**World Journal of Environmental Biosciences**
Available Online at: **www.environmentaljournals.org**

**Volume 15, Issue 2: 121-129**

https://doi.org/10.51847/jD6qNlerMh

**ISSN 2277- 8047**

# Mathematical Modeling of Ecotoxicant Behavior in “Soil–Vegetation Cover” Systems

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**ABSTRACT**

*Technogenic contamination of soils and vegetation by radionuclides, heavy metals, pesticides, and other ecotoxicants requires reliable tools for assessing pollutant redistribution and forecasting environmental risks. This study examines mathematical modeling approaches for describing ecotoxicant behavior in soil–plant systems and identifies the principal processes that should be incorporated into simulation algorithms, including vertical and lateral migration, transformation between physicochemical forms, fixation in soil, root uptake, biological redistribution, degradation, and removal from the system. Existing mathematical models of pollutant migration and bioavailability are analyzed to define general principles for model development and parameterization. Particular attention is given to low-parameter modeling as an approach suitable for situations where complete experimental datasets are unavailable. Based on the previously developed VERT_MIG and 3Dmig_mod_aut algorithms, the 3Dsoil_plants algorithm is proposed for simulating the spatiotemporal dynamics of ecotoxicants in soil–plant systems. The model represents soil as interconnected spatial cells and accounts for both vertical and horizontal pollutant transfer, as well as interactions with vegetation. Models based on this algorithm were implemented in the cross-platform QB64 environment, enabling their use as standalone software under Windows, Linux, and macOS. The proposed approach provides a flexible framework for forecasting ecotoxicant redistribution under spatially heterogeneous contamination conditions.*

**Keywords:** *Ecotoxicants, Mathematical modeling, Soil–plant systems, Simulation modeling, Spatiotemporal dynamics*

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**Received:** 13 March 2026
**Accepted:** 29 May 2026

## INTRODUCTION

Human economic activity has led to large-scale environmental contamination by radionuclides, heavy metals, pesticides, herbicides, insecticides, and other ecotoxicants that adversely affect biota and humans. Under conditions of active human interference in the established functioning of the biosphere, the input and subsequent redistribution of various technogenic pollutants in soil and vegetation cover become key factors ultimately determining the intensity of their impact on living organisms. It is essential to be able to forecast the consequences of this generally highly negative phenomenon.

To achieve this, mathematical modeling is utilized; this approach facilitates a formalized representation of the complex mechanisms dictating ecotoxicant behavior within soil–plant systems. It is essential to recognize that these dynamic processes can either mitigate or exacerbate the influence of pollutants on local biota. For instance, vertical migration, or burial, significantly dictates the extent of anthropogenic impact on living organisms. With radioactive contamination, soil-based shielding of ionizing radiation effectively decreases the dosage absorbed by surface-level organisms. Conversely, the transition of ecotoxicants into the rhizosphere enhances the probability of plant contamination via root uptake, potentially intensifying the systemic suppression of root growth. Consequently, precise modeling remains vital for evaluating the varied environmental consequences of such pollutants within diverse soil matrices and biological contexts.

Properly selected algorithms of mathematical models, once implemented, make it possible to dynamically represent the specific behavior, properties, and targeted effects of a pollutant on living organisms.

*Features of ecotoxicant behavior in “soil–plant” systems that must be considered when developing algorithms*

The full range of processes associated with the dynamics of technogenic pollutants in “soil–plant” systems can be divided into three main groups: behavior separately within each of the two components—soil (1) and plants (2)—and the set of processes governing the redistribution of the ecotoxicant between them (3). Mathematical models may represent these processes either in their entirety or according to the above groups.

It is important to consider certain key features of ecotoxicant behavior that influence model algorithm design in each specific case. In our view, the main factors and processes determining such behavior include the form in which the ecotoxicant enters the system; vertical and lateral migration in soil; transformation of the pollutant from one form in soil to another and its fixation in the soil-absorbing complex; deposition on the external tissues of plants followed by redistribution; root uptake from soil; degradation; or removal beyond the system boundaries.

