Journal of Theoretical and Applied Information Technology

15th November 2023. Vol.101. No 21

ISSN: 1992-8645 www.jatit.org E-ISSN: 1817-3195

REPRODUCTION OF COMBINED EFFECTS ON ECOLOGICAL SYSTEMS AND THEIR COMPONENTS IN SIMULATION MODELS

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ABSTRACT

The study aimed to develop an algorithm for reproducing the simultaneous impact of various factors, both biogenic and anthropogenic, on ecological systems and their components in simulation models. Simulation models are effective tools in predicting and understanding the complex interactions between biogenic and anthropogenic factors in ecological systems that help to develop conservation strategies and sustainable resource management. The authors constructed the EcoCombi model, which reproduced the dynamics of the number or biomass of living components of biological systems that are under the combined influence of two or more factors. The object of the simulation was a terrestrial ecosystem consisting of the following components: soil, herbaceous vegetation, herbivores, and predatory animals. As a result, an algorithm was developed for reproducing the multifactorial impact on the object, based on which simulation models can be built and implemented, allowing for the prediction or reconstruction of various environmental situations associated with the simultaneous impact of various factors, both biogenic and anthropogenic, on ecological systems and their components. Based on the results of numerical experiments, it was found that an exhaustive account of the object's properties played a key role in an effective assessment of the consequences and forecasting of the combined effects of factors on the object using a model. It is also important to consider the nature of the impact of the factor (mono- or poly-impact on the vital processes of organisms, single or chronic exposure). The proposed algorithm applies to any situation where there is a multifactorial impact on the object. In this respect, it can be effective for reproducing most of the environmental processes observed during technogenic pollution.

Keywords: *Factorial Ecology, Combined Impact, Simulation Modeling, Ionizing Radiation, Ecotoxicants.*

1. INTRODUCTION

In natural conditions, ecosystems and their components are exposed to a variety of environmental factors of biotic and abiotic nature, which, as a rule, have a combined effect on the ecological processes [1, 2]. This is the subject of interest in factorial ecology (autecology). In addition, the biosphere has long been under the influence of various kinds of anthropogenic factors that can also have a joint impact. Environmental pollution with several ecotoxicants at once [3, 4] and even in combination with ionizing radiation is a common phenomenon that is receiving increasing attention [5-7]. Thus, we can talk about expanding the sphere of interest of factorial ecology and including in it three groups of endogenous and exogenous factors: abiotic, biotic, and technogenic (anthropogenic).

To predict the simultaneous impact of several factors of different nature on individual organisms, their communities, ecological systems, and the biosphere, it is necessary to formalize our ideas about this phenomenon. Our research was aimed at developing a model for predicting the simultaneous impact of several different factors on individual organisms, their communities, ecological systems, and the biosphere. In factorial ecology, the formalization of ideas about the combined effects of environmental factors has already received its interpretation [8], but the disturbance in the already established conditions for the functioning of biological and bioinert systems caused by humans and the expansion of the spectrum of anthropogenic impacts has long dictated the need for a new approach to solving this issue.

2. LITERATURE REVIEW

2.1 Impact of Several Factors on the Object

The primary solution to formalizing information about the impact of several factors on a given object is to conduct a full factorial experiment and use multiple regression analysis [9]. However, the impact of factors may be nonlinear, and the interaction of factors with each other is also possible, which significantly complicates this task.

If we proceed from the definition of a combined action as the simultaneous impact of several factors, when considering the example of a two-factor impact, the following options are possible [10]:

1) Additive action (the action of factors is summed up). The total effect is equal to the sum of the effects of all the factors of influence;

2) Synergism (enhancing the effect, one factor enhances the effect of the other);

3) Antagonism (one factor weakens the effect of the other);

4) Independent action (the combined effect does not differ from the isolated action of each factor). The effect of the most potent factor prevails.

In the case of more factors, the picture will be more complex. It should also be considered that the impact of the same factor, depending on any internal or external conditions, can be multidirectional, and its interaction with other factors of influence can also be ambiguous. Furthermore, the methods of exposure to the same object may be different and have different effects (for example, the pathways of ecotoxicant entry into the body or internal and external exposure to ionizing radiation) [11].

