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NUMERICAL SIMULATION OF THE MASS TRANSFER IN A HEMODIALYSIS CELL MACHINE

Внедрение современных математических методов в изучение процессов биологических систем является характерным для нашего времени. Наработанный громадный научный потенциал точных наук и современная вычислительная техника позволяют решать сложные задачи с большим набором параметров. Одним из сложнейших направлений в современной науке является моделирование массообменных процессов в живых системах и, в частности, в организме человека и создание медицинской аппаратуры для выполнения тех или иных лечебных операций. Само создание такой аппаратуры невозможно без четкого понимания биофизических и химических процессов, как в аппарате, так и в организме, находящемся под влиянием работы аппарата. Наиболее ярким примером взаимосвязи организма и аппарата является процесс гемодиализа. Математическому описанию этого процесса посвящено уже немало работ. В данной статье представлена математическая модель, описывающая гидравлическую сторону процесса с учетом сопровождающих эффектов, а также конвективно-диффузионный массоперенос нейтральных компонентов при взаимодействии их с полупроницаемой мембраной. Проведенные расчеты показали важные особенности таких систем, а также влияние задающих параметров на распределение рассматриваемых величин в капилляре и диализном канале.

Ключевые слова: *Математическое моделирование, массоперенос, концентрации компонентов крови, онкотическое давление, гемодиализ*

Впровадження сучасних математичних методів до вивчення процесів біологічних систем є характерним для нашого часу. Напрацьований величезний науковий потенціал точних наук і сучасна обчислювальна техніка дозволяють вирішувати складні завдання з великим набором параметрів. Одним з найскладніших напрямків у сучасній науці є моделювання масообмінних процесів в живих системах і, зокрема, в організмі людини і створення медичної апаратури для виконання тих чи інших лікувальних операцій. Саме створення такої апаратури неможливо без чіткого розуміння біофізичних і хімічних процесів, як в апараті, так і в організмі, що знаходиться під впливом роботи апарату. Найбільш яскравим прикладом взаємозв'язку організму і апарату є процес гемодіалізу. Математичному опису цього процесу присвячено вже чимало робіт. У даній статті представлена математична модель, що описує гідравлічну сторону процесу з урахуванням супроводжуючих ефектів, а також конвективно-дифузійний массоперенос нейтральних компонентів при взаємодії їх з напівпроникною мембраною.

Проведені розрахунки показали важливі особливості таких систем, а також вплив заданих параметрів на розподіл розглянутих величин в капілярі і діалізному каналі.

Ключові слова: Математичне моделювання, масоперенос, концентрації компонентів крові, онкотичний тиск, гемодіаліз

The introduction of modern mathematical methods in the study of the processes of biological systems is characteristic of our time. The accumulated huge scientific potential of exact sciences and modern computer technology allow solving complex problems with a large set of parameters. One of the most difficult areas in modern science is the modeling of mass-exchange processes in living systems and, in particular, in the human body and the creation of medical equipment for performing certain medical operations. The very creation of such equipment is impossible without a clear understanding of biophysical and chemical processes, both in the apparatus and in the body, which is under the influence of the apparatus. The most striking example of the relationship between the body and the apparatus is the process of hemodialysis. A lot of work has already been devoted to the mathematical description of this process. This paper presents a mathematical model describing the hydraulic side of the process with allowance for accompanying effects, as well as convective-diffusion mass transfer of neutral components when they interact with a semipermeable membrane. The calculations carried out showed important features of such systems, as well as the influence of the control parameters on the distribution of the quantities under consideration in the capillary and the dialysis channel.

Keywords: *Mathematical modeling, mass transfer, concentration of blood components, oncotic pressure, hemodialysis*