First, let us briefly consider ecotoxicant behavior in soil. The vertical migration of chemical elements in soil—a porous medium—is a complex process comprising several components, primarily convective transport, sorption, diffusive mass transfer, and dispersive transport (Shein & Karpachevsky, 2007). Migration rates depend on a number of factors, including effective porosity, soil moisture, granulometric composition, and others. It should also be taken into account that the hydrochemical properties of soil vary along the profile, sometimes in opposite directions.

In soil, chemical elements or compounds containing them participate in various chemical reactions, may become fixed within the soil-absorbing complex, and can undergo transformation, shifting from one form to another. This affects their biological availability, may alter their mobility in soil, and can contribute to changes in toxicity.

An important role in ecotoxicant behavior in soil is also played by the initial physicochemical form of deposition, the amount of incoming pollutant, and its affinity for the soil-absorbing complex. For example, in the case of one of the most hazardous radionuclides—radiocesium—entering soil in trace quantities during releases, the phenomenon of gradual “aging” is observed, involving strong fixation of the radionuclide within the soil-absorbing complex, mainly in clay minerals. This renders it practically unavailable for uptake by plant root systems.

The nature of the ecosystem—whether natural or anthropogenic—serves as a critical determinant in evaluating pollutant behavior. In agrocenoses characterized by annual mechanical soil disturbance, analytical algorithms focusing on pollutant transformation within the tilled horizon are essential for predicting changes in ecotoxicant bioavailability and potential crop contamination. Conversely, "migration" mathematical models prioritize the vertical redistribution of pollutants throughout the soil profile. These models are particularly appropriate for undisturbed natural landscapes, including pastures and hayfields, where the primary soil structure remains intact. While the chemical evolution of pollutant species remains a relevant consideration in these non-tilled environments, the primary analytical focus shifts toward tracking the downward or upward transport of contaminants relative to the root-inhabited zone, which fundamentally influences the long-term ecological impact within such stable biosystems.

When analyzing pollutant behavior in vegetation cover, many influencing factors must also be taken into account. For example, as demonstrated by studies of the consequences of the Chernobyl Nuclear Power Plant accident, the dispersity of atmospheric fallout and the phenological stage of plants affect both the amount of ecotoxicant retained by vegetation and the rate of its removal (Shcheglov *et al*., 2001). Another factor is the species composition of the phytocenosis; different species have different retention capacities due to variations in surface roughness of external tissues, such as bark on tree trunks and branches.

The intensity of pollutant uptake through the root system depends on the depth of its penetration into the soil and its biological availability. It should be emphasized that model complexity is largely determined by ecosystem type. For example, the behavior of ecotoxicants in phytocenoses with a woody layer is considerably more difficult to reproduce. Perennial tree components may act as long-term depots. The retention capacity of structural parts of woody plants differs, and redistribution of the pollutant between external and internal tissues may occur over a prolonged period after deposition. This substantially complicates the model algorithm.

*Examples of mathematical models of ecotoxicant behavior in “soil–plant” systems*

A large number of mathematical models of varying complexity and implementation type (standalone models or full-featured software products with developed interfaces) have been designed to quantitatively predict pollutant behavior in soils and in “soil–plant” systems. Below are several examples of existing models.

For instance, the AquaSalt model (Guber & Shein, 1997) was previously used to simulate herbicide behavior in soil. Its algorithm reproduces vertical moisture movement and substance transport, taking into account possible transformation processes and interaction with the soil solid phase.

Models such as PEARL are widely applied for mathematical simulation of pesticide behavior in the environment. PEARL is a chromatographic flow model based on the convective–diffusive transport equation in soil and does not account for the presence of macropores and cracks (Leistra *et al*., 2001; Kolupaeva *et al*., 2006; Astaikina *et al*., 2016; Kolupaeva *et al*., 2017).

