About Two-dimensional Mathematical Model of Contaminant Migration in Unsaturated Catalytic Porous Media with Traps

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Abstract—This paper proposes an approach for the computer simulation of complex physical problem of contaminant migration through unsaturated catalytic porous media to the filter-trap. The corresponding mathematical model in the two-dimensional nonlinear case is presented. The model includes detailed considerations of the moisture transfer of saline solutions under the generalized Darcy’s and Cluta’s laws in different subregions of soil. The numerical solution of the boundary value problem was found by the finite difference method and proposed the algorithm for computer implementation. The proposed algorithm may be used for creating software with effective risk assessment strategies and predicting the cleaning and further useful use of the soil massifs.

Keywords—mathematical model; computer modelling; moisture transfer; boundary-value problem; numerical method; refinement; NanoSurface

I. INTRODUCTION

Contaminant sources occur in soil, from which the chemicals then migrate to air, surface water, and groundwater [1]. Predicting the movement of contaminants through porous media requires addressing the fate and transport processes that predominate in each sub medium and integrating the interactions between the media. This is a quite complicated problem [2–6].

In previous works, we investigated similar physical problems for saturated media [7, 8]. Therefore, in the zone of suspended water different processes became commensurate (e.g. the convective term and diffusion are almost identical due to the low velocity of moisture transfer). This fact opens a widespread use of colloid adsorbents in purification processes [9, 10]. Thus, the next mathematical model is presented for the first time and take into account a wide range of factors.

II. FORMULATION OF THE PROBLEM

The filter-trap located at a depth $CD$ of the soil. The pore spaces between the soil grain particles are partially filled with water and partially with air (zone of suspended water). There are dozens of colloid adsorbents with radius $R$ (micro or nanoparticles) in the layer of soil. Therefore, they may be used in for cleaning purposes as well. There is a piezometric pressure on the upper and filter-trap surfaces $H_1$ and $H_2$ ($H_1 > H_2$), respectively. The contaminants concentrations at the initial time $t = 0$: $\bar{C}^0_i(x, y)$ (for a saline solution in soil pore network, $>300 \mu m$ [11]), $\bar{C}^0_i(x, y)$ (soil surfaces hold water in soils and prevent rapid movement in smaller pores, thus the contaminant are held on the surface of the ground skeleton), $\bar{C}^0_i(x, y)$ (for contaminant located in the soil skeleton, the importance of such factor was presented in [12]), and $\bar{Q}^0(x, y, r)$ (for contaminant inside microparticles with radius $R$ [13]) are known.
The soil concentrations $\tilde{C}_1(t)$, $\tilde{C}_2(t)$ and $\tilde{C}_3(t)$ on the upper surface and $\tilde{C}_1(t), \tilde{C}_2(t), \tilde{C}_3(t)$ for the filter-traps are also known.

It is necessary to find out the $c_1(x, y, t)$, $c_2(x, y, t)$, $c_3(x, y, t)$ and $q(x, y, r, t)$ concentrations distribution over the soil.

### III. MATHEMATICAL MODEL

Due to the symmetry of the filtration picture a fragment of AB, B, BCD filtration area is considered. Therefore, the boundary value problem of the contaminant transport in a porous medium in a two-dimensional nonlinear case was solved using a mathematical model with the following equations [7, 14, 15]:

$$\frac{\partial}{\partial t} \left( D_1(c_1) \frac{\partial c_1}{\partial x} \right) + \frac{\partial}{\partial y} \left( D_1(c_1) \frac{\partial c_1}{\partial y} \right) = -\nu_1 \frac{\partial c_1}{\partial x} - \nu_2 \frac{\partial c_1}{\partial y} - \gamma_1 c_1 + \gamma_2 c_2 = \delta(0c_1),$$

$$\frac{\partial}{\partial t} \left( D_2(c_2) \frac{\partial c_2}{\partial x} \right) + \frac{\partial}{\partial y} \left( D_2(c_2) \frac{\partial c_2}{\partial y} \right) + \gamma_2 c_2 = \frac{\partial c_2}{\partial t},$$

$$\mu \frac{\partial h}{\partial t} = \frac{\partial}{\partial x} \left( K(h, c_1) \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( K(h, c_1) \frac{\partial h}{\partial y} \right) - \frac{\partial}{\partial x} \left( v_1 \frac{\partial c_1}{\partial x} \right) - \frac{\partial}{\partial y} \left( v_2 \frac{\partial c_1}{\partial y} \right) + f,$$

