Numerical solutions of the problem of salt-transfer in soils

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Abstract. Work is devoted to work out of effective numerical methods of the decision of problems of forecasting of mineralization of a soil solution taking into account of differential porosity and sorption and dissolution processes. The algorithm of the decision of a problem consists of the following sequence action. On time are used quadrature to the formula and regional problems with any boundary conditions dare a method of differential prorace. Testing of the program realising algorithm of the offered method of calculation it is carried out by the decision of the known problems, having practical application.

1 Introduction

For land reclamation, the further interest consider to the problems of predicting the salinity of a soil solution, taking into account differential porosity and sorption and dissolution processes. The salt solution in the soil is in two physical states: in the form of a solution firmly bound by molecular forces to the surfaces of the particles, and in the form of a free solution occupying the space inside the cavities of the pores. Among the mathematical models of soil-forming processes, salt-transfer models in the soil occupy an important place. The study of the migration of solutes in the ecological system "groundwater-soil" is one of the most important areas in modern soil science. It is a complex of scientific knowledge in mathematical physics, hydrodynamics, thermodynamics, physicochemical kinetics, molecular physics of dispersed systems, land reclamation, soil science, etc. Knowledge of the mechanism and patterns of transfer of solution substances makes it possible to develop effective measures to prevent soil salinization and desalinate saline lands for use in agriculture. This is due to the enormous theoretical and practical importance of the problem of soil salinity. In particular, mathematical models of salt transfer in soil can serve as a basis for solving the most important tasks of soil reclamation: determining the rate of washing of saline soils depending on the initial salt content, their composition, soil properties and hydrogeological conditions; identify the optimal level of groundwater, precluding soil salinization; calculating the maximum allowable salinity of irrigation water.

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2 Problem statement

It is known that for the simplest case of desalination of a soil-ground layer, the basic equation of motion of salts is [1,2]:

$$\frac{\partial C}{\partial t} = D^* \frac{\partial^2 C}{\partial x^2} - V \frac{\partial C}{\partial x} + \beta (C_n - C)$$  \hspace{1cm} (1)

where $C$ is the concentration of the soil solution, g/l; $t$ - time, day; $x$ - distance, m; $V = V_0/m$ - the actual speed of the movement of water in the pores of the soil, m / day; $V_0$ - filtration rate, m/day; $m$ - active porosity; $C_n$ - is the maximum saturation concentration, g/l; $\beta$ - dissolution coefficient, 1/day; $D^*$ is the coefficient of convective (filtration) diffusion, m²/day.

This equation assumes a linear (one-dimensional) movement of salts and water along the $x$ axis, a constant filtration rate $V_0 = \text{const}$ and independence of the dissolution rate of salts contained in the solid phase of the soil from their volume and surface. It follows from the equation that the change in salt concentration at a point in time is equal to the salt intake as a result of the difference in the concentration of the soil solution (diffusion term), salt transfer by moving water (convective term) and as a result of dissolution of the solid phase of salts and their intake into solution [3 - 5, 9, 10].

We consider equation (1) with initial

$$C = C_0 \text{ when } t = 0$$ \hspace{1cm} (2)

and boundary [6]

$$\begin{cases} 
VC - D^* \frac{\partial C}{\partial x} = VC_n \text{ when } x = 0 \\
\frac{\partial C}{\partial x} = 0 \text{ when } x = L
\end{cases}$$ \hspace{1cm} (3)

conditions.

3 Decision methods

The method of solving the problem (1) - (3) is based on the use of quadrature formulas in combination with the differential sweep method [8].

