APPLICATION OF COMPUTER MODELING FOR ANALYSIS AND FORECASTING OF RADIONUCLIDES' MIGRATION IN SOIL

Outlook of various methods of computer modeling application for the analysis and forecasting of radionuclides' migration in the soil are discussed. The new mathematical models of radionuclides' transport in near-surface layer of soil are considered. It is pointed out, that further progress in this field is connected with development of universal program facilities integrating analytical models, data bases, geo information and expert systems

1. Introduction

Nowadays, computer modeling is widely used in different spheres of human activities. In particular, its methods are applied in solving ecological (radioecological) tasks. It is due to great capabilities and versatility of computer modeling means. First of all it is the possibility to describe the operation and forecast the effect of a separate process without interfering into the process itself. Thus, it gives the possibility to determine the future effect of some physical phenomenon that in its turn provides large-scale possibilities for controlling, monitoring or forecasting functions [1].

Therefore, there is a great number of ways of designing the models. Firstly, it depends on the scope of application. According to the radioecological tasks, the models can be divided into the data-driven (empirical) and science-based (theoretical) models. Frequently, the combinations of these two approaches find practical application [2].

With reference to solving the ecological tasks and in particular to the soil pollution problems, we may distinguish a number of problems in their rigorous physical-mathematical description. It depends on different factors, such as:

- Soil dispersity.
- Variety of meteo conditions.
- A host of affecting forces.
- Chemical and radioactive transformations.

One method to solve the problem of computer modelling of contaminant behaviour in a ground-water system is the model of impurity migration in soils developed by the authors [3]. The distinctive feature of this model against previous models is the more rigorous description of non-isothermal water transport based on the laws of thermodynamics and physics. This is based on differential equations for convective diffusion, liquid and gas flow and thermal conductivity.

Using some simplifications (region localization, averaging-out of the influence values and forces, introduction of additional empiric coefficients) it is possible to obtain a qualitative theoretical model. However, the practical application of this model needs, in general, more flexible and dimensioned computations including high solving speed and visualisation. In that case it is reasonable to expand the computer model and to introduce there additional instruments which make it possible to realize a quick approximation and forecasting based on empirical, statistical and other approaches.

The selection of the forecasting instruments is determined by the available data on the current process as well as by the requirements imposed on the forecasting. In our case we have a bulk of data on the vertical migration of caesium and strontium in the soil. At the same time it is required to get the most qualitative and quick forecast on the migration of radioactive substances in the soil across the sizeable territory. In that case the most expedient way is to use the hybrid expert systems (HES) [4].

The power of the HES is explained by the use of advantages of expert systems (ES) and artificial neural networks (ANN) in them. Their functionality is based on the accumulation of experience in the experimental data base; on the adjustment of the solution due to the change in the experience, as well as saving all experimental data in the data base. Therefore it is the main condition for the future improvement of the model.

2. Hybrid expert system

The main mechanism of the HES is the self organisation and training. It is represented by the ANN and rule-based system or ES structures. There are several levels of the organisation and internal communication of the HES components, as the HES task solution requires. These levels are defined by the ratio between the "neural networks" and "rule-based system" [4].

In the current work the "Modular hybrid systems" structure is used. A key defining characteristic of it is the hierarchy of module configuration, the complexity of which determines the information flow between the modules. The communication between modules has a sequential organization. Sequential processes imply that one process must be completed before data may be passed to the next module. One module acts as a data pre-processor extracting features required for the next module. This structure allows to use all the advantages of ANN and ES. These include the speeding up of training process; high speed results; data accumulation, addition and registration capability (domain pool).

2.1. Creation of hybrid expert system

Fig. 1 shows the general structure of the HES, applied for the forecasting of radionuclides' migration in the soil.

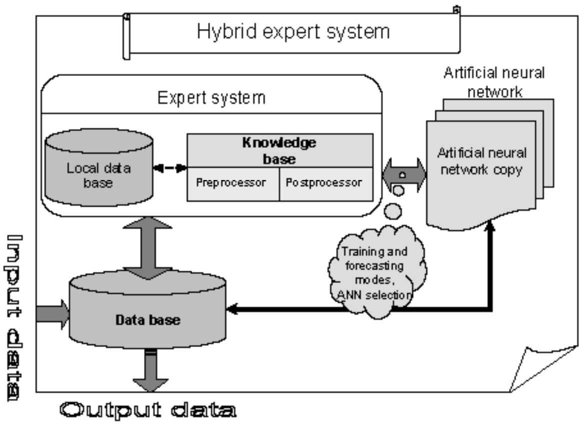

Fig.1. The hybrid expert system structure.

