

APPLICATION OF COMPUTER MODELLING FOR THE ANALYSIS AND PREDICTION OF CONTAMINANT BEHAVIOUR IN GROUND WATER SYSTEMS

Abstract. The application of the computer modelling for the analysis and prediction of the contaminant behaviour in ground-water systems is discussed. A new mathematical model of the impurity migration in soils and its application for the analysis of the accessibility of toxicants for the plants and the prediction of the ground water pollution is studied.

1. Introduction

Nowadays owing to the intensive development of the industry, the agriculture, the increase of domestic wastes and the influence of other factors, soil and ground water exhaustion and pollution achieved threatening scopes. For the Republic of Belarus soils contaminated by radionuclides became the most acute problem after the Chernobyl Accident. Therefore the study of the migration conditions and the contaminant reduction (radionuclides, heavy metals and organic compounds) in soils and ground-waters is the most actual problem for the environmental safety and environmental protection. The solving of this important problem is impossible without the scientific knowledge about dominating processes influencing on the migration and physical-chemical changes of the pollutants in different geological environment conditions. In our opinion the leading role in these researches on the contemporary stage should belong to the computer modelling methods that will help to understand this complicated and dynamic process more precisely as the influence of the polluted environment on human's health. The application of the modelling methods will help us to analyze different migration mechanisms and the toxicant reduction in soils and ground-waters, to determine the influence of the contaminated soil on the biosphere, to reduce the number of toxicants in crop production and to prevent their accumulation in human organism and animals (Serebryannyi, 2003).

The main purpose of the computer modelling methods is to formulate the mathematical model of the contaminant migration as an algorithm. In the future this model will be realized as a computer program that will help us to carry out numerical experiments on it and to get the necessary information (Kudryashov, 1998). Thus the researches on the influence of the factors such as weather conditions, physical-chemical characteristics of toxicants, etc. on the contaminant migration in soils are carried out with the help of the parametric study of the mathematical model and the determination of the dependence from any parameter. Such an experiment helps to investigate questions more deeply in the environment. Besides the use of the computer modelling methods can reduce a number of the expensive measuring experiments.

Keywords: mathematical modelling; contaminant transport; ground-water system

Thus the main objective of the work was the research of the possibilities of the application of the computer modelling for the analysis and prediction of the contaminant behavior in ground-water systems, in particular, radionuclides in soil.

2. Mathematical model of the contaminant behavior in ground-water systems

For the analysis and prediction of the migration, concentration of the contaminant content in soils it is necessary to create mathematical models providing the description of the main processes that influence on the transfer and redistribution of these substances (Fig. 1). The level of influence of processes can be differ from various geological surroundings and so on.