Introduction. One of the directions of the modern scientific development of the space industry is associated with a long stay and life support of a person in extreme conditions. The range of problems related to the creation of space technology currently includes not only the tasks of uninterrupted power supply and ensuring the reliability of mechanisms, but also, first of all, providing high-quality medical services based on modern medical equipment, in particular using membrane technology. Artificial blood purification (hemodialysis) in modern medicine has been universally recognized and is used as an effective method for ionic homeostasis, detoxification and dehydration of the body. The process of hemodialysis is associated with the occurrence of complex mass-exchange processes in the channels separated by membrane partitions through which the fluid is filtered and diffuses relatively low molecular weight blood components (muscular, creatine, toxic substances, allergens, etc.). One of the circuits of the hemodialysis apparatus used is a bundle of hollow fibers, the walls of which are semipermeable membranes. The blood of the patient is delivered inside the fiber, and the dialysis solution is injected into the interfiber space, as a rule, in countercurrent. Due to a certain pressure drop across the membrane, the fluid flow, which constitutes 90% of blood plasma, together with the metabolites, flows into the dialysis channel, as a result of which the concentration of the formed material and proteins in the fiber increases, which is accompanied by an increase in viscosity blood. Blood is a heterogeneous medium, it consists of blood particles (shaped material, dispersed medium) and dispersive fluid mass - plasma. Plasma is a biological colloidal solution that contains both low molecular weight substances and high molecular weight protein compounds (proteins). One of the most important effects associated with the hemodialysis process is the osmotic increase in pressure in the capillary pressure (oncotic pressure), which is due to the interaction of the plasma pro- teins with the membrane and the carrier fluid. In general, the hemodialysis process can be considered both from hydrodynamic positions and from the positions of diffusional mass transfer in the presence of molecular interaction of the components with each other and with the surfaces of the apparatus [1, 2]. At present, the hydraulic side of the theory of hemodialysis has acquired a relatively simple form, based on the solutions of the equations of hydrodynamics under the laser mode of flow in the channels [2–4].

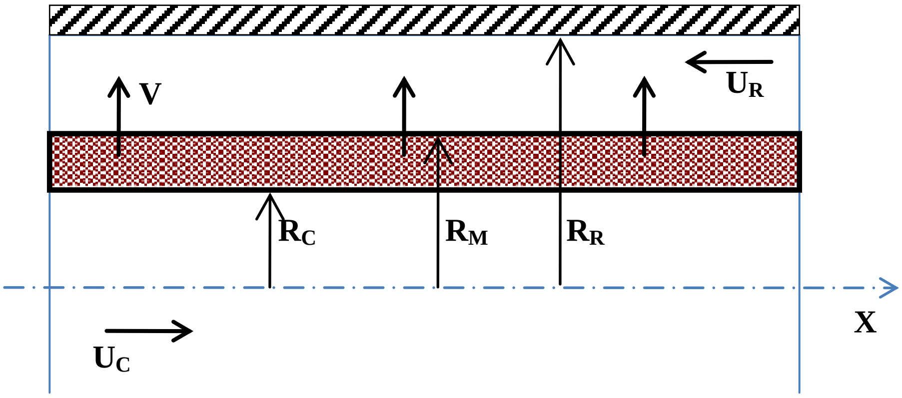


Fig. 1 Flow Chart

Mathematical formulation of the problem. Flow dynamics. If the cell shown in Fig. 1 is taken as the cell element, then the equations describing the dynamics of the fluxes and the preservation of the masses of the blood components can be written as follows (the Newtonian model of the liquid is considered):

$$G_C = -\frac{1}{8}\frac{\pi\rho_C}{\mu_C} R_C^4 \frac{dp_C}{dx}, \tag{1}$$

$$G_R = -\frac{1}{8}\frac{\pi\rho_R}{\mu_R}\left\{\left(R_R^2 - R_M^2\right)^2 - \frac{\left(R_R^2 - R_M^2\right)}{\ln\left(R_M / R_R\right)}\left[\left(R_R^2 - R_M^2\right) + 2R_M^2 \ln\left(R_M / R_R\right)\right]\right\}\frac{dp_R}{dx}, \tag{2}$$

$$\frac{dG_R}{dx} = 2\pi R_M \rho_R v_{MR}, \tag{3}$$

$$G_{PR} = Const, G_F = Const, \tag{4}$$

$$v_{CM} = K_M\left(p_C - p_R - p_{ONC}\right), \quad v_{MR} = \frac{R_C}{R_M} v_{CM}; \tag{5}$$

where G_C, G_R, G_S, G_{PR}, G_F - costs, respectively, of blood, dialysis fluid, liquid released from the blood into the dialysis channel, proteins, formulated material ; p_C, p_R is the pressure in the capillary and dialysis channel accordingly; ρ_C, ρ_R is density of blood, dialysis solution (the density of the emitted liquid is taken equal ρ_R); μ_C,

μ_R are the dynamic coefficients of viscosity, respectively, of blood and solution; R_C , R_M , R_R are radii (see fig. 1).