Various mathematical models of differing complexity and algorithmic structure have also been proposed for the formalized description of radionuclide and heavy metal behavior (Anokhin, 1974; Prokhorov, 1981; Muller & Pröhl, 1993; Velasco *et al*., 1993; Mamikhin, 1995, 2003; Spiridonov *et al*., 2005; Drichko *et al*., 2009; Kosheleva, 2009; Frid & Borisochkina, 2018; Kovalenko & Syromyatnikov, 2018; Perevolotskaya, 2019; Spiridonov *et al*., 2022).

To represent the dynamics of biological availability of ecotoxicants, some models consider their redistribution among different forms of occurrence (Fesenko *et al*., 1997; Konoplev *et al*., 1999; Mamikhin, 2004, 2007a, 2007b; Bulgakov & Konoplev, 2005; Spiridonov & Mukusheva, 2010).

There are also models describing two- or three-dimensional distributions of ecotoxicants in soil. We previously developed the simulation model 3Dmig_mod_aut, which reproduced radiocesium behavior in soils located on slopes (Mamikhin & Badawy, 2011). In addition, several specialized software packages are available for mathematical modeling of water flow and solute transport in saturated and unsaturated soil–ground media, including FEFLOW, Groundwater Modeling System, HYDRUS 2D/3D, and COMSOL Multiphysics: Earth Science Module (Kundas *et al*., 2011).

A special category comprises mathematical models whose algorithms allow a relatively comprehensive representation of ecotoxicant behavior in plants. This is a complex task requiring detailed knowledge of ecotoxicant metabolism in specific plant species and sufficient quantitative information for model construction. This can be illustrated by several radioecological models (Antonopoulos-Domis *et al*., 1990; Mamikhin & Kliashtorin, 1999; Avila *et al*., 2001; Mamikhin, 2003; Mamikhin & Manakhov, 2016; Spiridonov *et al*., 2021). To improve model adequacy, some models incorporate modules describing phytomass dynamics as the physical carrier of the ecotoxicant (Mamikhin, 2003).

There are also models addressing specific aspects of technogenic soil and vegetation contamination, such as impacts on soil biota (Vodopyanov *et al*., 2009; Harkat *et al*., 2022) or contamination under particular environmental entry conditions, for example, as part of organic waste (Kireycheva & Tingaev, 2009).

It is also important to mention soil erosion models. Erosion processes are accompanied by the transport of large quantities of technogenic pollutants within soil masses and their potential accumulation in lower relief elements or water bodies. A widely known example is the RUSLE2 model, based on the equation

$$A = R \times K \times LS \times C \times P, \quad (1)$$

In this equation, A represents the predicted mean annual soil loss, while R, K, LS, C, and P denote rainfall erosivity, soil erodibility, topography, vegetation management, and support practices, respectively (Renard & Freimund, 1994; Kuznetsova *et al*., 2024). Localizing this model facilitates precise erosion estimation, allowing researchers to effectively incorporate these findings into broader assessments concerning ecotoxicant transport within chemically contaminated geographical regions and landscapes.

*General approaches to model development*

Several general aspects deserve consideration. Models may be either point-based or distributed. In dynamic point models, variable values change only over time, whereas in distributed models, variables vary both temporally and spatially (Mamikhin & Shcheglov, 2020).

Despite the wide diversity of existing mathematical models that reproduce ecotoxicant behavior in soil at a point scale (per unit area), either autonomously or in combination with other processes, and their translocation within ecosystems, the modeling framework typically reduces to three main aspects: vertical (downward and upward) migration within the soil profile; transformation (transition between physicochemical forms); and removal beyond the soil profile (e.g., through crop harvesting or migration into deeper geological layers).

Simulation models describing two- or three-dimensional soil distributions form a separate category. Topologically, however, they can be regarded as complexes of communicating prisms forming a common volume, each prism corresponding to a point model of vertical migration.

The degree of detail in mathematical description depends on the completeness of initial information, knowledge of quantitative relationships governing modeled processes, and the feasibility of parameterizing the mathematical equations included in the analytical structure of the model.

Temporal discretization is also of significant importance. Some models simulate so-called "multi-year" dynamics with a one-year time step (Cardei *et al*., 2021), while others represent "seasonal" dynamics with daily time steps (Mamikhin *et al*., 2018). Naturally, a finer temporal resolution generally implies a more detailed representation of system functioning.

