MODELING OF UNDERGROUND
DISPOSAL OF LIQUID WASTES

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We consider a mathematical model of injection of a pollutant-containing solution into a stratum covered with a weakly penetrable clayey layer (water-confining stratum). The novelty of the statement of the problem lies in taking account of the linear action of pollutants on the buffer (protective) capabilities of the swelling clayey layer covering the stratum.

Introduction. Pleshchinskii et al. proposed a model of the rheological properties of porous media with a swelling skeleton and a model of the nonlinear effects of yield of water of the swelling clayey layer in pumping water out of the underlying stratum. Examples of swelling media in nature include, in particular, clayey rocks, which often play the role of weakly penetrable barriers (water-confining strata) between aquifers. The isolating (buffer) properties of water-confining strata have to be properly taken into account in calculating the characteristics of the underground disposal of liquid wastes (polluted solutions). In so doing, the basic requirement is the exclusion of ingress of pollutants from the stratum chosen for disposal into adjacent aquifers to prevent subsequent migration of pollutants in them. It is clear that the requirement of absolute isolation of the water-confining stratum is impracticable. Therefore, one has to calculate the process of penetration of the injected solution impurity through the clayey layer (water-confining stratum) into its adjoining aquifer to forecast the effective isolation of pollutants. The simplest approach to the description of the buffer properties of the water-confining stratum is to treat it as a binary medium (one system of pores, usually called cracks, is highly penetrable, and the second one, usually called blocks, is weakly penetrable). In so doing, the equation of impurity transport in such a medium without taking into account the diffusion (hydrodispersion) is described by the equations [3]

$$m_1 \frac{\partial C_1}{\partial t} + \mathbf{q}\nabla C_1 + \gamma(C_1 - C_2) = 0, \quad m_2 \frac{\partial C_2}{\partial t} = \gamma(C_1 - C_2). \tag{1}$$

Obviously, the assumption that the mass transfer between cracks and blocks is fast (the condition $\gamma \to \infty$ corresponds to this) leads to the equality $C_1 = C_2$. Then the first equation of system (1) reduces to the following equation:

$$(m_1 + m_2)\frac{\partial C_1}{\partial t} + \mathbf{q}\nabla C_1 = 0, \tag{2}$$

which describes the propagation of the retarded impurity (pollutant) front in a porous medium (effect of retardation of pollution by a biporous medium).

In the case where the impurity is sorbed by the solid phase, for the equilibrium sorption corresponding to the Henry isotherm with a distribution coefficient Ω we have the equation [3]

$$m\frac{\partial C}{\partial t} + \mathbf{q}\nabla C + \Omega \frac{\partial C}{\partial t} = 0. \tag{3}$$

It is mathematically equivalent to Eq. (2). Therefore, in hydroecology the coefficients of equilibrium adsorption (distribution coefficients) and absorption of impurity by the micropores of weakly penetrable blocks are often "identified"

and the so-called retardation factor $R_{\rm m} = m_1 + m_2$ or $R_{\rm m} = \Omega + m$ is introduced. Sometimes the retardation factor is introduced as follows: $m_1 + m_2 = m_1(1 + R')$, $R' = m_2/m_1$ (or $R' = \Omega/m$). In practice, it is difficult indeed to distinguish between the cases of true adsorption and absorption of impurity by the micropores of weakly penetrable blocks or aggregates. The most typical example of such a medium is clayey rocks characterized by an especially large specific fraction of micropores [4]. In other words, for clays with $m_2 \gg m_1$.

