Identification of Parameters of Mathematical Model Non-Isothermal Processes of Adsorption Surface-Active Substances in a Porous Medium Oil-Bearing Rock

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***Abstract*— In this paper we present the results of the identification of parameters of the mathematical model of non-isothermal adsorption of surfactants at the oil-bearing rocks of the porous medium. Developed the method to calculate the diffusion and kinetic coefficients of the models. The empirical formula for these coefficients is obtained in the form of polynomials.**

***Keywords*— identificationt; mathematical model; surface-active substance; effective diffusion coefficient; kinetic coefficient**

I. INTODUCTION

Many problems associated with the use of surface-active agents (surfactants) in oil, are still poorly studied. These include flood control operation of reservoir surfactant solutions, taking into account changes in temperature, which strongly depends on the complex approach to the modeling process. Under the integrated approach means a series of experimental and theoretical studies to develop optimal engineering and economic advice with respect to the specific conditions of the deposit. Solving these problems is impossible without mathematical modeling process.

It is known that temperature strongly influences the adsorption processes. Even a slight change in its effect on the further course of the absorption. Mathematical modeling of adsorption processes without the influence of temperature on the process leads to a large deviation from the theoretical results of the experimental data.

One of the difficulties of a mathematical model of non-isothermal adsorption of surfactant is to determine the adsorption and diffusion parameters of the model equations. These options allow you to select an effective mode of filtration of the solution, set the speed of the front points of the concentration of adsorption, control longitudinal and temporal distribution of the concentrations of surfactants on the solid and the mobile phase reservoir, depending on the initial concentration and solution flow rate.

Note that in many studies by the authors in describing the adsorption-diffusion process parameters such as the effective coefficient of kinetic, or given, or determined under static conditions using traditional methods.

II. METHOD FOR SOLVING

It follows that to study the regularities of the influence of temperature on adsorption and diffusion processes, the determination of their parameters is very important and has great practical and scientific importance. Consequently, it is necessary to determine the effective diffusion and the kinetic coefficients, which depends not only on the concentration of the target component, but also on the tem-perature, which significantly complicates the mathematical description of this process, and often makes it impossible to obtain analytical solutions. Therefore necessary to develop numerical methods for the determination of these parameters.

In this paper we present a method for determining the parameters of the equations of the mathematical model of non-isothermal adsorption of surfactant - oil soap from the aqueous solution in the oil sands using experimental data.

The essence of the method consists of the fact that the problem is reduced to the solution of several problems for the isothermal case. To solve these problems based functional residual with the appropriate choice of objective function and sought its extreme. And then using the solutions obtained by the method of least squares determined empirical formulas for the coefficients of the variables and the kinetics of diffusion in the form of polynomials depending on the concentration and temperature of the adsorptive layer.

The necessary experimental parameters - the equilibrium, kinetic and output data at different temperatures are calculated on the basis of experimental data at one temperature. Using the experimental parameters obtained at a temperature of 22^0C, the data calculated for other temperatures - 30, 35, 40 and 50^0C [1].

Analysis of experimental data in the field of surfactant adsorption on quartz and the oil sands has shown that they are best described by a model of non-equilibrium dynamics of adsorption on a fixed bed of adsorbent, which includes differential equation of material balance of the adsorbed substance in the one-dimensional movement of the solution in the porous medium, the equations of the kinetics and equilibrium adsorption. It takes into account that the coefficient of the kinetics and effective diffusion coefficient in a porous medium depends on the concentration of the target component and the temperature stratum. In the particular case, if you do not take into account the thermal diffusion, the resulting model equations are as follows:

material balance equation

$$m\frac{\partial C}{\partial t}+m\upsilon\frac{\partial C}{\partial x}+(1-m)\frac{\partial a}{\partial t}=m\frac{\partial}{\partial x}\left[D_E(C,T)\frac{\partial C}{\partial x}\right] \quad ,(1)$$

the equation of kinetics and equilibrium adsorption

$$\frac{1-m}{m}\frac{\partial a}{\partial t}=\beta(C,T)\cdot\left[C-\varphi(a_{eq},T)\right] \quad , \quad (2)$$

$$C_{eq}=\varphi(a_{eq},T) \quad , \quad (3)$$

where C, a; C_{eq}, a_{eq} are non-equilibrium and equilibrium concentration adsorptive and the adsorbate, respectively; υ - linear velocity of the flow of surfactant solution, injected into the reservoir; m - porosity of the reservoir; $\beta(C,T)$ is the kinetic coefficient; $D_E(C,T)$ is the effective diffusion coefficient; T is temperature; t is time; x is coordinate of the height of the adsorbent layer; φ is a function of adsorption equilibrium, which also depends the temperature, since the process non-isothermal.