Entering in (1) - (3) the following dimensionless values

$$\bar{x} = \frac{x}{L}, \quad \bar{t} = \frac{D^*}{L^2} t, \quad \bar{C} = \frac{C}{C_n}, \quad \bar{C}_0 = \frac{C_0}{C_n}$$

and keeping thus former a designation and accepting

$$\mu_1 = -\frac{V L}{D^*}, \quad \mu_2 = \frac{\beta L^2}{D^*}, \quad \mu_3 = -\frac{D^*}{LV}$$

will get

$$\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial x^2} + \mu_1 \frac{\partial C}{\partial x} + \mu_2 (1 - C) \hspace{1cm} \text{ (4)}$$

$$C = C_0 \text{ when } t = 0$$
\[
\begin{aligned}
\mathcal{C} + \mu_3 \frac{\partial \mathcal{C}}{\partial x} &= 1 & \text{when} & \quad x = 0 \\
\frac{\partial \mathcal{C}}{\partial x} &= 0 & \text{when} & \quad x = 1 .
\end{aligned}
\]

Integrating equation (4) over time in the interval \([0, t]\) we have:
\[
\begin{aligned}
\mathcal{C}(x, t) - C_0 &= \int_{0}^{t} \frac{\partial^2 \mathcal{C}(x, \tau)}{\partial x^2} d\tau + \mu_3 \int_{0}^{t} \frac{\partial \mathcal{C}(x, \tau)}{\partial x} d\tau + \mu_2 t - \mu_2 \int_{0}^{t} \mathcal{C}(x, \tau) d\tau \\
\end{aligned}
\]

taking here
\[
\begin{aligned}
t_m &= (m - 1) \Delta t, \quad m = 1, 2, 3 ... 
\end{aligned}
\]
and using the quadrature formulas of a trapezoid [8] we have
\[
\begin{aligned}
C_m(x) - C_0 &= \sum_{i=1}^{m} A_i \frac{d^2 C_i(x)}{dx^2} + \mu_3 \sum_{i=1}^{m} A_i \frac{dC_i(x)}{dx} - \mu_2 \sum_{i=1}^{m} A_i C_i(x) + \mu_2 \cdot t_m
\end{aligned}
\]
or
\[
\begin{aligned}
C_m(x) - C_0 &= A_m \frac{d^2 C_m(x)}{dx^2} + A_m \frac{dC_m(x)}{dx} + A_m C_m(x) + \\
&+ \sum_{i=1}^{m-1} A_i \frac{d^2 C_i(x)}{dx^2} + \mu_3 \sum_{i=1}^{m} A_i \frac{dC_i(x)}{dx} - \mu_2 \sum_{i=1}^{m-1} A_i C_i(x) + \mu_2 \cdot t_m
\end{aligned}
\]
\[\text{(5)}\]
where \(\Delta t\) – time step, \(A_j = \Delta t, (j = 2, 3, ..., m - 1); \ A_1 = A_m = \frac{\Delta t}{2}\).

From the last expression you can get the following system of equations

After some transformations in (5), you can get the following system of equations
\[
\begin{aligned}
\frac{d^2 C_m(x)}{dx^2} + \mu_1 \cdot \frac{dC_m(x)}{dx} + b_m \cdot C_m(x) &= f_m(x)
\end{aligned}
\]
\[\text{(6)}\]
where
\[
\begin{aligned}
b_m &= -\frac{\mu_2 A_m + 1}{A_m} \\
f_m(x) &= \frac{1}{A_m} \left[ \mu_2 \sum_{i=1}^{m-1} A_i C_i - \sum_{i=1}^{m-1} A_i \frac{d^2 C_i}{dx^2} - \mu_1 \sum_{i=1}^{m-1} A_i \frac{dC_i}{dx} - C_0 - \mu_2 \cdot t_m \right]
\end{aligned}
\]