We shall further proceed from the fact that in clays only impurity (pollutant) absorption by the micropores takes place, and, due to this, effective retardation of the penetration of the impurity through the clayey layer (isolating, or buffer, effect of water-confining strata) occurs. However, unlike the simple biporous medium, the impurity absorption by weakly penetrable blocks of a clayey rock obeys a nonlinear equation [1, 4]; therefore, the application of formulas of the type (2) or (3) will lead to a considerable error. To calculate the quantity of impurity retarded by blocks, let us use the corresponding relations from [1]. They are actually equivalent to the equation of nonlinear adsorption. The latter, as is known [3], leads to a smearing of the concentration fronts, as does the diffusion or hydrodispersion. Therefore, in order to investigate the contribution of the nonlinear absorption of the impurity by the micropores of blocks of a clayey rock to the buffer properties of the water-confining stratum independent of the diffusion smearing, we shall use the so-called diffusion-free approximation, i.e., assume that the diffusion coefficient (hydrodispersion) in the mass-transfer equation is equal to zero.

Of fundamental importance in describing the isolating (buffer) properties of clayey water-confining strata is the application of a theory that permits using both mechanical and physicochemical parameters of the clay. Moreover, it is necessary to take into account the influence of the swelling effects of clayey minerals on the ability of the solution to penetrate through the rock. The proposed models and their solutions [1, 2] make it possible to effectively realize the above-stated problems. It should be noted, however, that in this case two new unknowns appear: the impurity concentration of the polluting component in the water stratum and in the clayey layer. Thus, it is required to complement the system of equations describing the clayey layer and the water stratum in order to close it for a larger number of unknowns. Apparently, it is necessary to determine the impurity concentration in the water stratum and in the clayey layer. It is necessary to note that all designations of the quantities were taken by us from [1, 2], and the new ones were introduced so that the logical interrelation with the "old" designations is preserved.

Equation for the Impurity Concentration in the Clayey Layer. We shall describe the mass transfer in the clayey layer in the approximation of a biporous medium [3]. Let us write the mass-balance equation for the impurity density in the clayey layer. We assume that the value of the relative volume of transport (highly penetrable) pores in the clayey layer $m_{\rm c}$ is negligibly small, so the volume properties of the clay are determined by the volume of blocks. Thus, we can write

$$\frac{\partial (q_{\rm c} C)}{\partial z} + \frac{\partial (m_{\rm c.b} C_{\rm c.b})}{\partial t} = 0 \ . \tag{4}$$

For the cations and anions of a pore solution in clayey blocks, the equation [1, 4]

$$\overline{C}_1 = \frac{e'}{2} + \sqrt{\frac{e'^2}{4} + C^2} \ , \quad \overline{C}_2 = -\frac{e'}{2} + \sqrt{\frac{e'^2}{4} + C^2} \ , \tag{5}$$

where $e' = 2\pi/RT$; $\pi = eRT/2(V_0 - V_{\rm s})$, was obtained earlier. Observing that $C_{\rm c.b} = \overline{C}_1 + \overline{C}_2$, we have for the solution concentration in the clayey layer

$$\frac{\partial (q_{\rm c} C)}{\partial z} + \frac{\partial}{\partial t}\left[\left(1 - \frac{V_{\rm s}}{V_0}\right)\sqrt{(e')^2 + 4C^2}\right] = 0 \ . \tag{6}$$

Equation for the Impurity Concentration in the Stratum. As for the clayey layer, for the stratum it is required to introduce one more equation for determining the new unknown quantity — the impurity concentration in the filtering solution. Let us write the equation of impurity-concentration transfer in the stratum

$$m_a \frac{\partial c_w}{\partial t} + \operatorname{div}(\mathbf{q} c_w) = 0 , \tag{7}$$

which in the radial coordinate system has the form

$$m_a \frac{\partial c_w}{\partial t} + \frac{\partial}{\partial z}(q_z c_w) + \frac{1}{r} \frac{\partial}{\partial r}(r q_r c_w) = 0 .$$

Averaging this equation over z and taking into account that $q_r = -\dfrac{k_a}{\eta} \dfrac{\partial p}{\partial r}$ and $q_z(z_0, t) = -\dfrac{k_c}{\eta} \dfrac{\partial w}{\partial z}(0, t)$, we get

$$m_a \frac{\partial c_w}{\partial t} - \frac{k_a}{\eta} \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial p}{\partial r} c_w \right) = c_w \frac{k_c}{H\eta} \frac{\partial w}{\partial z} . \tag{8}$$