2.2 Simulation Modeling

In this case, from our point of view, the most adequate tool for displaying such situations in a formalized way is simulation modeling [12]. The implementation of a mathematical model in the form of a computer program allows us to consider and display the impact of almost any possible combination of factors, the reaction of the object which is represented in the form of particular response functions. Attempts to build such models have been made with variable success for a long time, since the 1970s. As for natural environmental factors, the consideration of their combined influence on biological processes is present in many ecological models of that period, for example, in models of carbon behavior in various terrestrial ecosystems [13]. There are much fewer models in this respect that also reflect anthropogenic influence. Nevertheless, they exist. As an example, let us recall the model of a three-species ecosystem [14], which implements an approach that allows considering the combined thermal effects and eutrophication of a reservoir on the dynamics of biota. Also interesting in this regard is a simulation model of a laboratory algal community built to study the effect of different concentrations of nitrogen and phosphorus on the structure and dynamics of phytoplankton biomass [15].

2.3 Possible Approaches to the Formalization of Combined Impact in Ecology

A common method of formalizing phenomena in factorial ecology is the use of multiple regression analysis [16]. This method is used in ecology to study the possibility of predicting changes under the influence of two or more factors of any parameter of the functioning of an ecological object based on data obtained during preliminary studies. It is assumed that the relationship between the values of the dependent variable (parameter or function of the object) Y and several independent variables (factors) X can be expressed by the following linear equation:

$$Y = b + b1x1 + b2x2 + \ldots + bnxn + e \qquad (1)$$

where Y is the variable; $x\ 1, x\ 2, \ldots.\ x\ n$ are factors; b, $b\ 1$, $b\ 2$, ... $b\ n$ are model parameters, and e is the prediction error. However, the impact of factors can be and most often is nonlinear. This requires us to take other approaches when formalizing phenomena that fall within the sphere of interest of factorial ecology.

Another way of formalization in this area can be an approach from the standpoint of mathematical analysis, i.e., the selection of a universal mathematical formula reflecting the observed patterns of the combined influence of environmental factors on organisms and ecosystems. In this case, specific factors with their share of influence are combined into complex factors. The proportion or otherwise the weight of factors reflects the local features of the environmental impact on the body [17]. However, the variety of factors and features of ecological systems and their components does not, in our opinion, adequately reflect the real picture formally in this case. From our point of view, the method of simulation modeling in such a situation is a more convenient and effective tool.

When simulating a set of impacts on an object, one can use the concept of the space of environmental factors [8] and operate within this space, selecting mathematical equations, the so-called response functions that quantitatively characterize the influence of one or several factors on the object as a whole or its individual properties, for example, growth rate, productivity, mortality, etc. The forms of particular response functions can be very diverse. The most typical dependences of the functions of a biological object on various factors in two-dimensional space can be displayed by straight lines, exponents, parabolas, and sigmoidal curves. Piecewise defined functions are often used, which may have thresholds, triggers, plateaus, etc.

The next key point in the formalization of the combined effects of several factors is the assessment of the importance of factors and variants for considering this. If we use the laws of Liebig's minimum and Shelford's tolerance and single out the most important factor that is most significant for our object, then the remaining factors can be neglected, and then the algorithm is reduced to including the corresponding equation reflecting the dependence of the functioning of the object on this limiting factor in the model. However, such situations practically never occur in nature. The importance of a factor is a variable value, and in certain conditions or at a certain time interval, another factor may come out on top. In addition, it is necessary to consider the possible interaction of factors, as already mentioned above. Ecological processes, by their very nature, fall under the law of the cumulative effect of the Mitcherlich-Baule factors, and their occurrence depends on the totality of the factors acting simultaneously. In this case, the effect of the two factors can be represented as follows:

$$\Delta C = a12 * f1 * f2 * C \tag{2}$$

where *a12* is the coefficient or function of the interaction of factors 1 and 2, *f1* is the influence of factor 1 on *C*, *and f2* is the influence of factor 2 on *C*.

In our simulation models [13, 18], we successfully used this approach in the equation of photosynthesis intensity. However, as noted earlier, in practice, the factors affecting the biological system are in various relationships with each other. This may require adding other elements to Equation 2.

