MATHEMATICAL MODELLING WITH USE INFORMATION-COMMUNICATION TECHNOLOGIES IN COURSE STUDYING ECOLOGICAL TOXICOLOGY

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Abstract

Ecological toxicology (ET) – one of is natural-scientific (NSE) courses for which studying theoretical knowledge of mathematics is necessary, for chemistry, biology and others NSE courses. Biological experiments are necessary for fastening of theoretical knowledge on laboratory animal and biological test objects. For carrying out of such experiments laboratory animals, biological objects are required, and also the necessary equipment, reactants, etc. Considering the humane relation to animals and restriction of their use in experiments, methods of mathematical modeling in course studying «ET» are offered. Besides, use of interactive control facilities by the information allows modeling some processes in ET. Authors conduct researches at engineering faculty of the Rezekne Higher Education Institution by preparation of engineers of protection of environment. As a result of the spent researches it is established that at students the greatest interest to studying as course ET, and a course – «Mathematical methods in environmental science» is shown. Students can visually see practical use of mathematical methods in is natural-scientific courses. ICT application supplements better mastering of a material at a studied course. Mathematical modeling with use ICT in course studying ET raises progress of students and gives the chance to use theoretical knowledge on the mathematician.
Keywords: *ecological toxicology, information-communication technology, mathematical modeling, Rezekne Higher Education Institution, study process.*

Introduction

To improve the quality of education, especially in the context of economic crisis, you must use a number of positive training methods, both in secondary schools and in universities. One such method is the mathematical modeling using ICT. Environmental toxicology (ET) – one of the NSE courses, for which the required theoretical knowledge of mathematics, chemistry, biology and other NSE courses.

ET studying reactions of biological systems, mainly Superorganismal level (population, ecosystem) to the effect of alien chemicals. In the area of her interests is the spread of physical and chemical agents and their transformation in the environment and the organism, biological accumulation, and akklimat-

sionnye cause toxic effects, the ways and forms of adaptation of biosystems to new physical and chemical components of the environment, the sustainability of ecosystems in terms of toxic load. Toxicology is the study of a variety of toxic effects at different levels of the organization of the biota - organismal, population and ecosystem (Безель,2002; Калинкина, 2008).

To consolidate the theoretical knowledge and solutions the aforementioned problems in the ET used in laboratory experiments. Such experiments can measure the effect of toxic substances on biota. Figure 1 shows the use of laboratory studies in ET (Калинкина, 2008).

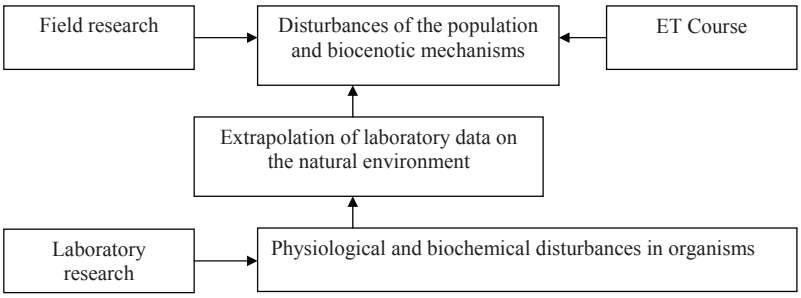

Figure 1. Methods for ecotoxicological studies.

These toxicological experiments (TE) are the key to understanding the mechanisms of functioning of populations and ecosystems under conditions of toxic effects. For the TE traditionally used laboratory animals (mice, rats, rabbits) and other biological test objects (Израйлет, Яриновский, Страпч, 1978; Фридман, 1982).

Implementation of TE, especially if they are connected with full toxicological evaluation of a large class of compounds presents considerable difficulties. It is connected first, with considerable economic costs and, secondly, long-term 2-3 years, such studies (Яриновский, Гредин, Замах, 1982). Experimental studies of toxicity of a large group of compounds showed that the toxicological characteristics of individual groups of compounds can be carried out mathematically. In this case, the authors used mathematical modeling using interpolation and extrapolation in the series of compounds with similar chemical structure, physico-chemical properties and biological effects.

In connection with the above (Яриновский, Кангро, 1999) study of the toxicological properties of new compounds should be conducted using mathematical methods with mandatory follow-up experimental justification toxicity of individual representatives of each class of compounds. Mathematical modeling of the valuation of new chemical compounds in the environment and food authors recommend the use in conducting laboratory and practical work of students in the specialty "Environmental Protection".

