

# COMPUTER SIMULATION OF NON-ISOTHERMAL WATER AND SOLUTE TRANSPORT IN SOIL

The mathematical model and results of the computer simulation of heat, water and solute transport in soil are presented in this paper. Non-isothermal moisture transport was described by the equations of heat conduction, the vapor and liquid transport. The solute transport was simulated by the convection diffusion equation in which the processes of sorption and reaction were taken into account. The finite-element method was used for the numerical solution of the obtained system of the differential equations. The results of the computer simulation of non-isothermal water and radionuclide Sr-90 transport in soil are represented and discussed.

## 1. Introduction

The major element of environmental safety is the problem of soil contamination with various chemical substances and, first of all radionuclides. The forecasting by using mathematical modeling of pollutant transport in contamination zone is a perspective direction of the solution of this problem. This method will allow beforehand to take the necessary measures providing decrease of receipt of these substances in crop production.

There are a large number of works which is devoted to the problem of mathematical modeling of solute transport in soil and migration of radionuclides including [1-3]. The analysis of physical mechanisms of solute transport in soil shows, that impurity migration is mainly defined by the dispersion in the soil water flow. But water transport in soil is not only the result of moisture gradient but and it is the result of temperate gradient. In this connection the problem of modeling of solute transport in soil is divided into two problems. The first problem is modeling of non-isothermal water transport in soil and the second one – modeling of impurity migration. Also the processes of sorption, reaction and meteorological conditions influence on the impurity migration in the soil. All above listed natural phenomena are not accounted in the mentioned works there. In the majority of them during the modeling the solute transport by the soil moisture the questions of the non-isothermal water transport (evaporation and redistribution of the moisture under action of the gradients of temperatures and gradients of moisture) are not taken into account. The problem of modeling of the non-isothermal water transport in porous medium in spite of that the first models have been published more then fifty years ago [4, 5] remains actual nowadays [6].

In this connection the attempt to describe more accurately the solute transport in soil taking into account non-isothermal water transport was made in this work.

## 2. Mathematical model's description

The unsaturated soil domain consists of soil-solids, liquid water and water vapor. The air content in the soil is not taken into account. The present approach to modeling solute transport in the soil domain considers heat conduction equation, convection diffusion equation and transport equations for liquid water and water vapor.

The liquid water mass balance is expressed as [7]:

$$\frac{\partial(\rho_L \theta_L)}{\partial t} = \nabla(\rho_L V_L) - I, \quad (1)$$

where  $\rho_L$  is the liquid water density, [kg/m<sup>3</sup>];  $\theta_L$  is the volumetric liquid water content, [m<sup>3</sup>/m<sup>3</sup>];  $t$  is time, [s];  $V_L$  is the liquid phase flux, [m/s];  $I$  is the phase change water flux, [(kg)/(m<sup>3</sup> s)].

The liquid phase flux is determined by the Darcy's law [7]:

$$V_L = \frac{K_o K_L}{\eta_L} \nabla(P_L - \rho_L g z), \quad (2)$$

where  $K_o$  is the intrinsic permeability of the porous medium, [m<sup>2</sup>];  $K_L$  is the relative permeability;  $\eta_L$  is dynamic water viscosity, [kg/(m s)];  $P_L$  is the pressure difference between the liquid and gas phases, [Pa];  $g$  is acceleration of gravity, [m/s<sup>2</sup>];  $z$  is the coordinate vertical elevation, [m].

For the modeling of the water and vapour transport the knowledge of the phase change water flux, the dependence of the relative permeability from the water content and the dependence of the pressure from the water content and temperature are necessary. The last relation can be received using moisture sorption isotherm. The sorption isotherm is the experimentally obtained dependence of the mass water content ( $u$ ) from relative humidity ( $\varphi$ ) at different temperatures.

The relative humidity and the vapour water pressure ( $P_V$ ) are related by the dependence:

$$\varphi = \frac{P_V}{P_S}, \quad (3)$$

where  $P_S$  is the saturation vapour pressure are function on the temperature.

And the mass water content  $u$  is connected with the volumetric liquid water content  $\theta_L$ :

$$\theta_L = \frac{\rho_s}{\rho_L} u, \quad (4)$$

where  $\rho_s$  is the soil density, [kg/m<sup>3</sup>];

Then using the sorption isotherm functional dependence of moisture content from vapour water pressure and temperature can be received:  $u = \psi(P_v, T)$ . From this dependence the function defining the change of the vapour water pressure from the mass moisture content and temperature is derived:  $P_v = f(u, T)$ .