To reproduce the functioning of ecological systems of different levels that are influenced by factors interacting with each other, we developed an algorithm that assumes that the object of modeling is a system that is a set of components subjected to a combined internal or external impact. The components can be interconnected and affect each other. Thus, the quantitative characteristic of a particular *i*th component of the system *Ci* (for example, biomass) that interests us is a variable that depends differently on *n* factors, for example, as in Equation 2, and the impact of other components may be included in the number of factors. The algorithm allows the connection of additional blocks that allow for reproducing the dynamics of factors to simulate a variety of environmental situations. The discreteness of consideration of ecological processes is determined by the specifics of the ecosystem, the time scale of the factors, and the availability of the necessary initial information. Models based on this algorithm can be either point-based or distributed.

The study aimed to develop an algorithm for reproducing the simultaneous impact of various factors, both biogenic and anthropogenic, on ecological systems and their components in simulation models.

3. MATERIALS AND METHODS

3.1 Exposure to Ecotoxicants and Ionizing Radiation

From our point of view, the combined effect of ecotoxicants and ionizing radiation is of particular interest. Based on the algorithm presented above, we developed the EcoCombi simulation model. As an example of a possible application of the model, let us consider its reproduction of a specific situation of exposure in a laboratory experiment to nitrates (addition of NaNO3 to water) and a single acute γ-radiation on the culture of cladoceran freshwater crustaceans *Daphnia magna L.*

It is assumed that the population in question is initially in a state of complete equilibrium with the environment and is supplied with food in an amount conducive to maintaining a constant number of the hydrobiont community (*Y*). Since the conditions are favorable, the community consists only of females, and reproduction occurs parthenogenetically. The average lifetime of each individual in the laboratory is 3 months.

The change in the number of crustaceans *Y* is described by a finite-difference equation of the following form:

$$\Delta Y = (a1 * (1 - ang * (fn + fg)) * Y - (b1 * (1 + bng * (jn + jg)) * Y \tag{3}$$

where: $a1$ is the fertility of one female per day; $b1$ is the mortality (in terms of one individual) per day; *a*ng is the coefficient of interaction of factors when they affect fertility; *fn(N)* is the proportion of fertility reduction depending on the concentration of nitrate ions; *fg(G)* is the proportion of decreased fertility depending on a single dose of gamma radiation; *bng* is the coefficient of interaction of factors when they affect mortality; *jn(N)* is the proportion of increased mortality depending on the concentration of nitrate ions; *jg(G)* is the proportion of increased mortality depending on a single dose of γ-radiation.

The functions *fn*, *fg*, *jn*, and *jg* are calculated using a Pearson curve of the first kind:

$$BELL = ((A - B)/(C - B))e*((A - D)/(C - D))e*((d - c)/(c - b)) \quad (4)$$

which describes the asymmetric bell-shaped dependence of the process on the value of the argument a and is equal to 0 for $a \leq b$, $a \geq d$, taking the maximum value of 1 for $a = c$. The argument e is responsible for the width of the bell, the smaller its value, the wider the bell.

The magnitude of the model parameters was determined using regression analysis and the iteration method during numerical experiments with the model based on data obtained during laboratory experiments by G.A. Tryapitsina et al. [19, 20].

3.2 An Ecosystem with a Full-Fledged Food Chain

The most interesting from an ecological point of view is the situation with the combined impact of anthropogenic factors on the ecosystem, the components of which form a full-fledged food chain. It is extremely difficult to conduct an experimental study of the consequences of such an impact on such an object, especially if the participants in such a chain are large long-lived animals. In this case, to get at least an approximate estimate of the possible damage, one can limit one's work to a general description of the situation.

To illustrate this approach, let us consider a version of the EcoCombi model designed to reproduce the combined effects of ionizing radiation and chemical pollution on the biota of the food chain. The object of modeling is a terrestrial ecosystem consisting of the following components: soil, herbaceous vegetation, herbivores, and predatory animals. The EcoCombi_FC (food chain) model includes the main unit for calculating the biomass dynamics of living system components and two auxiliary modules.

The topological structure of the model in the form of a flowchart is shown in Figure 1.