Dimensionless System of Equations for the Clayey Layer. Taking into account the previous results, let us write the dimensionless equations of the process for the clayey layer. We assume that the initial value of the concentration in the stratum is known to us and is equal at all points of the stratum. Denoting $\delta_1 = V_0^0/V_s$, $\delta_2 = eRT/(2\Gamma V_s)$, $\delta_3 = c_0 RT/\Gamma$, and $\bar{c}_c = C/c_0$, we write

$$\bar{\sigma} + \bar{w} = 1 ; \tag{9}$$

$$\frac{\partial \theta}{\partial \tau} + \frac{\partial \bar{q}_c}{\partial z} = 0 ; \tag{10}$$

$$\bar{q}_c = -\frac{\partial \bar{w}}{\partial z} ; \tag{11}$$

$$f = V_s (\delta_1 \exp \theta - 1) , \quad V_0^{(0)} = 1 , \quad V_s = \frac{2}{3} ; \tag{12}$$

$$\bar{\pi} = \frac{\delta_2}{\delta_1 \exp \theta - 1} , \quad \delta_2 \approx 2 ; \tag{13}$$

$$\frac{\partial f}{\partial \tau} = \bar{\alpha} (\bar{\Pi} - \bar{\sigma}) , \quad \bar{\alpha} = T_0 \alpha \Gamma ; \tag{14}$$

$$\bar{\Pi} = \sqrt{4\bar{\pi}^2 + \delta_3^2 \bar{c}_c^2} - \delta_3 \bar{c}_3 ; \tag{15}$$

$$\frac{\partial (\bar{q}_c \bar{c}_c)}{\partial z} + \frac{\partial}{\partial \tau} \left[\left(1 - \frac{1}{\delta_1 \exp \theta} \right) \sqrt{\frac{4\bar{\pi}^2}{\delta_3^2} + 4\bar{c}_c^2} \right] = 0 . \tag{16}$$

The initial conditions are

$$\bar{w}(\bar{z}, \bar{r}, 0) = \bar{p}(\bar{r}, 0) , \quad \bar{c}_c = 0 ; \tag{17}$$
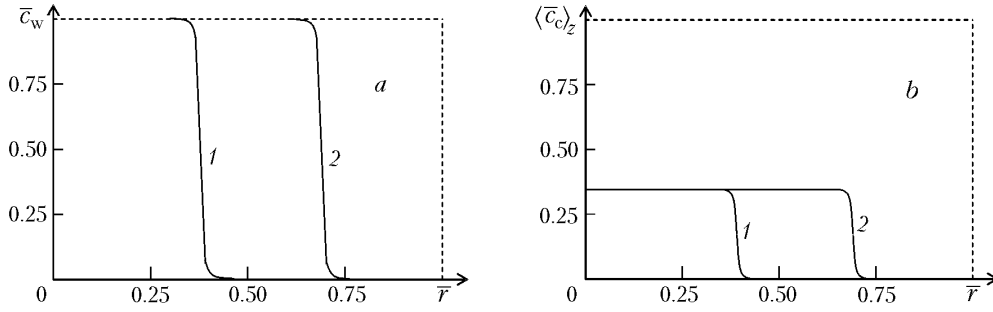
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Fig. 1. Impurity concentration in the stratum (a) and in the clay (b) versus the distance to the borehole: 1) concentration profile for $\tau = 0.5\tau_{st}$; 2) same, $\tau = \tau_{st}$.

and the boundary conditions are

$$\overline{c}_c\,(0,\tau) = \overline{c}_w\,, \quad \overline{w}\,(0,\tau) = \overline{p}\,, \quad \overline{w}\,(1,\tau) = \delta_4\,. \tag{18}$$

