One-Dimensional Numerical Modeling for Water Flow and Solute Transport in an Unsaturated Soil

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Abstract – A mathematical model that describes solute transport through the unsaturated soil, to prevent aquifer contamination is detailed in this paper. Indeed, this problem is the result of the combination of three key processes: water flow, heat transfer and solute transport. Resolution of such one-dimensional problem is performed using a numerical approach based on the finite difference method with an implicit scheme.

Keywords – Simulation, Finite Difference Method, Unsaturated Soil, Groundwater, Temperature.

I. INTRODUCTION

In the next few years, groundwater contamination is the most important risk for water resources. The pollution process can be started by the discharge of industrial waste or pesticides and insecticides used in agriculture. Numerous studies were devoted to the prediction of solute transport migration through the unsaturated zone reaching groundwater. Pérez Guerrero et al.[1], Xiong et al. [2] and Ghafoor et al. [3] considered the transfer phenomena as a one-dimensional problem and have determined the model parameters. These studies have led to analytic solutions, but always in the case of a simplified problem (homogeneity, isotropy, isothermal and saturated porous medium). Mori et al. [4], San Jose Martinez [5] and Guan [6] have focused on the description of the solute transport process in the soil and have evaluated the existed numerical models. Lessoff et al. [7] and El-Sadek [8] have proposed numerical and analytical models to solve the problem of groundwater contamination across different soil types. On the other hand the PRZM (Pesticide Root Zone Model) is designed to describe and simulate the one-dimensional movement of chemical pollutants in the unsaturated zone of the soil. Hilhorst et al. [9] treated the coupled transport of mass and energy in porous soil. They were able to solve, using the mixed finite element method, the equations of mass and heat transfers. The phenomenon of ground water contamination is the result of the instant combination of three processes: the water flow, the heat transfer and solute transport in the porous media. The problem is much more complex than the simplified case studied in the literature mentioned above. In this study, we propose a mathematical model that takes into account the unsaturated case of porous media and thermal gradient effect.

II. MATHEMATICAL FORMULATION

A. Water Flow

The geometry of the porous media is highly irregular, making the study of water movement very complex. In this paper, we restrict ourselves to the case of a homogeneous soil. In a known element of volume V of the studied soil, the law of conservation of mass is given by the equation:

\[ \frac{\partial}{\partial t}(\rho \theta) + \text{div}(\rho q) = S_1 \]  

Where: \( t \) is the time; \( \rho \) is the water density; \( \theta \) is the volumetric water content; \( q \) is the Darcy flux; \( S_1 \) is a sink term.

The Darcy Law in an unsaturated porous media is written as:

\[ q = K(x,y,z,\theta) - \text{grad} (h+1) \]  

Where: \( K(x,y,z,\theta) \) is a second order tensor expressing the hydraulic conductivity of the porous media; \( x, y, z \) are the Cartesian coordinates; \( h \) is the water pressure head.

The equation of van Genuchten (1980) for the retention curve is:

\[ \theta(h) = \begin{cases} \theta_r + \frac{\theta_s - \theta_r}{1 + 10^n h^m} & h < 0 ; m = 1 - \frac{1}{n} \qquad n > 1 \\ \theta_r & h \geq 0 \end{cases} \]  

Where: \( \theta_r \) is the residual water content; \( \theta_s \) is the saturated water content; \( h \) is the water pressure head; \( \alpha \) and \( n \) are shape parameters.

The MvG equation (Mualem and van Genuchten, 1980) to describe the hydraulic conductivity curve is:

\[ K(h) = \begin{cases} K_s r S_1^{1/2} [1 - (1 - S_1^{1/2})^n]^m & h < 0 \\ K_s & h \geq 0 \end{cases} \]  

Where: \( m = 1 - \frac{1}{n} \qquad n > 1 \) and \( S_1 = \frac{\theta - \theta_r}{\theta_s - \theta_r} \); \( K_s \) is the saturated hydraulic conductivity; \( S_1 \) is the effective saturation; \( r \) is the pore connectivity parameter, equal to 0.5 (Mualem, 1976).

Supposing the water pressure head is independent in space, the Darcy Law became:

\[ q = -K \frac{\partial h}{\partial \theta} \text{grad} \theta - K \frac{\partial h}{\partial T} \text{grad} T + 1 \]  

(1) and (5) combination gives the water flow model:

\[ \frac{\partial}{\partial t}(\rho \theta) = \text{div}[D_{at} \text{grad} \theta + D_{at} \text{grad} T] + S_1 \]  

with

\[ D_{at} = \rho K \frac{\partial h}{\partial \theta} \quad D_{at} \]  

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B. Heat Transfer

Heat transport in porous media is made by conduction in the solid matrix and by conduction and convection in the liquid phase. It is generally assumed that the temperatures of the solid and the fluid balance instantly and therefore we consider only the unknown temperature $T$ in the porous media.