To these equations it is necessary to add the dependencies of viscosity and oncocteric pressure on the corresponding parameters [5]:

$$\mu_C = \mu_{PL}\left(1 + 2.5H + 0.0735H^2\right), \tag{6}$$

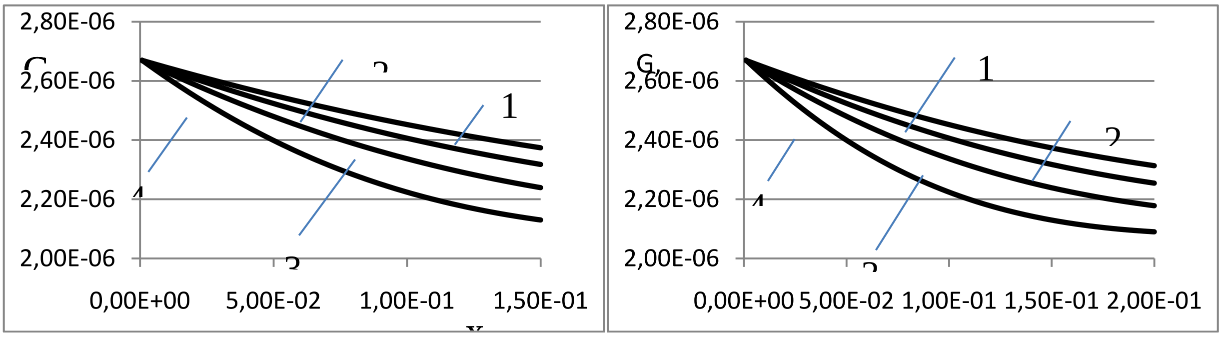
$$p_{ONC} = 0.21 \cdot c_{\Pr} + 1.6 \cdot 10^{-3} \cdot c_{\Pr}^2 + 9 \cdot 10^{-6} \cdot c_{\Pr}^3, \tag{7}$$

where μ_{PL} is dynamic coefficient of viscosity of the plasma; H is volume fraction of the form material (hematocrit); $c_{\Pr}$ is mass concentration of proteins in plasma. Somewhat more complex dependences of the dynamic viscosity on the hematocrit fraction are given in [2], the formula for the blood density is also given there.

$$\rho_C = 1030\left(1 - H\right) + 1090H\,. \tag{8}$$

The written system of equations forms the basis of the hydrodynamic theory of hemodialysis, and with varying degrees of simplification has been considered in contemporary literature [2–4, 6].

In fig. 2 - 5 shows the results of calculations of costs and pressures in the channels of the device (R_C = 0.3 mm; R_M = 0.34 mm; R_R = 0.7 mm).



А Б

Fig. 2 Changes in blood flow in the fiber (A - fiber length 15 cm; B - fiber length 20 cm):

1 – $K = 10^{-9}$, **2** – $2 \cdot 10^{-9}$, **3** – $3 \cdot 10^{-9}$, **4** – $4 \cdot 10^{-9}$.

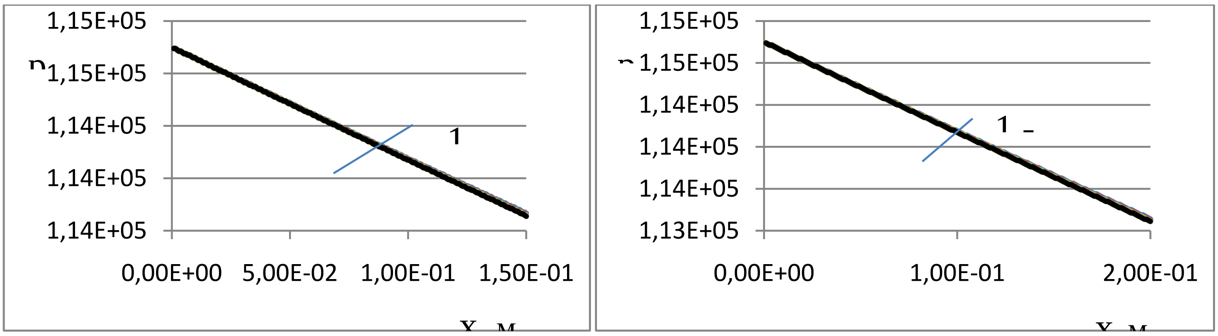


Fig. 3 Pressure drop in the fiber (same designations)