Dimensionless System of Equations for the Stratum. Now it is necessary to obtain the dimensionless form of the mass-transfer equations in the stratum. The initial value of the concentration at the stratum inlet is c_0. Denoting $\overline{c}_w = c_w/c_0$, we have from (8)

$$m_a\frac{\partial c_w}{\partial t} = \frac{k_a z_0 \Gamma}{\eta U r_\infty^2}\frac{1}{\overline{r}}\frac{\partial}{\partial \overline{r}}\left(\overline{r}\frac{\partial \overline{p}}{\partial \overline{r}}\,\overline{c}_w\right) = \overline{c}_w\frac{k_c \Gamma}{H\eta U}\frac{\partial \overline{w}}{\partial \overline{z}}\,.$$

Introducing the quantities $E = \dfrac{k_a z_0 \Gamma}{\eta U r_\infty^2} \approx 10^{-2}$ and $F = \dfrac{k_c \Gamma}{H\eta U} = \dfrac{k_c \Gamma \rho_w g}{H\eta U\rho_w g} = \dfrac{K\Gamma}{HU\rho_w g} \approx 1$, we write, with account for the designations of [2], the system of mass-transfer equations for the stratum

$$\overline{A}\frac{1}{\overline{r}}\frac{\partial}{\partial \overline{r}}\left(\overline{r}\frac{\partial \overline{p}}{\partial \overline{r}}\right) + \frac{\partial \overline{w}}{\partial \overline{z}} = 0\,, \quad \overline{A} = 10^{-1}\,; \tag{19}$$

$$m_a\frac{\partial \overline{c}_w}{\partial t} - E\frac{1}{\overline{r}}\frac{\partial}{\partial \overline{r}}\left(\overline{r}\frac{\partial \overline{p}}{\partial \overline{r}}\,\overline{c}_w\right) = \overline{c}_w F\frac{\partial \overline{w}}{\partial \overline{z}}\,. \tag{20}$$

The initial conditions are

$$\overline{c}_w\,(\overline{r},0) = 0\,, \quad \overline{p}\,(\overline{r},0) = \delta_5 + \left(\frac{p_b}{\Gamma} - \delta_5\right)\exp\left(-\frac{\overline{r}-\varepsilon}{\varepsilon}\right),\quad \varepsilon = \frac{r_b}{r_\infty}\,,\quad \delta_5 = \frac{p_\infty}{\Gamma}\,.$$

The boundary conditions of the first kind are

$$\overline{c}_w\,(\varepsilon,\tau) = 1\,, \quad \overline{p}\,(\varepsilon,\tau) = \frac{p_b}{\Gamma}\,, \quad \overline{p}\,(1,\tau) = \delta_5\,,$$

and of the second kind

$$\overline{c}_w\,(\varepsilon,\tau) = 1\,, \quad q_r\,(\varepsilon,\tau) = \text{const}\,, \quad \overline{p}\,(1,\tau) = \delta_5\,.$$

Results and Discussion. The problem has been solved numerically with the use of the same difference scheme as in [2]. One of the specific features of the process is the radial distribution of the impurity concentration in the stratum and in the clay. While in the first case the radial distribution plot of the impurity concentration in the stra-

tum has a rather traditional form (see Fig. 1a), in the second case it is unusual (Fig. 1b). The mean value of the impurity concentration in the clay layer is always lower than the stratum values. This is due to the nonlinear relations (5) for the impurity absorption by clay micropores and is not an averaging artefact. Another feature of the process showed up as different shrinkage values of the clay with and without account for the swelling effect ($\delta_2 = 0$ or $\delta_2 \neq 0$ respectively). For instance, with account for the swelling effect the shrinkage value of the layer is smaller than in the absence of the action of the swelling forces at equal rates of impregnation of the clayey layer with the polluted solution. Thus, the injection of polluted solutions into the stratum affects, in the first place, the deformation of the separating clayey layer rather than the dynamics of penetration of the solution through the clay. Actually, this effect is quite clear. Shrinkage in our model is realized by forcing out water from the clayey blocks. The osmotic pressure impedes the forcing out of water, which just shows up as smaller shrinkage values of the clayey layer.

