusion streams are directed in the opposite direction relative to the flow of the filtering solution. Such effects significantly reduce the membrane productivity, during separation processes [1, 2].

Therefore, it is advisable to investigate the phenomenon of concentration polarization, studying the distribution of concentrations and its change over time in the channel, to determine the optimal modes of rational operation of membranes. Since experimental determining concentration distribution during the filtration process is very difficult, methods of mathematical modeling are used. Unfortunately, there is no single theory capable of fully describing the processes that take place near the surface of the membrane for the processes of separation (concentration) of multicomponent solutions [3], so this task remains relevant. Among modern works, there are stochastic approaches [4], various semi-empirical models [3, 5], but in most cases the theoretical study of mass transfer processes is carried out by methods of continuum mechanics using finite difference approximation [3, 5-7].

The purpose of this work was to determine the level of concentration polarization in the membrane channels of barometric apparatus with methods of mathematical modeling.

Experimental. The phenomenon of concentration polarization related to mass transfer processes, namely the distribution of the concentration C (x, t) of the dissolved substance in solvent through height of the channel of baromembrane apparatuses is studied.

For one-dimensional models, the concept of linear concentration, kg/m, is introduced, that is, the mass of the dissolved substance per unit length of the segment on x-coordinate:

$$C_{line} = \frac{dM}{dx}, \tag{12.1}$$

For explicit schemes of finite-difference approximation the stability conditions are formulated by the Courant's criterion [6]. Physical meaning of this criterion is followng: the speed of movement along the grid should be less than the transmission rate of perturbations in the system. For this case, the relation determines the Courant's criterion:

$$\Delta t < \frac{\Delta x^2}{2D}, \tag{12.2}$$

where D is the diffusion coefficient, Δx, Δt is the spatial and temporal step according to the scheme, respectively. The concentration of the dissolved substance in the point x at time t is $C = C(x,t)$, kg/m. Change of its mass in volume $S \cdot dx$ for time dt equals $\frac{\partial C}{\partial t} \cdot dx$. Because of the movement of convective and diffusion streams, the concentration of the target component in the considered elemental volume changes (Figure 12.1) [7, 11, 12].

Diffusive fluxes are:

$$q_1^{diff} = -D\frac{\partial C}{\partial x}, \tag{12.3}$$

$$q_2^{diff} = -D\frac{\partial C}{\partial x} - \frac{\partial}{\partial x}\left(D\frac{\partial C}{\partial x}\right)dx, \tag{12.4}$$

Convective fluxes are:

$$q_1^{conv} = C \cdot v, \tag{12.5}$$

$$q_2^{conv} = C \cdot v + \frac{\partial (C \cdot v)}{\partial x} dx, \tag{12.6}$$

$q_e \cdot dx$ is the mass flow from external sources, kg/s, q_e is the flow density, kg/m s. Taking into account the balance of masses in the allocated volume, we obtain the equation of convective diffusion with an external source:

$$\frac{\partial C}{\partial t} = -\frac{\partial (C \cdot v)}{\partial x} + \frac{\partial}{\partial x}\left(\frac{D \cdot \partial C}{\partial x}\right) + q_e, \tag{12.7}$$

The solution $C=C(x,t)$ must satisfy the initial and boundary conditions set at the boundaries of the interval [0, h] at the points x=0, x=h and set the upper boundary of the channel and the surface of the membrane. $C(x,0)=C_0(x)$ - initial conditions, concentration of feeding solution [13].

Results and discussion. Consider a one-dimensional system simulating a portion of space (vertical line, with width $w \to 0$) of the channel of length *l*, height *h*, with a membrane with area *S* is completely filled with a flow of solution (carrier) in which the target component is present (Figure 12.1). From the bottom there is a membrane that completely passes by the carrier (solvent), but does not pass by the target component (Figure 12.2).

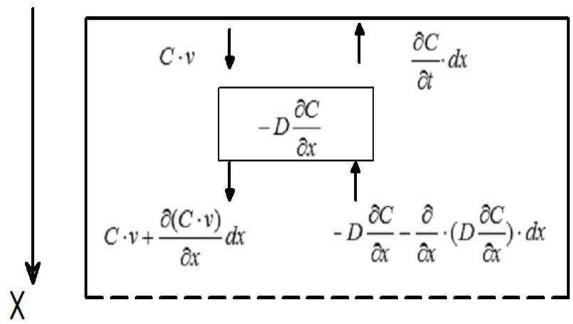

Fig. 12.1. *Scheme of flows in the membrane channel: X – spatial coordinate.*

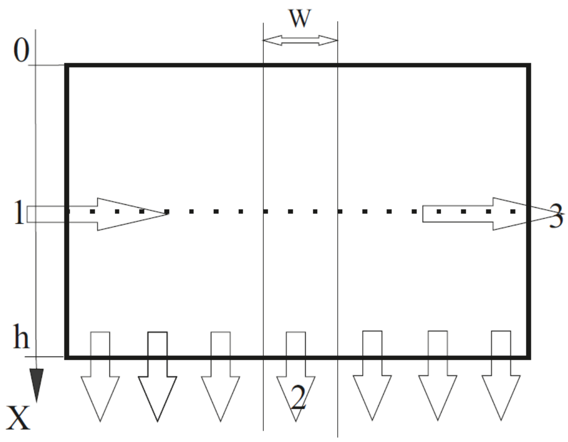

Fig. 12.2. *Scheme of the pressure channel: 1 – the flow of feeding solution; 2 – flow of permeate (filtrate); 3 – the flow of concentrate.*