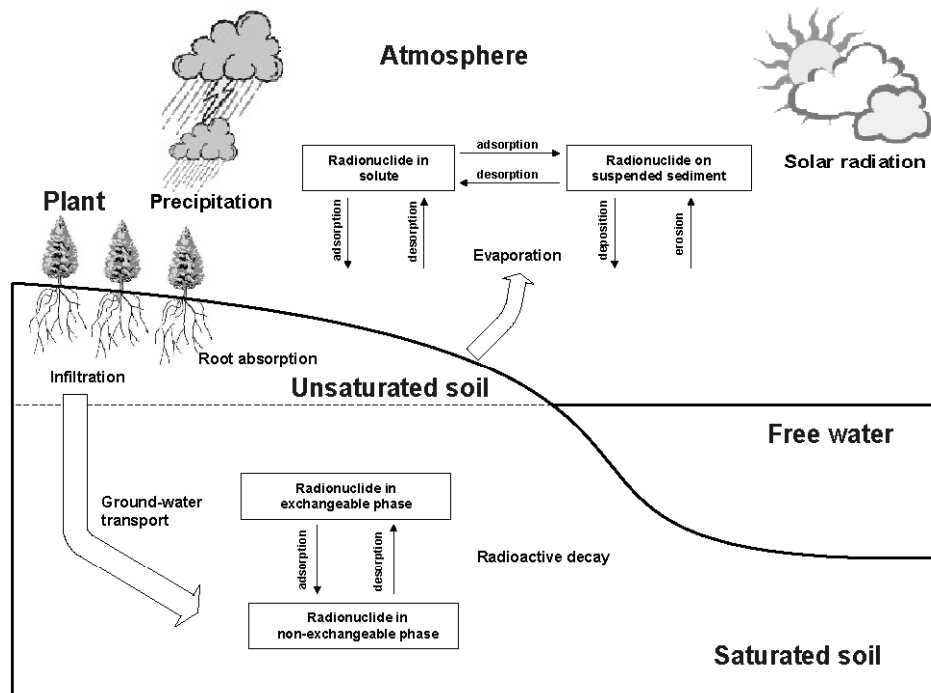


Figure 1. Basic processes determining the contaminants redistribution in ground-waters systems

The main physical-chemical processes determining the contaminant transport and redistribution in soils include: (Bulgakov, 1992):

- The convective-dispersion transport of contaminants in the solute form.
- The movement of the ground water in the liquid and gas phases under the influence of the gradients of the moisture and temperature.
- The redistribution between contaminants dissolved in water and absorbed by the matrix solid material.
- The contaminant diffusion in soils absorbed by the matrix solid material.
- The chemical and radioactive transformation of the contaminants.
- The aerosol fallout of the contaminants on the soil surface.
- The infiltration – the absorption of the water from the soil surface.

- The deduction of contaminants from the soil during the water evaporation.
- The absorption of toxicants by plants.
- The evaporation of the moisture from the soil surface.
- The loss of the moisture in the soil due to the moisture's absorption by plants and the its evaporation in the atmosphere during the living process of the plant system.
- The contaminant deposition on the soil surface and ingress to the atmosphere due to wind erosion.

The analysis of the foregoing processes shows that the dominating mechanism of the contaminant transport in soils is the dispersion and convection in the soil water flux (Kudryashov, 1998). Here the moisture in the soil exists both in the liquid and gas phases and its distribution is carried out under the influence of gradient of the moisture and the temperature. In this connection the modelling problem of the contaminant distribution in soil has two subproblems: the modelling of the non-isothermal water transport and contaminant migration.

In our opinion the progress in the sphere of the application of the computer modelling for the analysis and prediction of the contaminant behavior in ground-water systems is connected with the substitution of the purely empirical description for the informal one that is based on the physical mechanisms proceeded in the nature. It makes the model more adequate to the processes taken place in the nature.

One of the examples to solve the problem of the computer modelling of the contaminant behaviour in the ground-water system is the authors' developed model of the impurity migration in soils (Kundas, 2005). The distinctive feature of this model from the earlier existed is the more rigorous description of the non-isothermal water transport based on the laws of thermodynamics and physics. The model is based on differential equations: convective diffusion, liquid and gas flow and thermal conductivity.

The water flow in the porous medium representing the soil is defined by the following equation (Bear, 1997):

$$\frac{\partial(\rho_L \theta_L)}{\partial t} = \nabla \left(\rho_L \frac{K_o K_L}{\eta_L} \nabla (P_L - \rho_L g z) \right) - I - S_w \quad (1)$$

where ρ_L is the liquid water density, [kg/m³]; θ_L is the volumetric liquid water content, [m³/m³]; t is time, [s]; K_o is the intrinsic permeability of the porous medium, [m²]; K_L is the relative permeability; η_L is the dynamic water viscosity, [kg/(m·s)]; P_L is the pressure difference between the liquid and gas phases, [Pa]; g is the acceleration of gravity, [m/s²]; z is the coordinate vertical elevation, [m]; I is the phase change water flux, [(kg/(m³·s))]; S_w is the sink term representing root water uptake, [(kg/(m³·s))].

For the modelling 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 (φ) at different temperatures.

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

$$\varphi = \frac{P_v}{P_s} \quad (2)$$

where P_s is the saturation vapour pressure is the function from the temperature.