In the scheme of the experiment carried out the initial and boundary conditions for each fixed value of temperature, have the form:

$$C(0,t) = C_0 \ ; \quad a(x,0) = 0 \ ; \ C(x,0) = 0 \ ; \quad (4)$$

$$C(L,t) = C^{exp}(t); \quad \left.\frac{\partial C}{\partial x}\right|_{x=L}=0 \quad , \quad (5)$$

where C_0 - initial concentration of the adsorptive at the inlet of the adsorber; $C^{exp}(t)$ - the concentration of oil soap in the solution at the outlet of the adsorbent layer.

At each temperature the problem of determining the effective diffusion coefficient and the kinetic coefficient of adsorption is reduced to solving a system of differential equations (1) - (5).

In view of the nonlinear differential equations (1) - (5) to obtain an exact analytical solution is impossible. Therefore, for each value of the temperature problem is solved numerically by the grid method [2].

The problem of determining D (C) and β (C) is reduced to minimize functional [3]

$$I(D,\beta)=\int_0^T\left[C(L,t)-C^{\exp}(t)\right]^2 dt \quad , \quad (6)$$

where $C(L, t)$ is determined from the solution of (1) - (5).

III. The Results

By specifying the desired functions as polynomials

$$\beta(C)=\sum_{i=0}^{n}b_iC^i \quad , \quad D_E(C)=\sum_{k=0}^{n}d_kC^k \qquad (7)$$

problem of determining these functions is converted to the definition of constant coefficients b_i, d_k.

Minimization of the functional $I\ (D,\ \beta)$ is a method of descent [4].

Difference analog of the original system (1) - (5) is solved by the sweep method. The integral (6) is calculated by a trapezoid.

In the scheme, a program set forth in the language Fortran-IV. Based on the experimental and calculated (by the above method) data for SAW brand "oil soap" made program for the calculations.

For the numerical solution of the problem is written to the difference analogue of choosing a uniform in x and nerovnomerny in t steps. The choice of non-uniform step in t is associated with the experimental data, each temporary layer is selected in accordance with measurements made on an experimental setup.

Calculations were performed at the following temperatures - 22, 30, 35, 40 and 50 ^{0}C.

To obtain the dependence of β and DE on the concentration and temperature in an explicit form using the method of least squares. The functions $\beta\ (C,\ T)$ and $D_E\ (C,\ T)$ are given in the form of polynomials

$$\beta(C,E)=\sum_{i=0}^{n}\sum_{j=0}^{m}b_{i+j}C^iT^j \quad , \quad D_E(C,T)=\sum_{k=0}^{n}\sum_{l=0}^{m}d_{k+l}C^kT^l$$

With the obtained values of β and D_E at different temperatures and concentrations are the polynomial constant coefficients determined by the method of least squares.

As a result of numerical calculations for the required functions, the following empirical formula is obtained:

$D_E\ (C,T) = 0.3163+0.000182\bullet C^2-0.0322\bullet T + 0.00189\bullet C\bullet T +0.0002\bullet C^3+0.008\bullet T^2$

$\beta\ (C,T) = 0.1446\bullet 10^{-3} - 0.4\bullet 10^{-5}\bullet T - 0.664\bullet 10^{-8}\bullet C\bullet T - 0.6794\bullet 10^{-7}\bullet C^2 + 0.2373\bullet 10^{-10}\bullet C^2\bullet T^2$

The developed method is the calculation of a general nature and is justified for the class of surfactants. Similar results are obtained for the surfactant mark "sulfanol."

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