Another critically important issue concerns the combined impact of technogenic pollutants on biota and its representation in mathematical models. Algorithm selection in such cases is determined by the availability of necessary quantitative information, particularly equations describing relationships between object characteristics and impact factors (Mamikhin, 2023a, 2023b). For living organisms, these characteristics include individual or collective life parameters, such as biomass of an individual or population size. Ideally, a mathematical formula reflecting observed patterns of combined environmental factor effects would be available. However, the empirical data required to derive such equations are often lacking. In such cases, the impact of multiple factors may be assessed using an equidosimetric approach. This approach enables comparison of factor strengths affecting biota, identification of the most significant ones in specific situations, and evaluation of overall impact consequences.

Our findings indicate that the dynamics of ecotoxicants within the soil–plant interface can be effectively captured through mathematical modeling. Nevertheless, the central difficulty persists in accurately parameterizing these governing equations. Obtaining the comprehensive experimental datasets required to define such complex systems is frequently impractical. This limitation becomes significantly more pronounced when researchers attempt to scale these models to encompass vast geographical areas or account for the inherent heterogeneity across a diverse range of ecological and environmental systems.

A possible solution is the application of so-called low-parameter models (Frid & Borisochkina, 2018). Below, we propose for consideration a specific example of a tested and implemented algorithm based on the low-parameter approach, realized in several mathematical models.

*Algorithm for vertical migration of radionuclides in soil: VERT_MIG*

The low-parameter approach has for a long time been successfully applied by us in the VERT_MIG algorithm in various versions of simulation models of vertical migration of radionuclides in soil under radioactive contamination of different soils resulting from the Chernobyl NPP and Fukushima-1 NPP accidents (Mamikhin, 1995, 2003, 2007a, 2007b; Mamikhin *et al*., 2016; Mamikhin *et al*., 2018).

Since the description of the algorithm has already been provided in our publications, here we present it briefly and focus on the most important aspects in the context of this work.

It is assumed that models built on the basic algorithm are point models; the dimension of state variables is $kBq/m^2$. The models are systems of finite-difference equations. In the original version, the following state variables are used, which, with a 1-day time step, reflect the dynamics of $^{137}Cs$ content in the corresponding components:

*P* - content of $^{137}Cs$ in aboveground phytomass;

*Sao* - total content of $^{137}Cs$ in the uppermost layer of variable thickness (e.g., forest litter or sod).

*X(i)* – mobile component of $^{137}Cs$ content in soil,

*Y(i)* – low-mobility component of $^{137}Cs$,

where *i* = 1 , ... , *n* – is the soil layer number.

The low-mobility fraction of 137Cs is defined by its sequestration within subterranean biomass through root absorption, as well as its retention in the soil-adsorbing complex. This immobilization occurs via non-exchange sorption on clay minerals and clay–

humus matrices, ion-exchange processes with humic substances, and co-precipitation within insoluble salt structures. Conversely, the remaining inventory constitutes the mobile fraction, primarily comprising water-soluble and partially exchangeable radionuclide species. Furthermore, a theoretical distribution pool, designated as R, serves as an auxiliary state variable to model the relocation of 137Cs within the soil profile, driven by plant root networks, fungal hyphae, and the biological activities of soil micro- and mesofauna. It is postulated that the aggregate of fluxes directed into this specific pool remains in perfect equilibrium with the total outward fluxes, as established in the foundational framework of existing research (Mamikhin & Badawy, 2011).