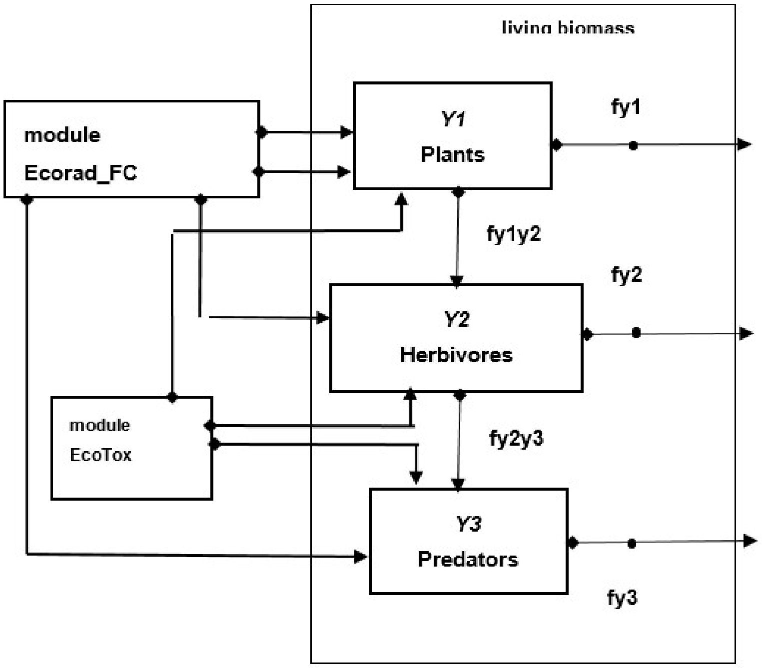

Figure 1: The Conceptual Scheme of the EcoCombi_FC Model. The Transfer of Matter is Shown by Solid Lines, and the Information Links are Dotted

As the first module, the previously developed Ecorad_FC (food chain) model is used, describing the behavior of 137Cs in the chain "soil – producers – consumers of the 1st order – consumers of the 2nd order", where the dynamics of the dose load on living organisms is also calculated [21, 22]. The EcoTox module reproduces the dynamics of the intake and maintenance of one or more ecotoxicants in the system.

The state variables of the main block of the model are *Y*1: vegetation, *Y*2: herbivorous animals, and *Y*3: predatory animals. Units of measurement: g*m-2. The model is deterministic and point-based, i.e., the values of variables are determined unambiguously, and the values of state variables change only in time. The time step *t* in this version of the model is equal to 1 day with a possible subsequent averaging over the year to neutralize the seasonal heterogeneity of radioactive and chemical contamination of food resources. It is accepted that in the absence of external influence, the ratio of biomass in terms of vegetation, herbivores, and predators corresponds to the ratio in the classical food pyramid of 100:10:1.

The model is described by the following system of finite difference equations:

$$\Delta Y1 = f11(sef, d, v1, \ldots, vn) - f12(d, v1, \ldots, vn) - f13(Y2) \qquad (5)$$

$$\Delta Y2 = f21(d, v1, \ldots, vn) - f22(d, v1, \ldots, vn) - f23(Y3) \qquad (6)$$

$$\Delta Y3 = f31(d, v1, \ldots, vn) - f32(d, v1, \ldots, vn) \qquad (7)$$

where *sef* is the natural environmental factors (solar radiation, air temperature, soil moisture, etc.), *d* is the dose load, and *v1,...,vn* is the pollution of the ecotope with ecotoxicants.

The functions of biomass growth and death of members of the food chain *f11*,*f12*,*f21*,*f22*,*f31*, and *f32* are described by Equation 2. Let us focus on the consumption functions *f13(Y2)* and *f23(Y3)*. Here phytophages and predators act as natural factors of influence, respectively, on the biomass of vegetation and phytophages. Therefore, the parameters of the equations were selected in such a way as to ensure the ratio of the biomass of the classical food pyramid. Depending on the availability of initial information, these functions can be represented by simple linear equations or more complex ones, for example, considering seasonal fluctuations in biomass and activity of animals, members of the food chain, or network. In each specific case, this should be solved by the objectives of modeling and with the specifics of the impact. In the considered version of the Ecorad_FC model, linear equations were used.

To test the validity of the EcoCombi model, we reproduced the impact situation of factors of varying severity for different members of the food chain.