In recent years, several researchers (Жмур, 2001) offer new methods used in ET. Thus, the definition of toxicity of water and water extracts from soils, sewage sludge, waste is recommended to examine changes in mortality and fertility tseriodafnies (Ceriodaphnia affinis, Cladocera, Crustacea). Determination of acute toxicity of water samples in laboratory conditions were studied for the reduction of chlorophyll fluorescence and reduce the number of green cells of algae of Scenedesmus quadricauda (Жмур, Орлова, 2001). The criterion for acute toxicity in this case is the suppression of the level of chlorophyll fluorescence of algae or a decrease in the number of algal cells by 50% or more compared with the control within 96 hours of exposure.

Usage a dynamic model on ET describes Коросов, 2002; Коросов, Калинкина, 2003. Dynamic model ET are used to describe the speed and the result of events occurring over time. They provide an opportunity to focus on every point (stage, step) implementation process, thus reveal the mechanism and allow us to understand the causes of phenomena. The task of mapping the dynamics of phenomena effectively handle the analytical model (a system of differential equations), requiring highly specialized knowledge, as well as simulation algebraic models, which under the force to build everything. This was made possible thanks to a widespread package of MS Excel, on the electronic pages that are built model formulas and calculations are carried out, and built-in program optimization Solver allows to find the best values of model parameters – the coefficients in the model equations. A simulation model designed

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to calculate and play on computer screens the same changes in the characteristics that were observed in experiments, for example, calculate how many animals must die to the current point in time or in the concentration of toxicant, that is to reproduce the curve «dose-of the effects».

Methodology of Research

Studies conducted in the Engineering Faculty of Rezekne Higher Education Institution (RHEI) since 2005, together with the students of 2 courses. Object of study - the process of training students 3 courses, specializing in engineering environment. To study the toxicological processes, mathematical modeling and prediction of toxicity of chemical compounds used mathematical calculations of acute toxicity ($DL_{50\%}$), maximum permissible concentration (MPC) and other parameters toximeters. In addition, were used existing computer programs (Kliedere, 2003). Programming ET performed in conjunction with the students of 2 courses of the speciality "Engineer-Programmer". According to the research a number of students (Lobazova, Avotina, 2007; Lobazova, Seimanovs, 2006; Pavlukevics, 2005; Seimanovs, Civkors, 2007) carried out research work under the guidance of the authors. The results of research students have been published in the student's scientific works.

Result of Research

In the ET used in laboratory experiments with biological objects. The main criteria for evaluation of the toxic substance is its toxicity, the danger. Toxicity of compounds is measured by indicators $DL_{50\%}$ (average fatal dose of a substance in a single dose which kills 50% of laboratory animals at 10-day observation period). For a preliminary assessment of toxicity and hazard of the compound sufficient to have the value $DL_{50\%}$, physico-chemical characteristics of matter, the possibility of pollution and literature data on the toxicity of compounds.

To calculate the DL50% of toxic substances using the formula:

$$DL_{50\%} = \frac{\Sigma(a+b)(m-n)}{200}, \text{ where} \qquad (1)$$

Σ – summation sign standing after the values; a, b – values of related doses; m, n – frequency of deaths, %; 200 – constant coefficient.

Table 1. Initial data for calculating $DL_{50\%}$ toxic compounds.

Group of animals	The dose of toxicant	Quantity of animals		% of death	Relevant probits
		alive	death		
I	550	7	0	0	3.2
II	1100	4	3	43	4.82
III	1550	2	5	71	5.57
IV	2000	0	7	100	6.8

Using the formula 1 and the initial data tables 1,2, it is easy to calculate $DL_{50\%}$ of the toxic substances in experimental animals.

Table 2. Expression of the death of animals in the experiment in probits.

Quantity of animals in group	Probits in fatal outcomes	
	0%	100%
3	3.62	6.38
4	3.47	6.53
5	3.36	6.54
6	3.27	6.73
7	3.2	6.8

From graphic (statistical) methods of calculating $DL_{50\%}$ convenient and simple method of probit analysis, which the authors used in their studies. Using this method we can construct a schedule for the indicators listed in Tables 1,2 and find $DL_{50\%}$ of the compound (Figure 2).

