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Numerical Simulation of Opposite Currents

The mathematical models of hydrodynamics processes in chemical reactors are based on Navier-Stokes equations. In direct current reactors the models that are most frequently used are models based on the approximation of boundary layer [1]. At the same time such an approximation for simulation of processes in opposite current reactors leads to non-classical problems of mathematical physics and so these problems were not sufficiently discussed in literature. The prototype of such problems is the parabolic boundary value problem with changing direction of time [2].

In this paper we propose the model that is mathematically correct for the description of hydrodynamics processes in opposite current reactor in approximation of boundary layer for two immiscible liquids. We have developed a calculating algorithm for the approximate solution of corresponding boundary value problem. The algorithm is based on the decomposition of calculated domain to two subdomains with iterative satisfying conditions on the boundaries of subdomains.

1. Formulation of the problem

Let x - be longitudinal and y - cross coordinates, u and v - corresponding velocity components. We consider stationary flow of two immiscible liquids. Let domain Ω_+ $(0 < x < 1, y > 0)$ be filled with one liquid and domain Ω_- $(0 < x < 1, y < 0)$ - with another liquid. Density ρ and viscosity μ of the liquid in Ω_+ are noted by ρ_+ and μ_+ correspondingly. Analogous notations (ρ_-, μ_-) are used for the characteristics of the second liquid. Liquids are supposed incompressible.

It is natural to use the approximation of the boundary layer for the description of the opposite current. After ordinary operations we come to equations:

$$\rho\left(u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y}\right) = \mu \frac{\partial^2 u}{\partial y^2}, \quad (x,y) \in \Omega_+ \cup \Omega_-, \qquad (1)$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \quad (x,y) \in \Omega_+ \cup \Omega_-, \qquad (2)$$

where p is pressure.

Equations (1), (2) are added by necessary conditions on the interface $y=0$. Opposite current corresponds to the input of the following boundary conditions for velocity:

$$u(0,y) = U_+, \quad y > 0, \qquad (3)$$

$$u(1,y) = U_-, \quad y < 0, \qquad (4)$$

where $U_+ > 0$, $U_- < 0$.

Besides the boundary conditions (3), (4) there are conditions of conjugation for tangential velocities and forces:

$$[u] = 0, \quad \left[\mu \frac{\partial u}{\partial y}\right] = 0, \qquad (5)$$

with the notation

$$[g] = g(x,y+0) - g(x,y-0).$$

The condition of immiscibility has the form:

$$v(x,0) = 0. \qquad (6)$$

The problem (1)-(6) corresponds to the description of the opposite current in the approximation of the boundary layer. Besides nonlinearity this problem has it's characteristic features. First of all it relates to the non-classical problems of mathematical physics - parabolic boundary value problems with changing direction of time [2]. In each isolated subdomain (in Ω_+ and in Ω_-) boundary conditions are taken for different values of x (the analogy of time).

Additional difficulties (possible incorrectness of problem) are generated by the fact that the sign of function $u(x,y)$ in equation (6) is not constant in each isolated subdomain. To avoid this difficulty the model of the boundary layer is made more precise. Instead of equation (1) we consider the equation

$$\rho\left(\tilde{u}\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y}\right) = \mu\frac{\partial^2 u}{\partial y^2}, \quad (x,y) \in \Omega_+ \cup \Omega_-, \qquad (7)$$

where

$$\tilde{u}(y,y) = \begin{cases} max\{u(x,y), 0\}, & (x,y) \in \Omega_+, \\ min\{u(x,y), 0\}, & (x,y) \in \Omega_-. \end{cases} \qquad (8)$$

Under conditions (8) the problem for equation (7) is correct.

2. Computing algorithm

The problem (2)-(8) is solved in dimensionless variables. Using for dimensionless variables the same notations as for dimensional variables we come to the system of equations

$$R(y)\left(\tilde{u}\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y}\right) = \frac{\partial^2 u}{\partial y^2}, \qquad (9)$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \quad 0 < x < 1, \quad -\infty < y < \infty \qquad (10)$$

where

$$R(y) = \begin{cases} 1, & y > 0, \\ \eta, & y < 0 \end{cases}$$

The system of equations (9), (10) is added by boundary conditions and conditions of conjugation:

$$[u] = 0, \quad \left[\frac{\partial u}{\partial y}\right] = 0, \tag{11}$$

$$v(x,0) = 0, \quad 0 < x < 1, \tag{12}$$

$$u(0,y) = 1, \quad y > 0, \tag{13}$$

$$u(1,y) = \vartheta, \quad y < 0. \tag{14}$$

The problems (9)-(14) are characterized by two dimensionless parameters:

$$\eta = \frac{\rho_- \mu_-}{\rho_+ \mu_+}, \quad \vartheta = \frac{U_-}{U_+}. \tag{15}$$

For the approximate solution of the problem, difference methods are used, especially the two-step iterative method [3] with external iterations on the non-linearity. Much attention was paid to the development of methods of linear problems solution. We have carried out methodological calculations on approximate simulation of some mass transfer processes in opposite current.