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 D_3(q) \frac{\partial q}{\partial r} \right) = \frac{\partial q}{\partial t},$$

$$u_x = -K(h, c_1) \frac{\partial h}{\partial x} + \nu_1 \frac{\partial c_1}{\partial x}, u_y = -K(h, c_1) \frac{\partial h}{\partial y} + \nu_2 \frac{\partial c_1}{\partial y},$$

$$\frac{\partial c_1}{\partial x} + \frac{\partial c_2}{\partial y} = 0,$$

$$q(x, r, t) \bigg|_{r=0} = \frac{k_f c_1(x, t)}{1 + \eta c_2(x, t)},$$

$$\frac{\partial h}{\partial n} \bigg|_{AB \cup B \cup BCD} = 0, \quad h_{ib} = H_1, \quad h_{AB \cup EF \cup FD} = H_2,$$

$$l_{c_1}|_{AB} = \tilde{C}_1(t), \quad l_{c_2}|_{AB} = \tilde{C}_2(t), \quad l_{c_3}|_{AB} = \tilde{C}_3(t).$$

The equations above describe the following transport mechanisms of contaminant with concentration: (1) $c_1$ in a convectively mobile pore solution; (2) $c_2$ in the water bound with the soil skeleton taking into account the intra-particle diffusion; (3) $c_3$ in the soil skeleton. Equation (4) describes moisture transfer; (5) the intra-particle transport mechanisms of contaminant with concentration $q$ [13, 16]; (6) the generalized equation of the Darcy-Cluta law in the two-dimensional case for moisture transfer of the salt solutions [17]; (7) the adsorption isotherm; (8) boundary conditions for piezometric head $h(x, t)$; (9)-(12) boundary conditions for concentrations $c_1(x, t)$, $c_2(x, t)$, and $c_3(x, t)$; (13) boundary conditions for intra-particle concentrations $q(x, y, r, t)$.

Transfer of contaminant dissolved in water (saline solution) by filtration flow occurs under the influence of the pressure gradients and the concentration of salts. The moisture and mass transfer of saline solutions occurs under the generalized Darcy’s and Cluta’s laws.

The boundary value problem (1)-(13) is set correctly (or correctly posed), because the conditions of existence and uniqueness of its solution are fulfilled [18].

### IV. NUMERICAL SOLUTION OF BOUNDARY VALUE PROBLEM

The computational mesh $0_{th,1,12,32,10}$ was built for finite-difference approximation with steps $h_1$, $h_2$, $h_3$ and $r$ by $Ox$-axis, $Oy$-axis, $Oz$-axis and Ot-axis for $x$, $y$, $r$, $t$ variables respectively [19–21].
where \( n_1, n_2, n_3 \) are steps count.

Let us show the solution algorithm on the example of an equation (2). According to a locally one-dimensional method, we represent the differential equation (2) as a system of two one-dimensional equations with locally one-dimensional method [14]:

\[
D_2 \frac{\partial^2 c_1}{\partial x^2} + \frac{\gamma_1 c_1}{2} - \frac{\gamma_2 c_2}{2} = 0
\]

(14)

\[
D_2 \frac{\partial^2 c_2}{\partial x^2} + \frac{\gamma_1 c_1}{2} - \frac{\gamma_2 c_2}{2} = 0
\]

(15)

where \((x, y) \in \Omega, r \in (0, R), t > 0\).