No less important indicator of ET is the maximum permissible concentration of harmful substances in the air, water, soil, and in food. Using mathematical modeling in ET, in the presence of data on the compound: physico-chemical properties, chemical structure, biological activity, $DL_{50\%}$, we can calculate the maximum permissible concentration of virtually any chemical compound. Studies have shown that computational methods for determining the MPC is not much different from the experimentally based (Яриновский, Кангро, 1999).

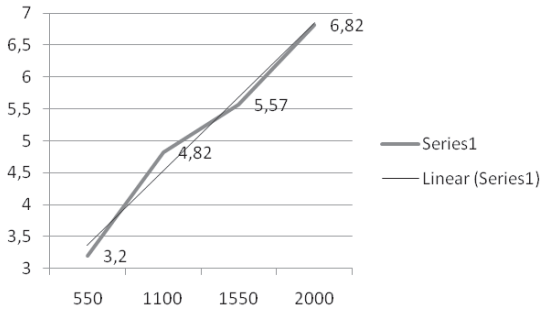

Figure 2. Calculation $DL_{50\%}$, using the method of probit analysis. Notes: Vertical - probits, horizontal - dose, mg / kg.

Evaluation of the concentration of hazardous substances in specific locations of water courses require many complex with a control measurement. This process can be simplified by using a mathematical solution - it is possible to predict the concentrations of hazardous substances, according to the characteristics of the substances instead of leakage, and taking into account the characteristics of the water bleeding. For this purpose it was created two computer programs that use mathematical algorithms and allow the situation to some extent, be modeled by setting each parameter and the effects of toxic substances in surface waters to the overall result. The Microsoft Excel program (Figure 3) was set up to work with the site and input the necessary values to calculate.

The program was implemented in Microsoft Visual Studio. NET environment, programming language C + + using object-programming and visual programming tools. Program (Figure 4) also provides the opportunity for input to make changes to the substance list, therefore, is seen as an individual presence of the substance and parameters affecting the overall toxic hazard. The advantage of this program is that the program can operate on any computer with the Windows operating system and does not need any additional software unlike Microsoft Excel tables. Both programs were tested with control examples and gave accurate and reliable results.

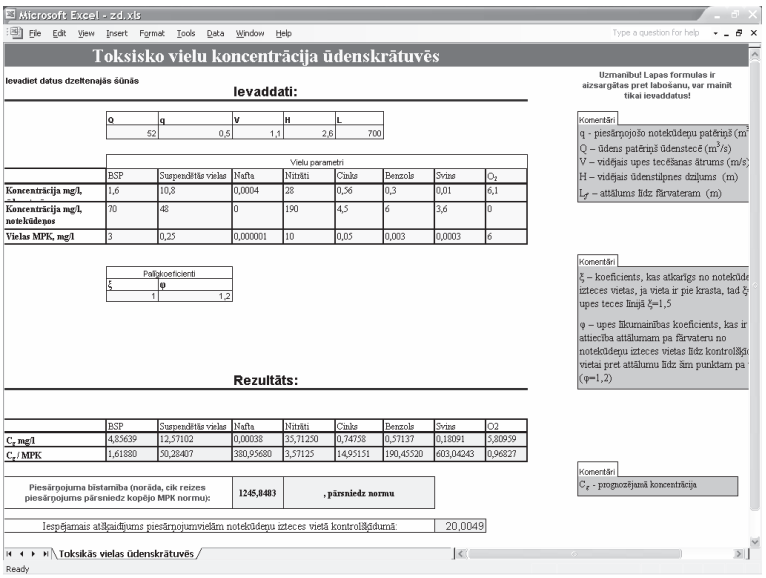

Figure 3. Excel program window.

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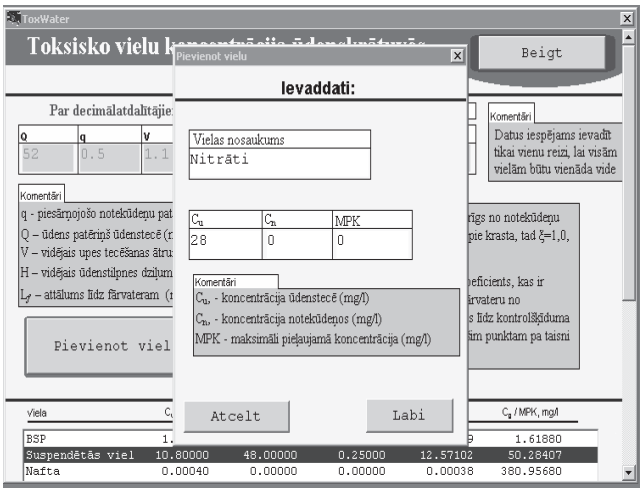

Figure 4. **C++ program window.**

Program "Contaminated groundwater, the volume and quantity of pollutants in the evaluation." The program developed the database management system, Microsoft Access 2003 (Figure 5, 6). The program for the average pollutant concentrations, the volume of contaminated water, the quantity of pollutants and compensation for groundwater pollution in the calculation.