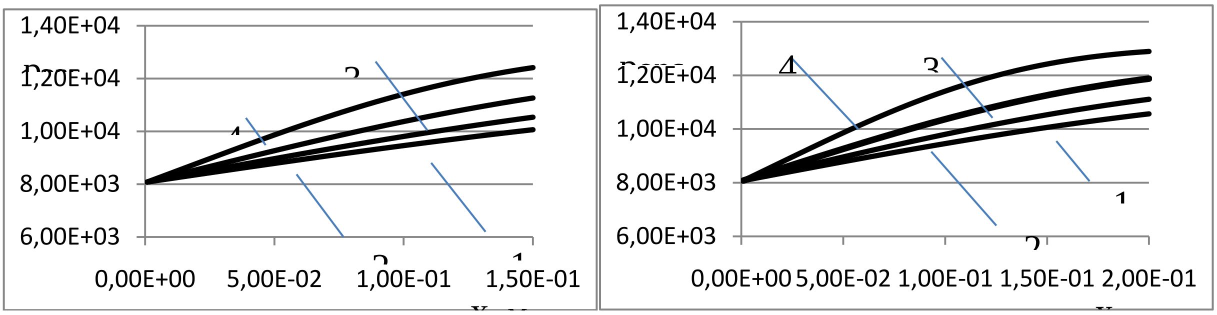


Fig. 4 The change of oncotic pressure in the fiber (the same designations)

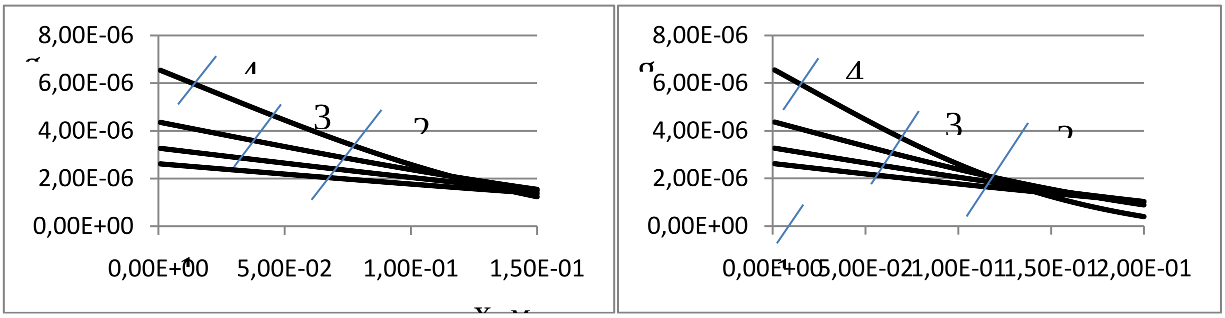


Fig. 5 Changes in the flow rate of fluid through the membrane (designations are the same)

The curves show qualitatively a change in the hydrodynamic parameters from the channel length and membrane resistance. From fig. 2 it follows that the costs in the capillaries, quite noticeably react to the magnitude of the flows. This is natural, because the flow rates themselves in the capillaries are not rational, as a result of which the membrane resistance must be clearly defined. Shown in fig. 4, the separation of oncotic pressure curves suggests that its values may be significant in the process. The calculations carried out in [3] for a more complex rheological model of a fluid, showed small differences in the pressure distribution in the channels compared to the Newtonian model, as a result of which the authors of this work - use the Newton model of a liquid to study mass transfer processes. The mathematical model and the method of successive approximations of this work allows one to determine the fluxes and pressures in the capillary and dialysis channels, depending on the driving parameters and hydraulic characteristics of the membrane.