The mathematical framework incorporates several transfer functions to describe the dynamics of 137Cs. Specifically, fap denotes atmospheric deposition of the radionuclide onto aboveground phytomass, while fwx and fwy represent the influx or erosion of 137Cs within the soil surface layer triggered by flooding or intense precipitation events. The parameter fsp characterizes the root uptake of 137Cs from the soil, whereas fps accounts for the accumulation of the isotope in the soil through atmospheric fallout and the decomposition of plant litter. Furthermore, F1 signifies the soil surface removal driven by organic mineralization, particulate leaching, convective flow, and downward levage. Vertical migration processes include "fi," representing convective transport, and "dfi," which models the quasi-diffusive movement of less mobile isotopes. Chemical transformations are defined by xyi, the immobilization of the mobile fraction via adsorption and complexation, and gi, the mobilization of the fixed component through desorption. Biological interactions involve xri, representing radionuclide assimilation by roots and soil biota, and rxi, which denotes the subsequent release of 137Cs into the soil environment during decomposition or via exudates. Finally, the coefficients dp, dxi, dyi, and dr encapsulate the physical process of radioactive decay across the respective compartments, as established in the referenced methodology (Mamikhin *et al*., 2022). The overall topological structure of the simulation model and the relationships among its state variables and transfer functions are presented in **Figure 1**.

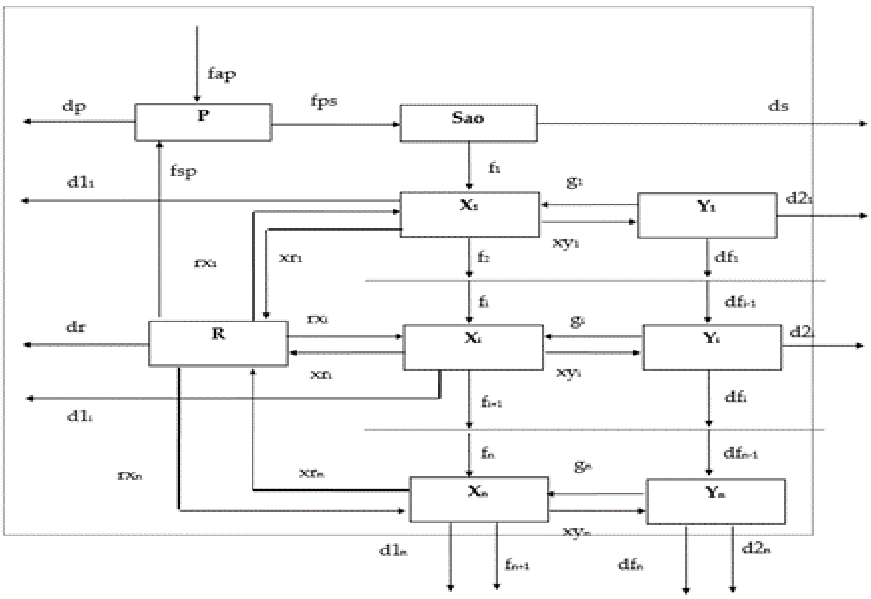


**Figure 1.** Flow diagram reflecting the topological structure of the simulation model of vegetation-cover contamination dynamics and vertical migration of $^{137}$Cs in Soil

As shown by the results of numerical experiments with models built on this algorithm, the most important integral flux determining the intensity of downward migration (burial) of radiocesium is the sum of convective transport and lessivage. In the model, it is determined by the value of the migration coefficient of the mobile component a3. By comparing its value obtained by the iteration method using field observation data, one can characterize the overall rate of radiocesium migration along the soil profile at different sites and estimate the approximate average intensity of vertical migration for the studied soils of the middle and low floodplain.

We used the model to conduct numerical experiments for forecasting, reconstruction, and investigation of $^{137}$Cs migration processes in "soil–plants" systems, with primary attention to soil processes, namely vertical migration and the dynamics of forms of occurrence.

Although the algorithm was developed for modeling radionuclide behavior, in our opinion it is sufficiently universal. When considering the dynamics of pollutants, which are often complex chemical substances, their transformation will also have to be taken into account, since during transformation mobility, biological availability, and the degree of hazard for biota representatives change. In the case of heavy metals, it is only necessary to exclude the radioactive decay function.