And the mass water content u is connected with the volumetric liquid water content θ_L :

$$\theta_L = \frac{\rho_s}{\rho_L} u \quad (3)$$

where ρ_s is the soil density, [kg/m³].

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

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

$$P_L = P_s + \frac{RT\rho_L}{M_L} \ln \varphi \quad (4)$$

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 water vapour pressure from the water content and temperature is written in the following form (Grinchik, 2003):

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

The expression (5) 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 of 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 (Grinchik, 2003):

$$I = \rho_s \frac{\partial u}{\partial t} = \rho_s \left[\left(\frac{\partial u}{\partial P_v} \right) \frac{\partial P_v}{\partial t} + \left(\frac{\partial u}{\partial T} \right) \frac{\partial T}{\partial t} \right] \quad (6)$$

The dependence of relative permeability from the water content is defined by following empirical equation (Genuchten, 1980):

$$K_L = \left(\frac{\theta_L - \theta_r}{\theta_s - \theta_r} \right)^b \left[1 - \left(1 - \left[\frac{\theta_L - \theta_r}{\theta_s - \theta_r} \right]^{\frac{1}{m}} \right)^m \right]^2 \quad (7)$$

where θ_r and θ_s denote the residual and saturated water contents, respectively, [m^3/m^3]; b and n are the parameters that denote soil characteristics.

The infiltration of the atmospheric precipitations can be modelled with the use of the above mentioned equation (1) by the way of the definition of specific boundary conditions. In the beginning of the precipitation when the soil is not saturated with water the water flux from the soil surface is defined by the rainfall rate (f):

$$\frac{K_o K_L}{\eta_L} \nabla(P_L - \rho_L g z) = f \text{ for } \theta_L < \theta_s \text{ and } \phi < 1 \quad (8)$$

When the near-surface soil layer approaches to the saturated state, i. e. pores in the soil is fully filled with water, boundary conditions on the surface of the soil are written in the form of

$$P_{Lsat}(t) = P_S + \frac{RT\rho_L}{M_L} \ln \frac{f(\theta_s, T)}{P_S} \text{ for } \theta_L = \theta_s \text{ and } \phi = 1 \quad (9)$$

where P_{Lsat} is the liquid pressure on the surface of the soil at the full saturation of the soil with the water [Pa].

The water vapour flow in the soil taking into account that the content of the air in pores contributes not significant influence on the moving of the water vapour can be described by the following equation: (Bear, 1991):

$$\frac{\partial(\rho_v \theta_v)}{\partial t} = \nabla \left(\rho_v \frac{K_o K_v}{\eta_v} \nabla(P_v - \rho_v g z) \right) + I \quad (10)$$

where ρ_v is the water vapour density, [kg/m^3]; θ_v is the volumetric water vapour content, [m^3/m^3]; K_v is the relative permeability; η_v is the dynamic water vapour viscosity, [$\text{kg}/(\text{m}\cdot\text{s})$]; P_v is the vapour pressure, [Pa].

The relative permeability of the water vapour is defined similarly to the relative permeability of water:

$$K_L = \left(\frac{\theta_L - \theta_r}{\theta_s - \theta_r} \right)^b \left[1 - \left(\frac{\theta_L - \theta_r}{\theta_s - \theta_r} \right)^{\frac{1}{m}} \right]^{2m} \quad (11)$$

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

$$\rho_v = \frac{MP_v}{RT} \quad (12)$$

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

$$\theta_v = m - \frac{\rho_s}{\rho_L} u \quad (13)$$

where m is the total porosity or the porosity decreased by the air content.

Using (12) and (13) the left part of the equation (10) is written in the form of

$$\frac{\partial(\rho_v \theta_v)}{\partial t} \approx \left(m - \frac{\rho_s}{\rho_L} u \right) \frac{M}{RT} \frac{\partial P_v}{\partial t} \quad (14)$$

The evaporation from the surface of the soil in the proposed model can be taken into account by the defining of the following boundary conditions:

$$P_v(t) = \varphi_{surf}(t) P_s(T) \quad (15)$$

where φ_{surf} is the soil surface relative humidity.