A relation between the pore pressure, the saturation vapour pressure and the relative humidity is given by Kelvin's equation:

$$P_L = P_s + \frac{RT\rho_L}{M_L} \ln \varphi, \quad (5)$$

where  $R$  is the universal gas constant, [8.31 J/(mol K)];  $M$  is the molar weight of water, [0.018 kg/mol].

This equation with the use of the dependence of the vapour water pressure from the water content and temperatures are written in a following kind [8]:

$$P_L(u, T) = P_s + \frac{RT\rho_L}{M_L} \ln \frac{f(u, T)}{P_s}. \quad (6)$$

The expression (6) reflects the physical and chemical properties of the liquid water, structural characteristics of the soil and is necessary for the solution of the equation of the water transport as the dependence between the pore pressure from the water content and temperature.

In compliance with the hypothesis of the local thermodynamic balance widely used in the theory of sorption the phase change water flux is defined by the equation [8]:

$$I = \rho_s \frac{\partial u}{\partial t} = \rho_s \left[ \left( \frac{\partial u}{\partial P_v} \right) \frac{\partial P_v}{\partial t} + \left( \frac{\partial u}{\partial T} \right) \frac{\partial T}{\partial t} \right]. \quad (7)$$

The dependence of relative permeability from the water content is defined by following empirical equation [8]:

$$K_L = \left( \frac{u - u_p}{m - u_p} \right)^n, \quad (8)$$

where  $m$  is the total porosity or porosity decrease by the air content;  $u_p$  is the quantity of bound moisture;  $n$  is the soil-dependent constant lied in the range of 3-4.

The equation of vapour water transport can be written in the form of [7]:

$$\frac{\partial(\rho_v \theta_v)}{\partial t} = \nabla \left( \rho_v \frac{K_o K_v}{\eta_v} \nabla(P_v - \rho_v g z) \right) + I, \quad (9)$$

where  $\rho_v$  is the vapour water density, [kg/m<sup>3</sup>];  $\theta_v$  is the volumetric vapour water content, [m<sup>3</sup>/m<sup>3</sup>];  $K_v$  is the relative permeability;  $\eta_v$  is dynamic vapour water viscosity, [kg/(m s)];  $P_v$  is the vapour pressure, [Pa].

The relative permeability of the vapour water is defined by the analogy with the relative permeability of water:

$$K_v = \left( \frac{m - u}{m - u_p} \right)^n. \quad (10)$$

The general gas law relates the vapour density with the vapour pressure:

$$\rho_v = \frac{MP_v}{RT}. \quad (11)$$

And the relation between the mass water content and the volumetric vapour water content is:

$$\theta_v = m - \frac{\rho_s}{\rho_L} u, \quad (12)$$

Using (11) and (12), the left part of the equation (9) is written in the form of:

$$\frac{\partial(\rho_v \theta_v)}{\partial t} \approx \left( m - \frac{\rho_s}{\rho_L} u \right) \frac{M}{RT} \frac{\partial P_v}{\partial t}, \quad (13)$$

The state equation for the temperature distribution in the soil, considering latent heat of the phase change is given by:

$$C_{eq} \frac{\partial T}{\partial t} = \nabla(K_{eq} \nabla T) + qI, \quad (14)$$

where  $C_{eq}$  is the volumetric heat capacity, [J/(m<sup>3</sup> K)];  $K_{eq}$  is the soil thermal conductivity, [W/(m K)];  $q$  is the latent heat of the phase change, [J/kg].

Volumetric heat capacity of the soil,  $C_{eq}$ , is the sum of the volumetric heat capacities of the soil constituents:

$$C_{eq} = \frac{\sum \theta_i \rho_i C_i}{\sum \theta_i}, \quad (15)$$

where  $\rho_i$ ,  $C_i$  and  $\theta_i$  are the density, specific heat capacity and volumetric fraction of the  $i^{th}$  soil constituent i.e. soil-solids, water, vapour water and air.

The thermal conductivity of soil can be calculated in the following way

$$K_{eq} = \frac{\sum \theta_i k_i}{\sum \theta_i}, \quad (16)$$

where  $k_i$  and  $\theta_i$  are the thermal conductivity, and volumetric fraction of the  $i^{th}$  soil constituent.