Conclusions. The solution of the problem on the underground disposal of liquid pollutants with account for the features of the swelling and deformation of the higher-lying isolating clayey layer has shown that how the process proceeds strongly depends on the physical characteristics of the layer being deformed. Since the swelling clayey layer "resists" shrinkage, its value decreases as the pollutant passes through this layer. The high shrinkage values may cause crack extension in the clayey layer. Consequently, we can speak of preferable conditions for disposal of liquid wastes in strata isolated from the other ones by clayey rocks with swelling mineral phases present in them.

NOTATION

$\bar{A}$, dimensionless complex; C, solution concentration in a highly penetrable system of pores (cracks) of clay; $C_{c.b}$, solution concentration in weakly penetrable clayey blocks; $\bar{c}_c$, dimensionless concentration of solution in a highly penetrable system of pores (cracks) of clay; c_w, solution concentration in the stratum; $\langle \bar{c}_c \rangle_z$, layer-height-averaged dimensionless solution concentration in a highly penetrable system of pores (cracks) of clay; $\bar{c}_w$, dimensionless solution concentration in the stratum; c_0, concentration of the solution injected into the stratum; C_1 and C_2, solution concentrations, respectively, in highly and scarcely penetrable zones in a biporous medium; $\bar{C}_1$, cation concentration in clay; $\bar{C}_2$, anion concentration in clay; E, F, dimensionless complexes; e, content of cations-compensators of the clayey particle charge in volume $V_0^{(0)}$; e', specific exchange capacity of clay; f, content of bound water in volume V_0; g, gravitational acceleration; H, aquifer power; k_a, penetrability of the aquifer; k_c, penetrability of the clayey layer; K, filtration factor in the stratum, m/day; m, medium porosity; m_a, aquifer porosity; m_c, porosity of cracks in the clay; $m_{c.b}$, porosity of clayey blocks; m_1 and m_2, porosity of highly and poorly penetrable zones in a biporous medium; p, pressure in the aquifer; p_b, pressure in the borehole; p_∞, pressure on the feed contour; $\mathbf{q}$, vector of the speed of filtration in the stratum; q_c, speed of filtration in the clayey layer; q_r and q_z, radial and vertical components of the speed of filtration in the aquifer; R, universal gas constant; $R_m(R')$, retardation factor; r, radius; r_b, borehole radius; r_∞, contour radius; T, temperature; t, time; T_0, characteristic time of the process; U, characteristic speed of filtration in the stratum; V_0, representative volume of the medium; $V_0^{(0)}$, initial value of the representative volume of the medium; V_s, volume of the solid phase in the V_0 composition; w, pressure in the clayey layer; z, vertical coordinate; z_0, clay-layer thickness; α, constant of mass transfer (absorption rate of water by clay blocks) in swelling; δ_i ($i = 1, 2, 3, 4, 5$), dimensionless complexes; Γ, rock pressure; γ, constant of mass transfer of blocks and cracks in a biporous medium; ε, ratio r_b/r_∞ (dimensionless size of the borehole); η, water viscosity; θ, shrinkage; ρ_w, water density; π and Π, osmotic pressure for zero and nonzero impurity concentration; $\bar{\sigma}$, normalized (dimensionless) effective tension; τ, dimensionless time; τ_{st}, time of going to the stationary stage; Ω, Henry adsorption constant (distribution coefficient). Subscripts: 0, characteristic scale; 1, parameters of the highly penetrable porous medium (cracks); 2, parameters of the poorly penetrable porous medium (porous blocks); a, aquifer; b, borehole; c, clay; c.b, clayey blocks; ∞, feed contour; m, entire medium; r, radial component of the speed of filtration in the aquifer; z, vertical component of the speed of filtration in the aquifer; s, solid phase; st, stationary stage of the process; w, water; overscribed bar, dimensionless quantity (except for the concentrations of ions and anions in the clay); angle brackets, averaging over the layer height.

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