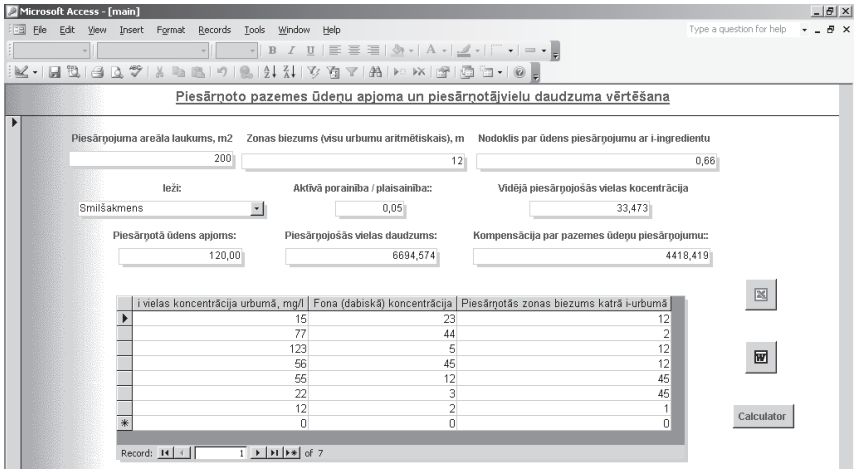

Figure 5. **Database program window.**

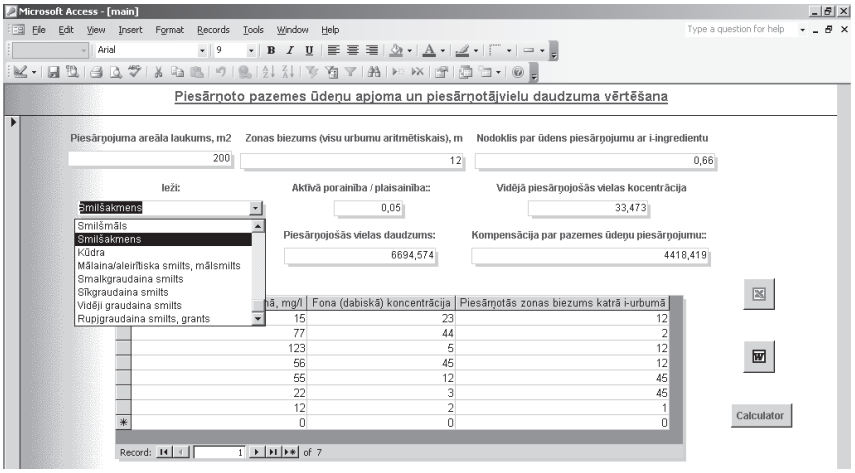

Figure 6. **Database form menu.**

The program allows the user to obtain the desired results much faster and without mistakes, which significantly facilitates the processing of data for groundwater contamination and the amount of pollutant inventory.

Conclusions

- To improve the quality of education at the rate of ET is proposed to use mathematical modeling using ICT.
- Most audiences of RHEI equipped with ICT (computer, interactive boards, etc.) that allows you to demonstrate how the lecture material, and modeling of many processes in ET.
- Use of simulation models in the learning process allows one to calculate and reproduce the same changes in the characteristics that are observed in laboratory experiments. The model reflects the successive changes of the biological system used in the test objects.
- Featured in the program we know ET allow relatively quickly and correctly handle the initial data obtained from experiments and demonstrate the action of toxic compounds on biological test facilities and environmental systems (water, air, soil, food, etc.).
- Use of mathematical modeling with the use of ICT in the learning process increases the interest and students performance, facilitates the presentation of new material and allows a better understanding of many biological and biochemical processes in environmental toxicology.

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