The state equation for the temperature distribution in the soil considering latent heat of the phase change is given by (Grifoll, 2005):

$$C_{eq} \frac{\partial T}{\partial t} = \nabla(K_{eq} \nabla T) + qI \quad (16)$$

where C_{eq} is the volumetric heat capacity, [J/(m³·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:

$$C_{eq} = \frac{\sum \theta_i \rho_i C_i}{\sum \theta_i} \quad (17)$$

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

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

$$K_{eq} = \frac{\sum \theta_i k_i}{\sum \theta_i} \quad (18)$$

where k_i and θ_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:

$$q = \frac{RT^2}{M} \left(\frac{\partial \ln P_v}{\partial \ln T} \right) \quad (19)$$

The heat exchange of the soil with the atmosphere is defined by the following boundary conditions:

$$T(t) = T_{surf}(t) \quad (20)$$

where T_{surf} is the temperature on the soil surface.

The contaminant transport taking into account sorption is described by equation (Serebryannyi, 2003)

$$\frac{\partial(\theta_L C)}{\partial t} + \frac{\partial(\rho_b N)}{\partial t} = \nabla(\theta_L D_{LS} \nabla C - V_L C) - R - S_s \quad (21)$$

where C is the dissolved concentration, [kg/m³]; N is the mass of the adsorbed contaminant per dry unit weight of the soil, [kg/kg]; ρ_b is the bulk density [kg/m³]; D_{LS} denotes the combination of the hydrodynamic dispersion tensor for water and diffusion in soil-solid [m²/s]; V_L is the water velocity, [m/c]; R is the term representing the change of the concentration due to radioactive disintegration or chemical reactions [kg/(m³·s)]; S_s is the sink term representing the root solute uptake, [kg/(m³·s)].

The solute spreading includes the mechanical dispersion in the water plus the molecular diffusion for the water and the soil-solid. These three processes appear in the liquid-solid dispersion tensor:

$$D_{LS} = \alpha \frac{V_L}{\theta_L} + \tau D_m + \rho_b K_d \frac{D_s}{\theta_L} \quad (22)$$

where α is the soil dependent constant for the dispersivity, [m]; τ is the soil dependent constant for the tortuosity; D_m is the molecular diffusion coefficient, [m²/s], D_s is the diffusion constant in the soil-solid [m²/s].

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

$$N = K_d C \quad (23)$$

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

The ingress of the contaminants in and from the soil into the atmosphere defined by the boundary conditions of the second type:

$$\theta_L D_{LS} \nabla C = q \quad (24)$$

where q is the flow of the contaminants between the soil and the atmosphere. The value of the flow is calculated according to appropriate expressions depending on the ingress of the toxicants in and from the soil (the aerosol fallouts of the contaminants, the fallout on the surface of the soil and the ingress of contaminants into the atmosphere due to the wind erosion etc.). If the contaminant transport from the soil into the atmosphere and vice versa is insignificant, the flow on the boundary is equal to zero: $q=0$.

The above mentioned mathematical model in the one-dimensional formulation is realized with the use of MATLAB and FEMLAB and allows to perform the computer modelling of the contaminant migration in the ground-water system.

3. Results of the computer modelling and its discussion

The prediction of the radionuclide penetration depth in the soil and the analysis of the contaminated ground waters that is a drinking water source is of the practical interest the Republic of Belarus after the Chernobyl Accident. It is also interested in the prediction of the change of radionuclides amount available for absorption by plants. In this connection the application of models given above for the prediction of the vertical migration of the radionuclides in the soil will be discussed further.

It is supposed that as a result of the nuclear fallouts the surface of the soil is contaminated by ^{90}Sr that under the influence of the rainfall migrates deep into the soil. It is necessary to determine the quantity of the radionuclides remained in the root layer and the ones that have got in ground waters after the specified period of time. Experimental measurements in this case allow to determine the concentration of the radionuclides in the soil at a certain depth, their content in ground waters and crop production, but they don't give any chance to predict the development of the situation in the future.