4. RESULTS

In the absence of specific information on each factor, an integrated approach to accounting for their impact is possible, using coefficients of the total impact of factors (suppressing or stimulating). Given that the peculiarities of the impact of complex pollutants on natural objects have been studied little, perhaps this is the most rational approach in this case. Figure 2 shows the results of reproducing such a version of the model of the impact situation of varying severity for different members of the food chain. In variant A, all members of the food chain are suppressed to varying degrees, and in variant B, consumers of the 1st order are stimulated.

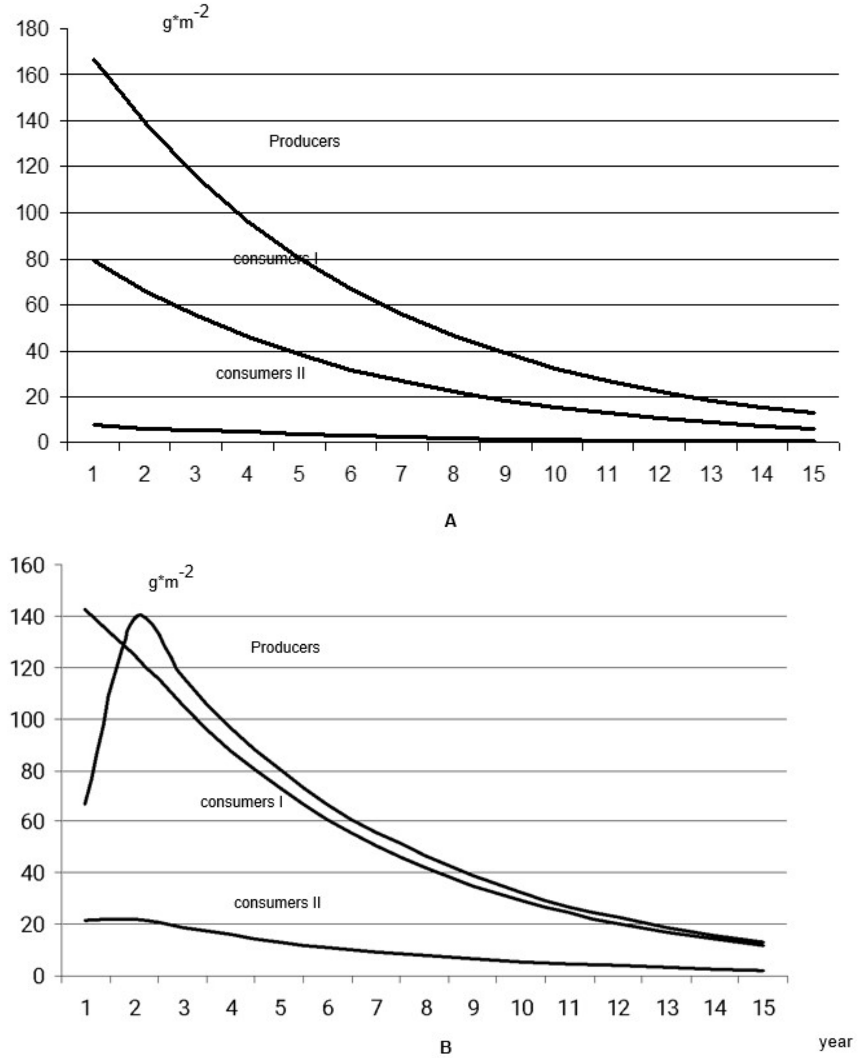

Figure 2: Forecast of Biomass Dynamics of Food Chain Members for 15 Years. A: The factor impact coefficients are equal to 0.0005, 0.001, and 0.003, respectively, for producers, consumers of the 1st order, and consumers of the 2nd order. B: They equal respectively 0.0005, 0.004, and 0.003. The value of the biomass of producers on the graph is reduced by 5 times relative to the actual one for the convenience of comparing the behavior of state variables

5. DISCUSSION

In the course of debugging the model and numerical experiments with it, important aspects were identified that determine the fate of a biological system exposed to combined effects and should be considered when adapting the algorithm for each specific scenario.

The key role in simulation is played by considering the properties of the object (for example, lifetime, sensitivity to the effects of each factor individually, and their totality) [23, 24]. In addition, the sensitivity of the body to the effects of the factor may vary according to age or phenological stage.