Mass transfer. In addition to flow distribution during hemodialysis, an important issue is the distribution of blood components in the dialysis cell. In the previous section, emphasis was placed on the separation of flows due to the corresponding pressure drops, which determine the hydraulic behavior of media, i.e. it was assumed that the diffusion fluxes are small compared to the dynamic ones. In real cases, the gradients of the components can be significant, and the filtration hydrodynamic velocities are small, which should lead to an increase in the weight of the diffusion component. In addition, diffusion processes may also be of self-interest, since With the help of the introduction of some active components that prevent, for example, blood coagulation, it is possible to regulate the process itself, either to fix the output of the desired component, or, for example, to regulate the patient's calcium-phosphorus metabolism [one]. Finally, significant scientific interest are ion-exchange processes in which the presence of membranes or phase supernotes has a great influence on the dynamics in general and on mass transfer [7,8]. Here we consider the diffusion processes of neutral components, one of which (1) is associated with blood, the other is distributed from the dialysis channel (component 2). A similar problem related to calcium metabolism was considered in [3]. The basic equation can be written as:

$$\frac{\partial\left(\rho_j c_j\right)}{\partial t}+u\frac{\partial\rho_j c_j}{\partial x}+v\frac{\partial\rho_j c_j}{\partial r}=\left[\frac{\partial}{\partial x}\left(\rho_j D_j\frac{\partial c_j}{\partial x}\right)+\frac{\partial}{r\partial r}\left(\rho_j D_j r\frac{\partial c_j}{\partial r}\right)\right]+J_j, \qquad (9)$$

where t is time; x, r - coordinate system; u, v - speed components derived from the hydraulic task; c_j - concentration of the j-th component; D_j - diffusion coefficient; J_j determines the change in concentration due to reactions. We further assume that the densities and diffusion coefficients are constant $J_j = 0$, and the initial values of the concentrations are zero. As the boundary conditions, we use the following relations.

In capillary:

$$c_1(0,r)=c_{10}, \quad (\partial c_1/\partial x)_{x=L}=0;$$
$$(\partial c_2/\partial x)_{x=0}=0,\ (\partial c_2/\partial x)_{x=L}=0; \qquad (10)$$

in the membrane:

$$(\partial c_1/\partial x)_{x=0}=0, \quad (\partial c_1/\partial x)_{x=L}=0;$$
$$(\partial c_2/\partial x)_{x=0}=0,\ (\partial c_2/\partial x)_{x=L}=0; \qquad (11)$$

in dialysis channel:

$$\left(\partial c_1/\partial x\right)_{x=0}=0,\ \left(\partial c_1/\partial x\right)_{x=L}=0;$$
$$\left(\partial c_2/\partial x\right)_{x=0}=0,\ c_2(L,r)=c_{20}. \tag{12}$$

At the boundaries of the regions, in accordance with the theory of mass transfer, we accept the corresponding equality of the concentrations and fluxes of the components [9].

On the axis of the capillary symmetry conditions

$$\left(\partial c_1/\partial r\right)_{r=0}=\left(\partial c_2/\partial r\right)_{r=0}=0; \tag{13}$$

on the border of the capillary membrane: $c_j(x,r)_{r=Rc+0}=H_{MC\,j}c_j(x,r)_{r=Rc-0}$,

$$\left(vc_j-D_j\frac{\partial c_j}{\partial r}\right)_{r=Rc-0}=\left(vc_j-D_j\frac{\partial c_j}{\partial r}\right)_{r=Rc+0}; \tag{14}$$

on the border of the membrane - dialysis channel:
$c_j(x,r)_{r=Rm-0}=H_{MR\,j}c_j(x,r)_{r=Rm+0}$,

$$\left(vc_j-D_j\frac{\partial c_j}{\partial r}\right)_{r=Rm-0}=\left(vc_j-D_j\frac{\partial c_j}{\partial r}\right)_{r=Rm+0}; \tag{15}$$

on the canal wall $\left(\partial c_1/\partial r\right)_{r=Rr}=\left(\partial c_2/\partial r\right)_{r=Rr}=0$. The written system of equations and boundary conditions is sufficiently general. It makes it possible, through the use of certain quantities or other, to model interesting, complex cases of mass exchange, and also to move to simpler equations. In particular, in a number of papers, for example, in [10, 11], mass transfer coefficients are used for mass fluxes of components between channels (through a membrane). In this paper, a model problem is considered — the transfer of a low-molecular complex from the blood to the dialysis channel and, conversely, some component from the diamal solution to the capillary when the speeds and Henry coefficients change **Hmc** and **Hmr**.