The heat flux vector $\phi_i$ passing through an elementary volume $V_i$, $\phi_i$ the heat flux by conduction through the solid grains and $\phi_{\omega}$ the sum of the heat flux by conduction in the liquid phase, and the convection due to the water velocity are given by:

$$
\phi_i = (1- \varepsilon) \phi_{\omega} + \theta \phi_{\omega},
\phi_{\omega} = -\lambda_s \text{grad}T + \rho \gamma_s T \frac{q}{\theta}
$$

Where: $\varepsilon$ is the porosity; $\lambda_s$ and $\rho \gamma_s$ are respectively the thermal conductivity of the solid matrix and the water; $\gamma_s$ is the specific heat coefficient of water.

Taking into account the equations (5) and (7):

$$
\phi_i = -(1- \varepsilon) \lambda_s \text{grad}T + (1- \varepsilon) \theta \lambda_s + T \gamma_s \text{grad}T - [T \gamma_s D_{\omega}] \text{grad}T + \rho \gamma_s TK
$$

The heat transport equation is written, in analogy with equation (1):

$$
\frac{\partial}{\partial t} \left[ C_s (1- \varepsilon) \frac{q}{\theta} \right] = \text{div} \left[ D_{\omega} \text{grad}T + D_{\omega} \text{grad}T - \rho \gamma_s TK \right] + S_2
$$

Where: $\rho \gamma_s$ is the specific heat coefficient of the solid matrix; $S_2$ is a second sink term.

C. Solute Transport

The total flux of solute through an elementary volume can be written as:

$$
\phi_3 = -D_i \text{grad}C + C q_x
$$

Where: $D$ is the hydrodynamic dispersion coefficient of the liquid phase the sum of $D_{\omega}$, the molecular diffusion coefficient and $D_i$ the mechanical dispersion coefficient.

By analogy with the equations (1) and (8), the solute transport equation is:

$$
\frac{\partial}{\partial t} \left[ C_s (1- \varepsilon) \frac{q}{\theta} \right] = \text{div} \left[ D_{\omega} \text{grad}T + D_{\omega} \text{grad}T - \rho \gamma_s TK \right] + S_3
$$

In the case of linear sorption:

$$
C_s = K_d C
$$

Where $K_d$ is the adsorption coefficient.

By putting the equations (5), (10), (12) in (11) the solute transport model is written as:

$$
\frac{\partial}{\partial t} \left[ C_s (1- \varepsilon) \frac{q}{\theta} \right] = \text{div} \left[ D_{\omega} \text{grad}T + D_{\omega} \text{grad}T - \rho \gamma_s TK \right] + S_3
$$

D. Boundary Conditions

At the soil-atmosphere interface there is a dynamic coupling between the three transport processes and the climatic conditions. The principle of the conservation of mass is expressed of the total water flow through a thin boundary layer of thickness $\sigma_z$ at the soil-atmosphere interface ($z = 0$):

$$
q_x = q_w
$$

Where $q_w$ is the water flow expressed by the generalized Darcy's law (7), at $z = 0$:

$$
q_w = \rho u(t)
$$

Where $u(t)$ is the rainfall velocity.

(5), (15) and (16) give:

$$
B_i \left( \sigma_z, \theta, T \right) = \int_{-\sigma_z}^{0} K \frac{\partial h}{\partial \theta} \left| \frac{\partial \theta}{\partial z} \right|_{z = 0} + \int_{-\sigma_z}^{0} K \frac{\partial h}{\partial T} \left| \frac{\partial T}{\partial z} \right|_{z = 0}
$$

We express, using the principle of conservation of heat through the thin boundary layer of thickness $\sigma_z$ of the soil-atmosphere interface as:
III. NUMERICAL SIMULATION

For solving the equations (6), (9) and (13), we adopt an implicit finite difference scheme centered in space and delayed in time. After discretization we obtain the following algebraic equations systems:

\[ A_w u_{w}^{i+1} + B_w u_{w}^{i+1} + C_w u_{w}^{i+1} + D_w = 0 \]

where \( i = 1, 2, 3 \)

\[ A_w = \left[ \frac{D_w}{\Delta z^2} + \frac{\partial D_w}{\partial z} \frac{1}{2 \Delta z} \right] \]

\[ B_w = \left[ \frac{2 D_w}{\Delta z^2} \right] \]

\[ C_w = \left[ \frac{D_w}{\Delta z^2} + \frac{\partial D_w}{\partial z} \frac{1}{2 \Delta z} \right] \]

(21)

Where \( i \) is the index of space discretization and \( t \) is the index of time discretization.