It is shown that HES does not focus on the class and type of contaminant substances during the forecasting process. Specific features of this domain are considered at low levels of the HES structural organization; specifically, when the knowledge base for the expert system is being built.

Fig. 1 shows that one of the main components of the HES is ES. Its functions include the data preliminary classification and organization, as well as further data postprocessing. This role is assumed by the preprocessor and postprocessor which are parts of the knowledge base which also includes logical links between numerical and symbolic data, as well as various methods which make use of it. The ES has a static organization and doesn't include a modification function.

Local data base is used for saving and keeping intermediate, initial and most successful ANN conditions. Besides, it keeps specific information (rules, symbolic forms and so on) for the knowledge base operation. The structure of HES also includes the general data base. It stores input, experimental, training and calculated data. Besides, it saves and keeps output data (forecast data). Availability of this data during the operation of the system is the main prerogative for the reorganization of the ANN's conditions, which fact determines a dynamic work of the HES as a whole.

ANN module is the central part of HES. It is the main forecast element of the system. It has its own structural specificity and instruments. Its dynamic aspect is connected with the creation of several copies of ANN, each of them characterizing different self conditions required for solving specific tasks. A significant feature of the neural network is that it has two operating modes: training and forecasting [5]. A specific feature of the current ANN configuration in the training mode is that it saves an old condition in the local data base for the future comparison of the conditions. The purpose of the comparison is to find the best ANN's condition which is more valid for the current task.

The pre-processor, together with the post-processor, classifies the ANN's copies in conformity with the knowledge base principles. During the system operation, it appears as a concrete definition of the task being solved (radionuclide type selection) and error estimation from some ANN (only in the system testing mode). If the ANN produces an erroneous result, the HES correction mechanism will be enabled. Its function is to retrain an additional neural network in order to increase forecasting accuracy.

2.2. Tasks and structure of Artificial Neural Network

As it was noted before, the HES main computing part is the ANN. The description of the basic elements, their operation principles and the ANN training algorithms are to be found in different respective publications. The main accent of the current work falls on the ANN's structure with regard to the task being solved.

It is proposed to use one copy of ANN for each radionuclide (for example ^{137}Cs, ^{90}Sr) because there are a lot of radioactive elements, and the classification capability of the ANN will be totally decreased. Following this architecture, the ES solves the problem of the ANN selection and its training algorithms. Furthermore, the ES implements the input and output data normalization tasks.

It is significant to note, that the ANN is a formal language that describes the interconnection between input and output parameters using well-known and understandable functional dependences.

The most popular ANN architecture is multi-layer perceptron (MLP). It is a type of ANN with a specific structure and training procedure. The main component of MLP is the formal neuron, which sums the inputs, and performs a transform via the activation function. The activation function (or non-linear transformer) may be given by any continuous, bounded and non-decreasing function, such as the commonly used exponential sigmoid or hyper tangent. Activation function was employed only in hidden unites – output neurons have linear function. MLP of such structure is a universal approximator.

In a standard MLP neurons are arranged in input, hidden and output layers. The number of input and output layer neurons depends on the data dimension. The number of neurons in the hidden layers can vary and it is the user's task to choose the optimum configuration. As long as the aim of MLP in the present work is to extract large-scale trend, the number of hidden neurons was chosen as small as possible to be able extract the non-linearity. Further increase of the number of hidden neurons leads to extracting more detailed local peculiarities of the pattern, then in such case not only general trend will be modeled by MLP that contradicts the idea of the approach. Choosing too many hidden neurons will then lead to over-fitting (or over-learning) when MLP looses its ability to generalize the information from the samples. On the other using too few hidden neurons does not provide explicit extraction of the trend, hence some large-scale correlation will remain in the residuals restricting further procedure. Also the complexity of the MLP must be consistent with the amount of information for training – there should be enough data to match every connection.

As a result, the following (fig. 2) architecture of ANN for forecasting radionuclides' migration is proposed.

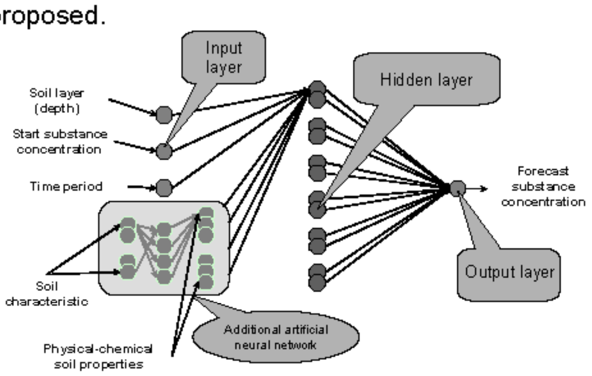

Fig. 2. The structure of artificial neural network.