*Algorithm of a low-parameter model of the spatiotemporal dynamics of ecotoxicant behavior in the "soil–plants" system: 3DSOIL_PLANTS*

Under non-uniform technogenic contamination, forecasting the three-dimensional distribution of an ecotoxicant in soil becomes relevant. This is possible on the basis of integrating modified algorithms underlying the VERT_MIG and 3Dmig_mod_aut models. Let us briefly consider the practical implementation of such an approach using the example of the spatiotemporal dynamics model of ecotoxicant behavior in the "soil–plants" system, 3D soil_plants. The migration field (a certain soil volume with vegetation presented on its surface) is divided into standardized "prisms," for each of which a point model is built based on an algorithm similar to VERT_MIG. The elementary cell (voxel) from which the "prisms" consist is shown in **Figure 2** (Ganea *et al*., 2024; Soman *et al*., 2024; Castellano-Rioja, 2025; Mikail *et al*., 2025; Petronis *et al*., 2025; Zulkarnain *et al*., 2025; Batra & Rajasekar, 2026; Merzouki *et al*., 2026; Mohammad, 2026; Shon & Yang, 2026).

Each "prism" can exchange substance and information with neighboring prisms. This is handled by the corresponding transfer functions that take into account the concentration gradient of the ecotoxicant. The coefficients included in the transfer-function equations may be either constants or functions. For example, diffusion coefficients may change depending on the physicochemical properties of soil horizons (Souza *et al*., 2024; Ahn *et al*., 2025; Cavero & Ferraz, 2025; Khalil & Nassar, 2025; Rani & Gehrke, 2025; Rivas & Molina, 2025; Shen & Bao, 2025; Silik, 2025).

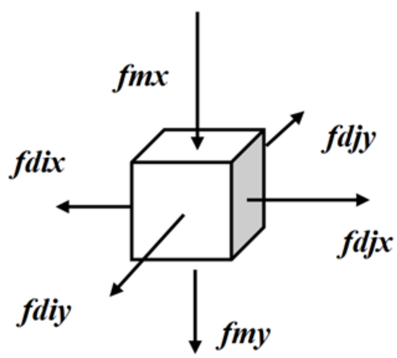


**Figure 2.** Elementary cell of the model of three-dimensional dynamics of ecotoxicant redistribution in soil for variable X(k,i,j).

Here, compared to models built on the VERT_MIG algorithm, new functions appear—*fdjx, fdix, fdjy, fdiy*—which reproduce horizontal migration of the ecotoxicant as a result of the combination of convective–diffusive processes occurring in soil. In the simplest version, the equations of these functions may look as follows:

$$fdjy = d * (X(k,i,j) - X(k,i,j+1)), \qquad (2)$$

where d is a coefficient reflecting the rate of equalization of pollutant concentrations in two neighboring cells of the same horizontal layer. With the necessary source information to describe both vertical and horizontal migration of the ecotoxicant, more complex equations can be used that account for factors such as porosity, granulometric composition, and soil moisture. Spatial redistribution of the fixed form of ecotoxicant occurrence *Y(k,i,j)* is calculated in the same way (Danchin *et al*., 2024; Essah *et al*., 2024; Hillman, 2024; Eid *et al*., 2025).

Thus, by implementing the considered algorithm as a model of ecotoxicant behavior in the "soil–plants" system 3Dsoil_plants, we obtain four-dimensional arrays of values *Xt(t,k,i,j) and Y(t,k,i,j)* describing the spatiotemporal dynamics of ecotoxicant content in soil, and can further forecast this process under various conditions of pollutant input onto the soil surface or even directly into its thickness, for example with groundwater (Agrawal *et al*., 2024; Bona & Lozano, 2024; Braun *et al*., 2025; O'Brien *et al*., 2026; Tran & Pham, 2026).

To describe ecotoxicant behavior in plants, initial information on the temporal dynamics of biomass of structural plant parts may be required. For example, in one modification of the 3Dsoil_plants model, the production model EcoGrass is used as a built-in module for this purpose. In this module, with a one-hour time step, phytomass stocks of aboveground and belowground parts of herbaceous vegetation (green phytomass, rhizomes, roots) and the substance fluxes that determine changes in these stocks are calculated (Mamikhin *et al*., 2022).