The latent heat of the phase change is computed with the use of the Clausius-Claperon equation:

$$q = \frac{RT^2}{M} \left( \frac{\partial \ln P_v}{\partial \ln T} \right). \quad (17)$$

The solute transport taking into account sorption and reaction is described by equation [3]:

$$\frac{\partial(\theta_L C)}{\partial t} + \frac{\partial(\rho_b N)}{\partial t} = \nabla(\theta_L D_{LS} \nabla C - V_L C) + R_L + R_p, \quad (18)$$

where  $C$  is the dissolved concentration, [kg/m<sup>3</sup>];  $N$  is the mass of adsorbed contaminant per dry unit weight of soil, [kg/kg];  $\rho_b$  is the bulk density [kg/m<sup>3</sup>];  $D_{LS}$  denotes the combination of hydrodynamic dispersion tensor for water and diffusion in soil-solid [m<sup>2</sup>/s];  $V_L$  is the water velocity, [m/c];  $R_L$  represents reactions in water [kg/(m<sup>3</sup>s)]; and  $R_b$  denotes reactions involving solutes attached to soil particles [kg/(m<sup>3</sup>s)].

The solute spreading includes mechanical dispersion in water plus molecular diffusion for the

water and soil-solid. These three processes appear in the liquid-solid dispersion tensor:

$$D_{LS} = \alpha \frac{V_L}{\theta_L} + \tau D_m + \rho_b K_d \frac{D_s}{\theta_L}, \quad (19)$$

where  $\alpha$  is the soil dependent constant for dispersivity, [m];  $\tau$  is the soil dependent constant for tortuosity;  $D_m$  is the molecular diffusion coefficient, [m<sup>2</sup>/s],  $D_s$  is the diffusion constant in the soil-solid [m<sup>2</sup>/s].

The distribution of impurity between soil-solid and liquid phases is described by using the distribution coefficient  $K_d$ :

$$N = K_d C. \quad (20)$$

The value of  $K_d$  can be determined experimentally or calculated by using the available information about the sorption properties of the system.

### 3. Modeling of solute transport

The solute transport in the soil under falling of the rain is modeled by the use of the developed model. The temperature gradient set in the profile of the soil and distribution of the concentration of the pollutants set on the surface of the soil (fig. 1). The impurity concentration in the profile of the soil in ten years was taken as the results of the modeling (fig. 2). From the results of the modeling it is visible that the velocity of the impurity migration in the vertical direction is several orders greater than in the horizontal direction. Therefore, the application of the one-dimensional model is acceptably under the modeling of the solute transport in the soil.

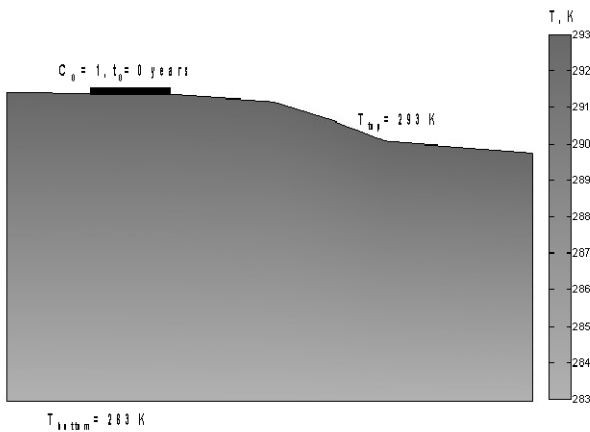


Fig. 1. Initial distributions of impurity concentration and temperature

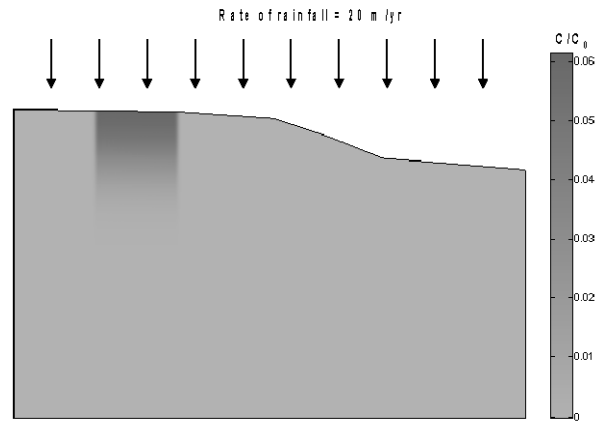


Fig. 2. Modeling result of solute transport in the soil

In the second case, the vertical migration of radionuclides in the soil is modeled. In this case, the change of the temperature and the change of the water content in the near-surface layer of the soil from the time according to the harmonic law was set. And the dynamics of the change of the initial distribution of <sup>90</sup>Sr (fig. 3) within six years was modeled [9].