The numerical algorithms developed above are used for modelling of mass transfer in oposite currents. We consider here the problems with a given velocity fields. These problems can be solved by using the above mentioned numerical technique. Let the flow be a shear one, e.g. only the velocity component along axis x is different from zero. In this case mass transfer is governed by the following equation for concentration c(x,y):

$$R(y)\ u(y)\ \frac{\partial c}{\partial x} = \frac{\partial^2 c}{\partial y^2}, \quad -1<y<1. \tag{16}$$

The linear profile of velocity component u(y) is used in the numerical experiment. The boundary conditions for concentration c are constant contamination for $y>0$ ($c(0,y)=c(x,1)=1$) and zero contamination for $y<0$ ($c(1,y)=c(x,-1)=0$).

The curves of equal concentration in the case when $\eta=1$ are shown in Fig.1. The dependence on the concentration field of velocity difference η is illustrated by Fig.2 and Fig.3, where the same curves are shown in cases $\eta=2$ and $\eta=4$, respectively.

Reference

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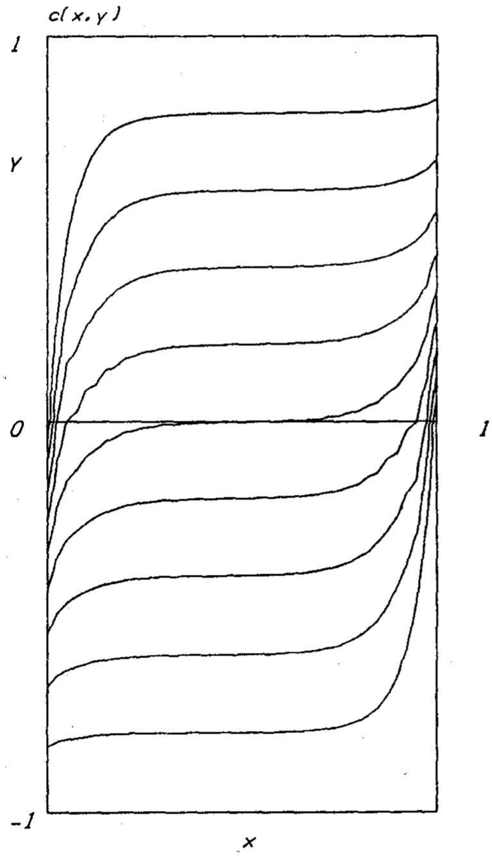

Fig.1

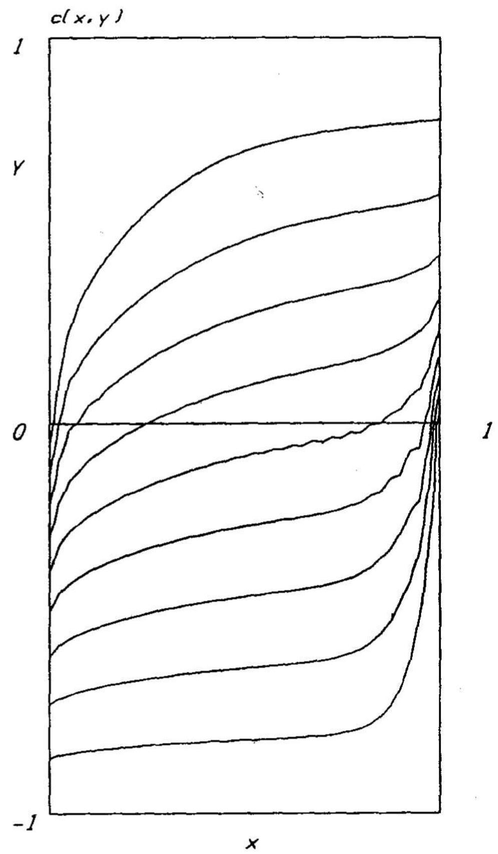

Fig.2

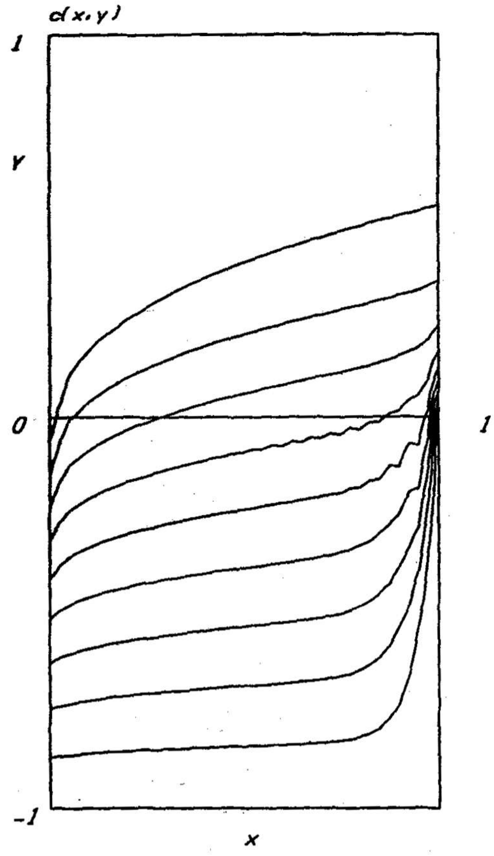

Fig.3