Physical-chemical soil properties determining the process of migration were set for the podzolic soil. The influence of the climatic factors was taken into account by the definition of the temperature and rainfall intensity change in time.

As a result of the modelling there were obtained different changes of ^{90}Sr content with respect to the total amount of the deposited radionuclides. (Fig. 2a).

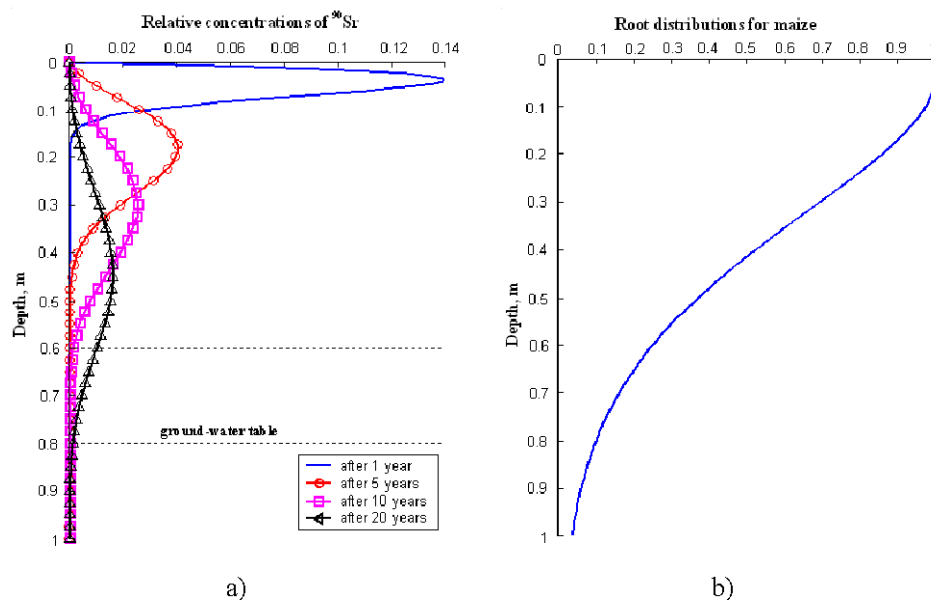


Figure 2. The distribution of ^{90}Sr (a) and root system for the maize (b) in the soil

Comparing the radionuclide distribution in the soil with the root system distribution of the crop production (Fig. 2b) it is obvious that during the analyzed period of time – 20 years the most part of the nondecayed radionuclides remain in the soil layer: 0 - 0.60 m and they are available for plants during root's absorption. At the same time it can be mentioned that there is no danger of the radionuclide ingress in the ground waters that is situated at the deeper level: 0.8 - 2.0 m.

The analysis of the results of the modelling (Fig. 3) shows that the contribution of the vertical migration process to the purification of the root-inhabited layer (0 - 0.6 m) of the analyzed soil from radionuclides on the first stage (20 years) is not significant in comparison with the role of the radioactive decay. But in the next period of time due to the vertical migration of radionuclides to the lower soil layer it is observed the sharp decrease of ^{90}Sr in root-inhabited layer.

The decrease of the radionuclides' content in the root-inhabited layer in 2 times from the total amount of fall-out on the surface of the analyzed soil due to processes of the radioactive decay and vertical migration can be expected in 19 years and the decrease in 100 times – in 78 years (Fig. 4a).