Equation (6) with boundary conditions
\[
\begin{aligned}
\frac{dC_m(x)}{dx} &= 1 & \text{when} & \quad x = 0 \\
\frac{dC_m(x)}{dx} &= 0 & \text{when} & \quad x = 1
\end{aligned}
\]
\[\text{(7)}\]
is solved by the differential sweep method [8], according to which the solution is sought in the form:
\[
\begin{aligned}
\alpha_m(x)C_m(x) + \beta_m(x)C_m(x) &= \gamma_m(x)
\end{aligned}
\]
\[\text{(8)}\]
where \(\alpha_m(x), \beta_m(x), \gamma_m(x)\) are the driving coefficients, which are found as a solution to the following Cauchy problem:
\[
\begin{aligned}
\alpha_m'(x) - \mu_1 \cdot \alpha_m(x) + \beta_m(x) &= 0 \\
\beta_m'(x) - b_m \cdot \alpha_m(x) &= 0 \\
\gamma_m(x) &= \alpha_m(x) \cdot f_m(x)
\end{aligned}
\]
\[
\begin{align*}
\alpha_m(0) &= \mu_3 \\
\beta_m(0) &= 1 \\
\gamma_m(0) &= 1
\end{align*}
\]

Taking in (8) \(x = 1\) and using the second condition (7), we have:

\[C_m(1) = \gamma_m(1)/\beta_m(1) \quad \text{and} \quad C'_m(1) = 0.\]

Solving equation (6) with the initial conditions (9), we find \(C_m(x)\) - the concentration of the soil solution.

The solution of the corresponding Cauchy problems can be carried out using the fourth order Runge – Kutta method [8,11].

4 Results

Based on the above algorithm, a program was compiled that is implemented as a standard program in the ABC Pascal algorithmic language. Testing of the program that implements the algorithm of the proposed calculation method was carried out when solving the following problem:

\[
\begin{align*}
\frac{\partial C}{\partial t} &= \frac{\partial^2 C}{\partial x^2} + \frac{\partial C}{\partial x} - 2C - x \cdot e^{-2t} \\
C &= 0.5x^2 - x + 2 \quad \text{when} \quad t = 0 \\
C + 2 \frac{dc}{dx} &= 0 \quad \text{when} \quad x = 0 \\
\frac{dC}{dx} &= 0 \quad \text{when} \quad x = 1
\end{align*}
\]

which has the exact solution:

\[C(x, t) = (0.5x^2 - x + 2) \cdot e^{-2t}.
\]

Table 1 shows the numerical values of the solutions obtained by the proposed method and is compared with the exact solution at different time intervals.

| \(x\) | \(t=1\) | \(t=2\) | \(t=3\) |
|-------|---------|---------|---------|
|       | Exact solution | Approached decision | Exact solution | Approached decision | Exact solution | Approached decision |
| 0     | 0.27067 | 0.27056 | 0.03663 | 0.03660 | 0.00496 | 0.00495 |
| 0.1   | 0.25781 | 0.25771 | 0.03489 | 0.03486 | 0.00472 | 0.00471 |
| 0.2   | 0.24631 | 0.24621 | 0.03333 | 0.03330 | 0.00451 | 0.00450 |
| 0.3   | 0.23616 | 0.23607 | 0.03196 | 0.03193 | 0.00433 | 0.00432 |
| 0.4   | 0.22736 | 0.22727 | 0.03077 | 0.03074 | 0.00416 | 0.00416 |
| 0.5   | 0.21992 | 0.21983 | 0.02976 | 0.02974 | 0.00403 | 0.00402 |
| 0.6   | 0.21383 | 0.21375 | 0.02894 | 0.02891 | 0.00392 | 0.00391 |
| 0.7   | 0.20909 | 0.20901 | 0.02830 | 0.02827 | 0.00383 | 0.00382 |
| 0.8   | 0.20571 | 0.20563 | 0.02784 | 0.02781 | 0.00377 | 0.00376 |
5 Conclusions

The received results shows high efficiency of a method of differential prorace of the decision of regional and initial-regional problems for the differential equations of the second order at performance of any linear boundary conditions. Thus factors of the resolving equations can be variables that is especially important at the decision of applied problems as problems of the forecast of water, thermal, salt modes and a problem by an estimation and updating of the various parametres entering into the equations.

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