For a numerical solution of equation (12.7), we apply the finite difference method. It is necessary to switch from continuous variables to discrete ones:

$$x \to x_j, j = 0,1,...,n, \qquad t \to t_i, i = 0,1,...,m \tag{12.8}$$

$$\Delta x = \frac{h}{n}, \qquad \Delta t = \frac{t_{\max}}{m}, \tag{12.9}$$

Similarly for concentration:

$$C(x,t) \to C(x_j,t_i) = C_{i,j} . \tag{12.10}$$

We apply marginal and initial conditions. At the initial moment of time (at t=0) the concentration is equal to the concentration of feeding solution:

$$C(x,0) = C_0, \tag{12.11}$$

The key component does not pass through the membrane and the upper boundary of the channel:

$$C(0,t) = C(h,t) = 0, \tag{12.12}$$

we approximate derivatives by difference schemes:

$$\frac{\partial C}{\partial t} \approx \frac{C_{i+1,j} - C_{i,j}}{\Delta t}, \qquad D\frac{\partial^2 C}{\partial t^2} \approx D\frac{C_{i,j+1} - 2C_{i,j} + C_{i,j-1}}{\Delta x^2}; \tag{12.13}$$

Consequently, by substituting expressions (12.13) into equation (12.7), we obtain the one-dimensional equation in discrete variables with initial and boundary conditions:

$$C_{i+1,j} = C_{i,j} + D\frac{\Delta t \cdot (C_{i,j+1} - 2C_{i,j} + C_{i,j-1})}{\Delta x^2}, \quad (12.14)$$

$$C_{0,j} = C_0, \qquad C_{i,0} = C_{i,n} = 0 \quad (12.15)$$

Using an explicit finite-difference scheme, with a given concentration value $C_{i,j}$ at a given point for fixed *i,j*, we can calculate $C_{i+1,j}$ and, thus, obtain the distribution of concentrations along the entire height of the pressure channel, and its change over time (Figure 12.3).

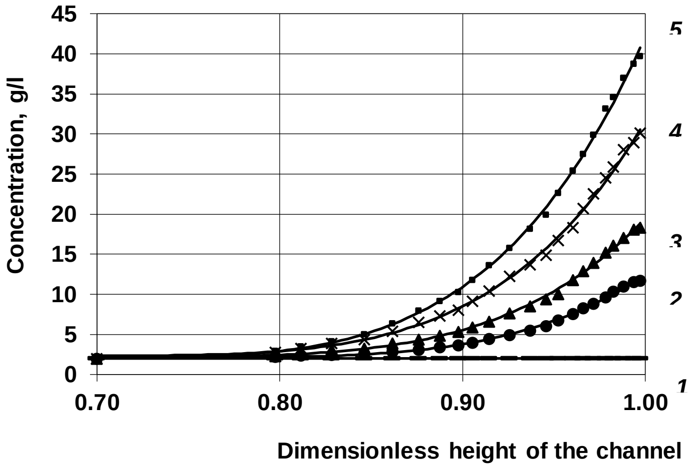

Fig. 12.3. *Distribution of concentrations by the height of the channel: 1 – 0 sec, 2 – 32 sec, 3 – 384 sec, 4 – 448 sec, 5 – 512 sec.*

Conclusions. The distributions of concentrations of the target component by height of the membrane channel were obtained and analyzed. The character of the curves coincides with physical representations of the process, with the exception of the region located near surface of the membrane. This is explained by the fact that in real systems the convective flow, having a turbulent flow pattern, makes the distribution of concentrations more uniform, diverting the mass flows of the target component into the volume of the channel from membrane surface. As a result, the effect of concentration polarization decreases and the sediment is formed less intensively.

The one-dimensional model that is presented does not consider the effects associated with turbulence, but can be applied to a dead-end separation scheme.

The scientific novelty consists in the determination of the kinetic changes in the level of concentration polarization in the membrane channels of barometric apparatus in the separation of food industry liquids.

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МАТЕМАТИЧНЕ МОДЕЛЮВАННЯ МАСООБМІНУ В БАРОМЕМБРАННИХ ПРОЦЕСАХ

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Резюме. *Застосовуючи відповідні граничні умови, що характеризують фізичну сутність баромембранних процесів, а також чисельні методи розв’язку диференціальних рівнянь, отримано систему алгебраїчних кінетичних рівнянь, які дозволяють визначити розподіл концентрації розчиненої речовини по висоті напірних каналів, що практично неможливо зробити експериментально. Встановлено, що залежно від тиску, характеристик мембрани та турбулізації потоку, величина концентраційної поляризації може перевищувати значення 10, що необхідно враховувати з метою унеможливлення утворення осаду на поверхні мембрани.*

Ключові слова: *мембрани, моделювання, розділення, концентраційна поляризація, масообмін.*