Models based on the presented algorithm are implemented in the freely distributed cross-platform programming environment Qb64 (https://www.qb64.org/portal/), which makes it possible to use them as standalone software packages on any currently used version of the Microsoft Windows operating system, as well as on Linux and Mac OS systems. Modeling results are displayed by the program on the screen in text-numeric and graphical form **(Figure 3)**, and a separate text file, data_gr.dat, is also generated containing calculation data in a format convenient for further processing in other programs.

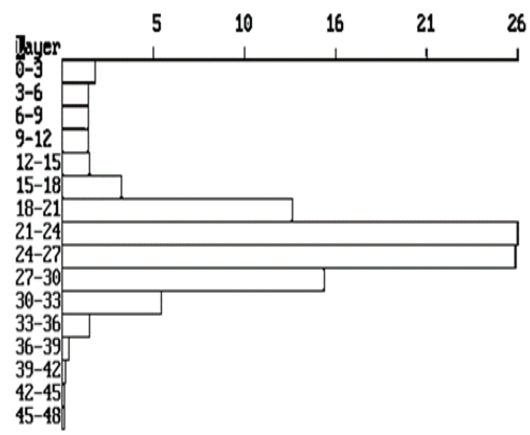


**Figure 3.** Forecast of ecotoxicant distribution along the profile of hydromorphic soil obtained using a model built on the 3Dsoil_plants algorithm.

## CONCLUSION

Since the method of mathematical modeling makes it possible to create effective tools for studying and forecasting ecotoxicant behavior in "soil–plants" systems and their impacts on biota, this scientific direction is receiving increasing attention from ecologists worldwide. Often, the main obstacle to developing localized ecological models is the lack of necessary initial data and the unknown values of quantitative parameters included in the equations. The development of simulation modeling based on implementing models on a computer as a program has somewhat reduced the severity of this problem by allowing parameter values to be determined using the model itself via the method of successive approximations (iterations), but it has not eliminated it completely. A possible way out in this situation may be the generalization of the processes under consideration and the construction of so-called "low-parameter" mathematical models. This makes it possible, albeit in simplified form, to formalize our understanding of ecotoxicant behavior and impacts and to obtain at least an approximate assessment of potential ecological risk.

Standard point models characterize processes based on a single unit of soil surface, an approach suitable for uniform contamination scenarios. In practical environments, however, non-uniform fallout typically prevails. While point-based methodologies remain acceptable when broad, averaged forecasts suffice, scenarios involving severe spatial variability or significant surface slopes necessitate the deployment of spatially distributed and three-dimensional modeling techniques. The primary challenge remains the robust parameterization of these complex models. Our evaluation of a low-parameter framework indicates that even when initial data is constrained, it is feasible to develop simulation models that capture ecotoxicant dynamics within a defined soil volume with a high degree of empirical adequacy.

The proposed 3Dsoil_plants algorithm represents a compromise solution that allows both a simplified description of the vertical and lateral migration of ecotoxicants in soil and their uptake by plants, and a more detailed representation when more complete input data are available. Transfer functions can be formulated at different levels of complexity depending on the available knowledge of the processes governing the modeled system. Additional auxiliary variables may be introduced to account for the influence of various factors; the thickness of individual soil layers can be varied; and an upper layer of variable thickness can be specified when necessary.

To collect information on the effects of possible ecotoxicant impacts, we created the database "Factorial Ecology," in which quantitative data are accumulated (LD50, LC50 parameters, and mathematical equations of dependence of the characteristics of the impacted object on ecotoxicant content or radiation level). This information can be used in models of the behavior of specific technogenic pollutants to calculate possible damage to biota from the standpoint of the equidosimetric approach with the identification of the leading factor and, in some cases, also using equations of multifactor impacts.

**ACKNOWLEDGMENTS:** None

**CONFLICT OF INTEREST:** None

**FINANCIAL SUPPORT:** This research was developed under the 2024-2026 targeted funding program commissioned by the Ministry of Science and Higher Education of the Republic of Kazakhstan. It specifically supports the scientific project (BR24992839) focused on evaluating the effects of ecotoxicants and advanced agricultural methodologies on crop yields and soil health within the Kostanay region.

**ETHICS STATEMENT:** None

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