From the results of the modeling (fig. 4) it is visible that migration <sup>90</sup>Sr in the depth of the soil passes slowly: for the considered period more than 90 percent from the general concentration of radionuclides remains in the 10-centimetric layer of the soil and is accessible to root absorption by plants. The speed of the penetration of radionuclides in the depth of the soil correlates with the experimental researches [10].

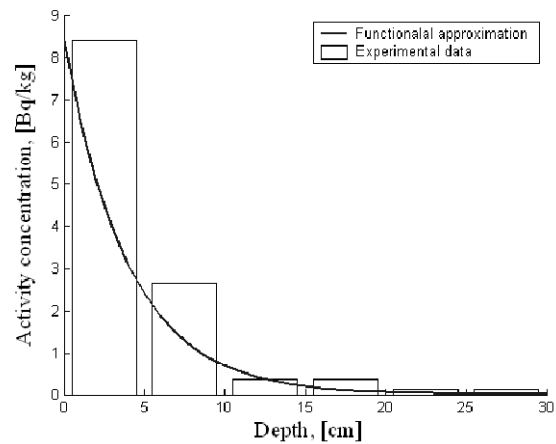


Fig. 3. Initial distributions of <sup>90</sup>Sr in the soil profile

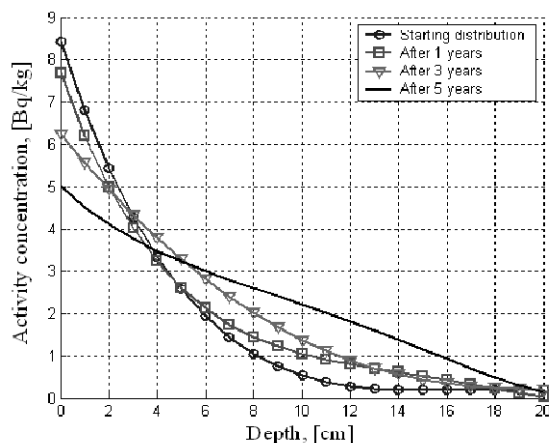


Fig. 4. Variation of the  $^{90}\text{Sr}$  distribution in the soil

#### 4. Conclusion

The mathematical model of the impurity migration in the soil is offered. The model takes into account the basic physical factors influencing on the substance and the thermal transport in the soil (convective diffusion, sorption, reaction and meteorological conditions). It allows to approach in the greater extent the phenomenological model to a real environment. Conducted numerical researches have shown that the model can be used for the prediction of the radionuclide vertical migration in the soil.

#### Acknowledgements

This work was supported by Ministry of Education of the Republic of Belarus.

#### References

- [1] Schuller P., Ellies A., Kirchner G.: Vertical migration of fallout  $^{137}\text{Cs}$  in agricultural soils from Southern Chile. *The Science of the Environment* 193, P 197-205. 1997.
- [2] Kudryashov N.A. and Alekseeva I.K. Numerical Simulation of Migration of Radionuclides in Soil after Radioactive Fallout. *IFZh*, Vol. 71, No. 6, P. 976-982. 1998.
- [3] Serebryannyi G.Z. and Zhemzhurov M.L. Analytical Model of Migration of Radionuclides in Porous Media. *IFZh*, Vol. 76, No. 6, P. 146-150. 2003.
- [4] Philip JR, de Vries DA. Moisture movement in porous media under temperature gradients. *Transactions American Geophysical Union* 1957, 38(2): 222-231.
- [5] Lykov A.V. *The drying theory*. Moscow: Energiya, 471 p. 1968.
- [6] Jordi Grifoll, Josep Ma. Gastó and Yoram Cohen. Non-isothermal soil water transport and

evaporation. *Advances in Water Resources*. In Press.

- [7] Bear J, Bachmat Y. *Introduction to Modeling of Transport Phenomena in Porous Media*. Dordrecht: Kluwer, 584 p. 1991.
- [8] Grinchik N.N., Akulich P.V., Kuts P.S. and others. On the Problem of Non-isothermal Mass Transfer in Porous Media. *IFZh*, Vol. 76, No. 6, P. 129-141. 2003.
- [9] Kundas S.P., Grinchik N.N., Gishkeluk I.A. Mathematical model of radionuclides' migration in soil. *The Bulletin of Polotsk State University, Applied sciences*. No. 3, P. 56-60, 2005.
- [10] Arastovich T. Influence of the soils property on the process of vertical movement of radionuclides. *The News of National Academy of Sciences, Agrarian sciences series*. No. 2, P. 62-65, 2004.