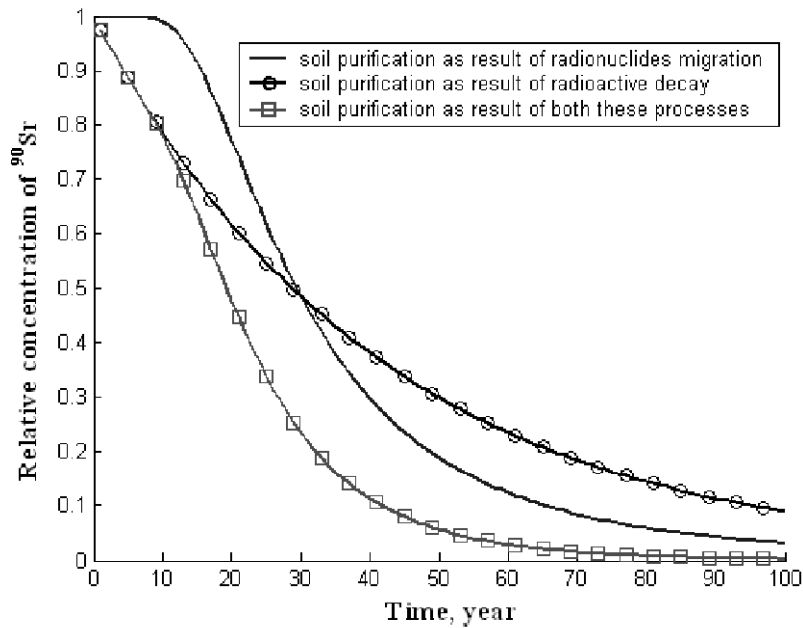


Figure 3. The role of the vertical migration and radioactive decay in the removal of ⁹⁰Sr from the soil level: 0 - 0.6 m

At that time the radionuclides fallen on the soil surface will reach the level of ground waters (the level of ground waters – 1.4 m) in 40 years. And the maximal accumulation of ⁹⁰Sr by ground waters will be observed in 110 years after nuclear fall-outs and will be 25 % from the total amount of the radionuclides fallen on the soil surface (Fig. 4b).

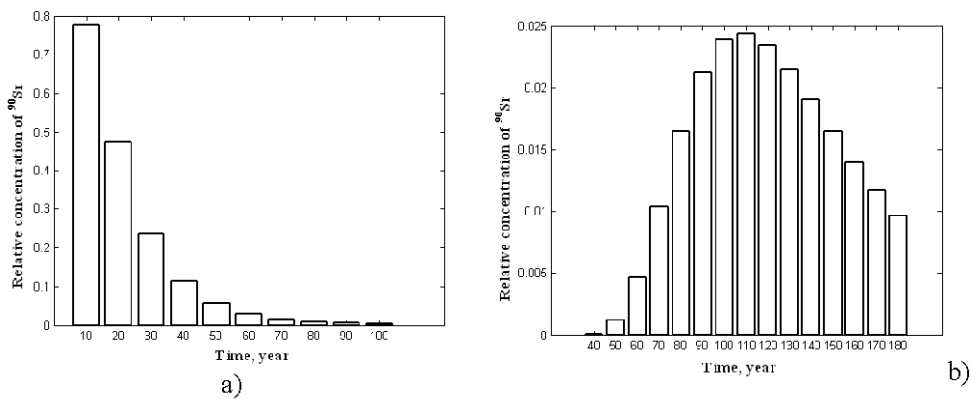


Figure 4. The dynamics of the relative concentration of ⁹⁰Sr in root-inhabited layer (a) and ⁹⁰Sr pollution density of ground waters (b)

4. Conclusion

It is shown that the application of the computer modelling for the analysis and prediction of the contaminants' behavior in ground-water systems is the effective instrument to solve the problem of environmental safety.

The contaminants' migration model in the soil was discussed and analyzed in the article. The model was based on the strict mathematical description taking into account physical processes and environmental factors exerting the essential influence on the examined process.

The results of the modelling of radionuclides' vertical migration in the soil have been obtained with the use of the proposed mathematical model that evidences of the possibility of its effective application for the solving of problems of the prediction of the long-term change of the radiological situation in the definite area.

The progress in the use of the computer modelling methods to research the radionuclides' migration in the environment can be achieved with the use of the universal software integrating mathematical models, databases with the information about different soil types and long-term hydrometeorological conditions for the definite area and geographic information systems.

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