In fig. 6 - 9 shows the distribution curves of the considered compounds in the capillary and the dialysis channel for various cases (**Hmr=1;** $v=\partial\left(u_C/U_{C0}\right)/\partial\left(x/L\right)$ was taken constant along the capillary, the diffusion coefficients in the membrane are an order of magnitude smaller than in solutions). The main changes of the setting parameters and the corresponding numbers of curves are given in the table.

Table 1. The main changes of the setting parameters

	1	2	3	4	5	6
Uc0	0,01	0,01	0,01	0,01	0,01	0,01
Ur0	0,02	0,02	0,04	0,04	0,02	0,02
v	0,1	0,2	0,1	0,1	0,1	0,2
Hmc	1	1	1	2	2	2

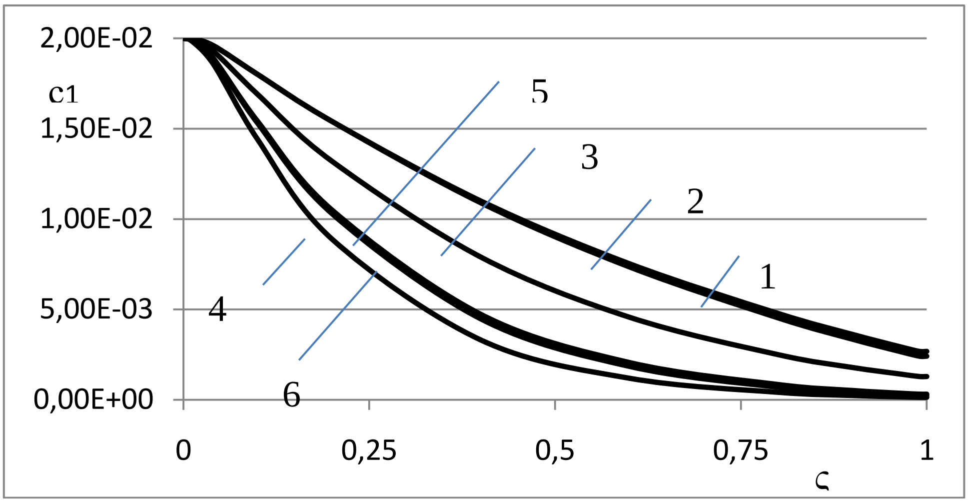


Fig. 6 - The distribution of the concentration of C1 in the capillary

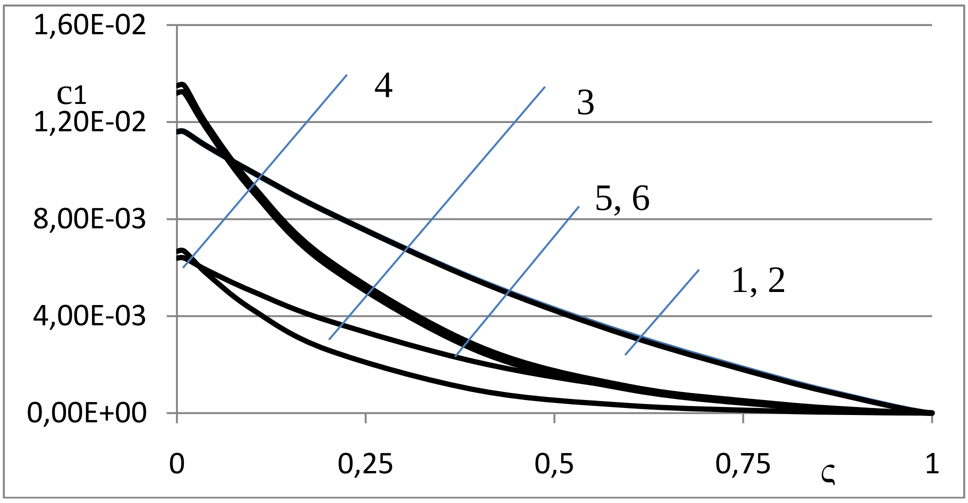


Fig. 7 - The distribution of the concentration of C1 in the dialysis channel

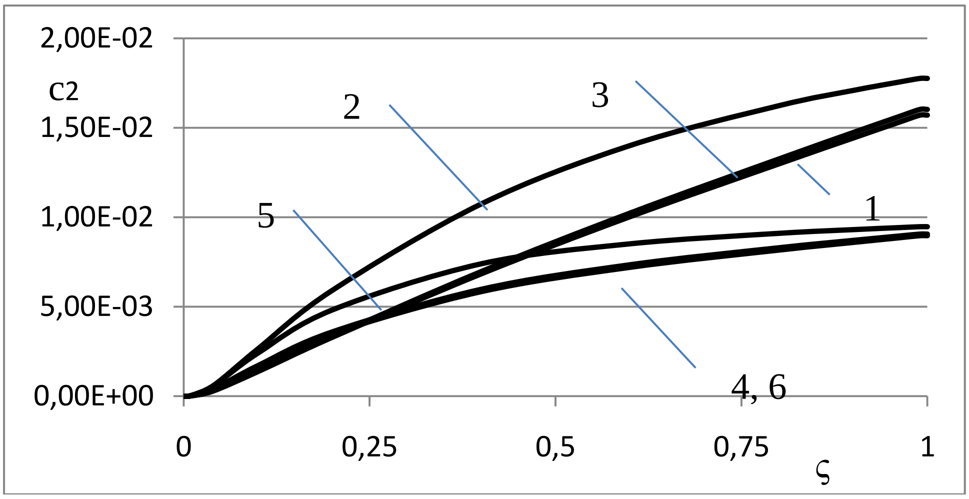


Fig. 8 - Distribution of C2 concentration in the capillary

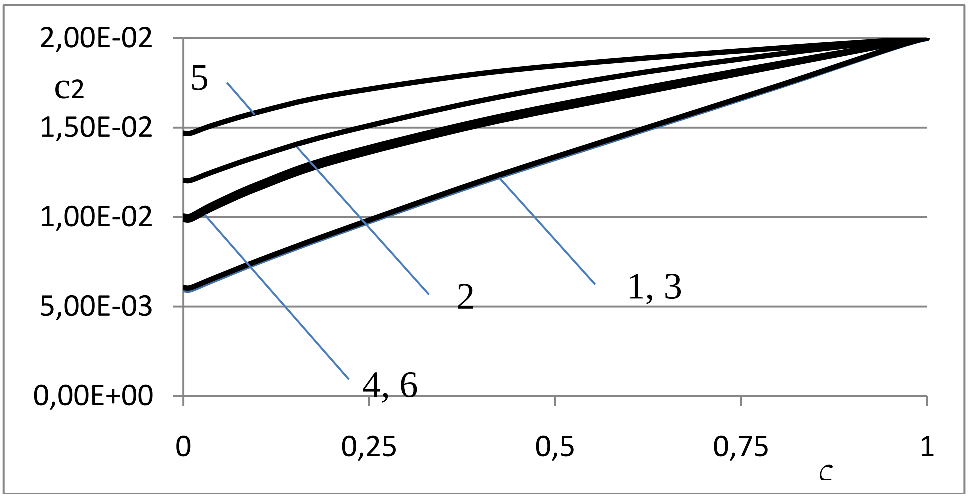


Fig. 9 - Distribution of C2 concentration in the dialysis channel

The given concentration curves of the considered components give an idea of their distribution in the channels, depending on the input velocities, filtration filtration flows in the membrane and Henry coefficients. Here, an important circumstance is the transition of component 2 from the dialysis solution to the capillary with blood, which is generally undesirable. This issue requires special attention and must be carefully developed. The second important point is related to the magnitude of the Henry coefficient, which has a significant effect on the distribution of the companion under consideration. This formulation of the problem and the numerical solution method allow calculating the distribution of blood components and dialysis solution in the capillary and dialysis channel depending on the determining parameters of the convective-diffusion process.

Conclusions. In the most general form, the problems of fluid hydraulics and convective-diffusive mass transfer in a cell of a hemodynamic apparatus are formulated. The performed numerical solutions have shown the effect of flows on the

flow of fluid in the channels and on the change in oncotic pressure of the blood. The distributions of the considered components of blood and dialysis solution in the channels are found, the effect of Henry overflows and coefficients on the concentrations of these substances is shown.

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