Each factor can affect several processes of the functioning of an object at once [25] and in different ways, for example, to stimulate the flow of some processes and disrupt the flow of others. This makes it difficult to quantify its impact on the integral characteristics of the object. There are other important points. In particular, the results of single and chronic exposure with the same total load differ significantly. The consequences of a single exposure can be one-time or chronic or have a delayed effect, depending on the properties of the object and the characteristics of the factor.

Approaches to the formalization of combined effects from the standpoint of classical mathematics [17], in our opinion, carry too many uncertainties compared to simulation algorithms that directly consider the mechanisms, direction, and degree of influence of factors. Simulation models in this case have a pronounced applied nature, which allows them to be used for practical purposes to solve environmental problems.

At this stage, the presented version of the EcoCombi_FC model demonstrates the capabilities of the algorithm. To parametrize the equations of future models for reproducing specific situations of anthropogenic pollution, we created the CombiData information system, which is designed to collect, store, and analyze data on the combined effects of various types of factors on biota. Working with the system allowed us to draw some conclusions related to the topic under consideration. According to preliminary data, the situation of combined effects of anthropogenic factors is most often found in the territories adjacent to industrial and household waste disposal sites and large enterprises, as well as in places where liquid waste is drained into reservoirs. There are very few studies of the combined effects of anthropogenic pollutants on natural objects at the ecosystem level. The present studies mainly focus on the effects on individual organisms or their organs [26, 27].

Our results, in addition to the advantages, revealed several difficulties associated with using simulation models in modeling environmental problems. Other researchers have encountered these problems and discussed them in scientific publications [5 ,7, 17]. Among the difficulties that we identified during the development of the EcoCombi simulation model, we primarily distinguish:

Data limitations. One of the main challenges is the availability and quality of data needed to parameterize and validate simulation models.

Model complexity. Ecological systems are often complex and involve many interacting components and nonlinear relationships, which influence the accuracy of predictions.

Validation and verification. Validation and verification of environmental systems simulation models is a major challenge. Ensuring that models accurately reflect real-world processes and make reliable predictions is often difficult due to the limited ability to conduct experiments at large scales.

6. CONCLUSION

An algorithm for reproducing multifactorial effects on an object was developed based on which simulation models can be built and implemented to allow forecasting or reconstructing various environmental situations associated with the simultaneous impact on ecological systems and their components of various factors, both biogenic and anthropogenic.

We constructed the EcoCombi model, which reproduces the dynamics of the number or biomass of living components of biological systems that are under the combined influence of two or more factors. The work on the model demonstrated the following points:

– the main problem of adapting the model to a specific environmental situation is the determination of quantitative dependencies of life processes of organisms on the factors of influence;

– the properties of the object play a key role in assessing the effects of exposure and predicting the behavior of an object under the combined influence of factors;

– the nature of the factor's impact is important (mono or poly-impact on the vital processes of organisms, single or chronic exposure).

The proposed algorithm is in principle applicable to any situation where there is a multifactorial impact on the object. In this respect, it can be effective for reproducing most of the environmental processes observed in anthropogenic pollution. The successful use of models built on the above algorithm depends on the completeness of information about the impact of factors on the functioning of a biological object and their interaction in this process.

To parametrize the equations of future models for reproducing specific situations of anthropogenic pollution, the CombiData information system was created, which is designed to collect, store, and analyze data on the combined effects of various types of factors on biota.

Our future work is associated with the need to integrate simulation models into environmental policy and decision-making processes, in particular in Kazakhstan and Russia. Even though in the academic environment, there is an understanding of the effectiveness of using simulation models, their development in practice is a difficult task. Decision makers, especially in government bodies, have a limited understanding of the intricacies of the models. They are reluctant to develop integration mechanisms based on specific recommendations for applications of these models and opportunities for future development associated with specific regional problems.

ACKNOWLEDGMENTS

The study was carried out within the framework of research, development, and engineering project (NIOKTR) No. AAAA21-121012290189-8, carried out on a state assignment, with the support of the Interdisciplinary Scientific and Educational School of M.V. Lomonosov Moscow State University "The Future of the Planet and Global Environmental Changes".

CONFLICT OF INTERESTS

The authors declare that there is no conflict of interest.

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