\[ D_x = \frac{\partial h}{\partial z} \left( D_t \frac{\partial T}{\partial z} - \rho K \right) + \frac{L}{\Delta z} \theta + S_1 \]

\[ D_y = -\left[ \frac{\partial}{\partial z} (\rho \gamma \gamma + \rho \gamma (1 - e)) - \frac{\rho \gamma \gamma \theta + \rho \gamma (1 - e)}{\Delta z} \right] T \]

\[ + \frac{\partial}{\partial z} \left( D_y \frac{\partial \theta}{\partial z} - \rho \gamma TK \right) \]

\[ D_z = \left[ \frac{\partial}{\partial z} (\rho \gamma \gamma + \rho \gamma (1 - e)Kd) - \frac{\rho \gamma + \rho \gamma (1 - e)Kd}{\Delta z} \right] C \]

\[ + \frac{\partial}{\partial z} \left( D_z \frac{\partial \theta}{\partial z} - D_{Tz} \frac{\partial T}{\partial z} - KC \right) + S_3 \]

(22)

\[ \chi_1 = \rho \]

\[ \chi_2 = \rho \theta + \rho \gamma (1 - e) \]

\[ \chi_3 = \theta + (1 - e)K_d \]

With \( L \) is the depth of the studied domain.

The resolution of each of the systems (21), is performed using the Cholesky method. Indeed, the calculation is started by an initial profile, according to the boundary conditions. The convergences are tested respectively on the water content, \( \theta \), and the temperature \( T \). The water content and the temperature at the interface \( z = 0 \) are obtained by solving, using the method of Newton – Raphson, from equations (17) and (18). We obtain then:

\[ \theta_{op} = \theta_{op-1} + \Delta \theta_0 \]

\[ T_{op} = T_{op-1} + \Delta T_0 \]

\[ p = 1, 2, 3, \ldots \]

(23)

This process is repeated until convergence, obtained when: \( \theta_{op}, T_{op} \approx \theta_{op-1}, T_{op-1} \).

IV. RESULTS

The results below were obtained for the following data:

\[ \theta_s = 0.422 \ cm^{-3} \cdot cm \]

\[ K_{sat} = 2.7 \times 10^{-5} \ m.s^{-1} \]

\[ \lambda_s = 5.72 \ J.m^{-2}.s^{-1}.K^{-1} \]

\[ \varepsilon = 0.422 \ cm^{-3} .cm^{-3} \]

\[ \rho_s = 1630 \ Kg.m^{-3} \]

\[ S_0 = S_1 = S_2 = 0 \]

In Fig. 2, the profiles of the water content for three values of the rainfall water velocities, \( v(t) \), are presented, in the case rainfall water temperature = 298 °K. It is noted that for a determined \( v(t) \), the water content is constant for depths less than 0.6 m, and it is close to the residual water content of the porous media. Indeed, the water infiltrated is redistributed under the effect of the soil pressure head. While, for depths greater than 0.6 m, the pressure head is "disturbed" by the gravitation, and water content increases until complete saturation, obtained on the upper surface of the aquifer, where suction potential is zero. Also, the increase of the rain water speed results in a slight increase in the water content due to the increased flux provided from surface.
The profiles of solute concentration, corresponding to the profiles of the water content and temperature respectively shown in Figures 2 and 3, are given in Fig. 4. for a temperature of rainfall water $T = 298 \, ^\circ \text{K}$. We find that, for a solute concentration at the surface of the water table $z = L = 0$, the profiles have a maximum depth at 0.3 m which corresponds to a maximum desorption and a minimum adsorption. The change in rain velocity does not affect the concentration profile.

We present, respectively, in Figures 5, 6 and 7, the influence of heating and cooling, on the profiles of the water content, temperature and concentration of solute, to a rain velocity $v(t)$ set at $15.28 \times 10^{-7} \, \text{m.s}^{-1}$. We note, from Fig. 5, such a temperature variation causes no effect on the water content of the environment due to the low temperature gradient induced heat conditions to the soil surface, in the unsaturated zone of the soil. However, in Fig. 6, there is a variation in the temperature of the porous media due to the heat flux provided by the rainwater to reach different temperatures, but which is not able to change the water content of the environment. On the other hand and according to Fig. 7, we see that increasing the temperature of the rainwater promotes increase of the concentration of the solute in water and migration of chemical pollutant in the soil. Indeed, in the absence of the influence of temperature on the water content of the medium, increasing the hydrodynamic dispersion is causing changes in solute concentration in water.
Fig.7. Evolution profiles of the concentration of the solute as a function of depth and temperature beyond rain at $v(t) = 15.28 \cdot 10^{-7}$ m.s$^{-1}$.

V. CONCLUSION

The numerical study that we conducted on water flow, heat transfer and solute transport in unsaturated and homogeneous porous media shows that climatic conditions and water movement in the surface are acting on the transport phenomena in the unsaturated soil region. Furthermore, it was found that the water temperature at the surface has an influence on the temperature and the solute profile in the soil. This result allows us to confirm that the cooling water, on the surface of an unsaturated soil slows the migration and contamination of groundwater.

REFERENCES