Finite-difference analogues of equations (14), (15) are tacking the following form:

\[
f^{(k+0.5)}_{i,j} = \frac{e^{(k+0.5)}_{i,j} - e^{(k-0.5)}_{i,j}}{\tau} = D_2 \left( \frac{\partial^2 e^{(k+0.5)}_{i,j}}{\partial x^2} - \frac{\gamma_1 e^{(k+0.5)}_{i,j}}{2} + \frac{\gamma_2 e^{(k+0.5)}_{i,j}}{2} \right) + b_{i,j}.
\]

(16)

\[
f^{(k+1)}_{i,j} = \frac{e^{(k+1)}_{i,j} - e^{(k-1)}_{i,j}}{\tau} = D_2 \left( \frac{\partial^2 e^{(k+1)}_{i,j}}{\partial x^2} - \frac{\gamma_1 e^{(k+1)}_{i,j}}{2} + \frac{\gamma_2 e^{(k+1)}_{i,j}}{2} \right) + b_{i,j}.
\]

(17)

where \( i = 1, n_1 - 1, j = 1, n_2 - 1, k = 0, n_3 \).

To find the solution (16) by the Thomas method we present it in following general way:

\[
\begin{align*}
\alpha_{i,j}^2 &= e^{(k+0.5)}_{i,j} - e^{(k-0.5)}_{i,j} + \beta_{i,j} e^{(k+1)}_{i,j} - f^{(k+1)}_{i,j}, \\
\beta_{i,j} &= \frac{\gamma_2}{\gamma_1}, \\
\gamma_{i+1,j} &= \frac{\gamma_1}{2}, \\
\gamma_{i,j} &= \frac{\gamma_2}{2}, \\
\gamma_{i-1,j} &= \frac{\gamma_1}{2}, \\
\gamma_{i,j+1} &= \frac{\gamma_2}{2}, \\
\gamma_{i,j-1} &= \frac{\gamma_1}{2}.
\end{align*}
\]

where \( \gamma_{i,j} = \frac{\gamma_2}{2}, \beta_{i,j} = \frac{\gamma_1}{\gamma_2}, \)

Then the stability conditions of the Thomas method are fulfilled -

\[
\left| a_i^2 \right| > \left| b_i^2 \right| + \left| b_i^2 \right|.
\]

The concentration value \( c_2(x, y, t) \) at the time steps \((k+1)\) is calculated using the next ratio:

\[
c^{(k+1)}_{i,j} = c^{(k+1)}_{i,j} + f^{(k)}_{i,j} - f^{(k+1)}_{i,j},
\]

where \( c^{(k+1)}_{i,0} = 0, c^{(k+1)}_{i,n_3} = 0, \beta_{i,0} = \frac{\gamma_1}{\gamma_2}, \beta_{i,n_3} = \frac{\gamma_2}{\gamma_1}. \)

Let us write the next finite-difference equations for the initial condition as well as for boundary condition for \( c_2(x, y, t) \):

\[
\begin{align*}
c^{(0)}_{i,j} &= C_0 i,j, \\
c^{(k)}_{i,j} &= C_i^1 (i,j, k \tau),
\end{align*}
\]

where \( k = \frac{0,n_3}{2} \).
Thus, the all necessary mathematical manipulations were performed for programming language implementation of the Thomas algorithm for $c_t(x,y,t)$.

Similarly, we split the sub-boundary-value problems (1), (3), (4), (5) and (6) with corresponding boundary and initial conditions (7)-(12) into the systems of one-dimensional equations. Mathematical conversions for similar one-dimensional boundary-value problems are described in previous works [7, 22]. In computation algorithm we need to find out the piezometric head distribution $h(x,y,t)$ first, then the Darcy-Clute moisture velocity $u(x,y,t)$ and finally the distribution of concentrations $c_1(x,t)$, $c_2(x,t)$, $c_3(x,t)$ and $q(x,r,t)$ . Each Thomas algorithm calculations we perform at half time step $(k+0.5)$ at $Ox$-axis and then at time step $(k+1)$ at $Oy$-axis. This approach allows us to solve the entire solution in the two-dimensional case and implement the corresponding software algorithm.

V. CONCLUSIONS

Since the mathematical modelling using colloidal adsorbents to the purification processes is new, the importance of new mathematical models become obvious. The statement and the mathematical modelling of the new corresponding two-dimensional problem of contaminant migration in unsaturated porous media was formulated. The numerical solution of the boundary value problem was found by the finite difference method using locally one-dimensional Samarsky's method and monotonic difference schemes and a computation algorithm is proposed as well. The results might be used to build effective risk assessment strategies for cleaning and further useful use of the soil massifs.

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