As is shown (fig. 2), in the ANN simple version the input layer has four signals (neurons). The first signal means a layer or a depth of the soil (metres) where the substance concentration is determined. However, as it was noted before, the ES normalizes this value as the interval (0,1]. The second parameter is the initial substance concentration at the start time. The third parameter characterizes a time period (months, years) expired from the start time to the forecasting period. As for the fourth parameter it is multiple. It includes a type and a class of porous media, meteo conditions, grading of soil, moisture and saturation. As an alternative to the soil characteristics data, there can be more specific physical and chemical soil properties.

It is efficient to build an additional ANN (fig.2) for the filling up the data base of the information about the soil properties. The function of this ANN is to forecast physical and chemical soil properties through the type and class of porous media, meteo conditions, grading of soil, moisture and saturation. The outputs of this additional network are connected to the main ANN inputs. Besides, the information obtained from these outputs can be used in the mathematical model.

The output value from the main ANN is the percentage of the forecasted substance concentration. This value characterizes the change of the substance concentration during the certain time period (which is entered into the input of ANN) in the given soil layer and type. The output value is required to do the normalization in the interval of (0 - 100].

For the ANN training it is planed to use the error back-propagation algorithm. It is applied to calculate gradient of MSE on adaptive weight. Various optimization algorithms, which employ back propagation, can be used such as the conjugate gradient descend method, second-order pseudo-Newton Levenberg-Marquardt method, or the resilient propagation method [6].

3. Program development for forecasting migration of radionuclides in the soil

The specific feature in the application of computer modeling methods in the domain under consideration, as it was noted before, lies in formulating algorithms, objects and classes diagrams of the mathematical migration model and HES, with their subsequent program realization. This allows to carry out computational experiments, train and modernize the system, collect experimental data using minimal time-consuming and resource-intensive experimental tests [7].

An algorithm of the system application is as follows: by using the HES, a user can get an approximate estimation (the accuracy is within the limits of 20-30%) of radionuclides' migration in the soil taking into account meteorological conditions, a specific type and characteristics of the soil in the given region and the type of flora. After that, in case the results provoke interest for further analysis, there is a possibility to make more accurate estimates of radionuclides' migration with the use of a formalized mathematical model (if there is a need to specify additional boundary conditions).

Fig. 3 presents an application framework, including the formalized HES and a mathematical model.

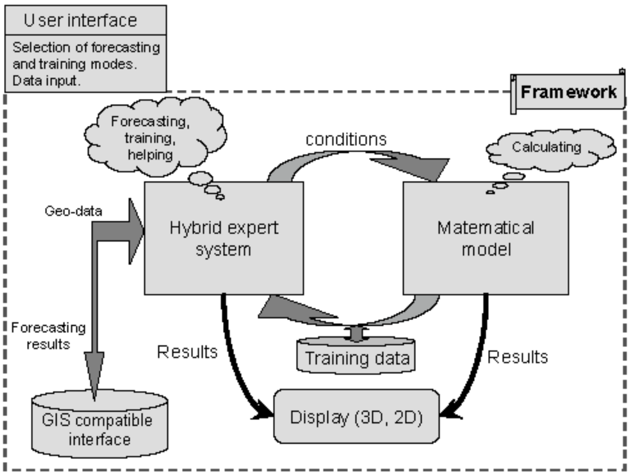

Fig.3 – Framework for forecasting radionuclide`s transport in the soil.

When working with the system a user can set different modes of its operation. These are the forecasting and training modes. The first one involves the use of the HES and a mathematical model. As it was discussed above, the HES makes a dimensioned approximate forecast, and for its future specification it is assumed to use a mathematical model. However, the input data for the estimates it will get from the HES.

This action simplifies the use of the system (in the automatic mode it will enter a boundary conditions by itself; in the manual mode a user can control the entering of the data).

The analysis of the obtained results can be made by means of the program-integrated tools (fig. 3) like two- and three- dimensional result visualizations or by the external geo-information systems (GIS). A GIS integration function will perform a separate module of the program. In addition, it will have a possibility to receive the geo-data from GIS to forecast the function realization.

The second mode of the system is the training one. It is used for upgrading the HES condition in order to get the more qualitative forecast information.

4. Conclusions

In the course of work, the issues in regard to the application of computer modeling methods for the analysis and forecasting of radionuclides' migration in the soil were considered.

Specifically, available means for the construction of computer models in the field of radioecology were analyzed.

Within the framework, a joint use of HES and a mathematical model in the object domain was proposed.

This will allow to use all advantages with respect to the speed and self-organization of HES as well as the forecasting accuracy of mathematical models.

Thus, such structure will allow flexibly, effectively and quickly enough to solve issues with regard to the analysis and forecasting of migrations of radioactive substances in the soil.

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