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THE ROLE OF MATHEMATICAL MODELING IN RESEARCH IN THE FIELD OF BIOACCUMULATION OF HEAVY METALS

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Abstract: This article presents the role and mathematical modeling importance in research and development of experimental plan. Although the results presented refer only to the field of biology, the presented method is valid for any field of activity. The results refer to research about bioaccumulation of heavy metals in plants. It is exposed how the mathematical modeling of the phenomenon, even under the most elementary form, suggests the basics of the experimental plan. The experiments performing, taking into account the mathematical models suggestions, lead to the correction and the development of mathematical models. These will be able to give new predictions and utilities.
Keywords: bioaccumulation, heavy metal, mathematical model

1. INTRODUCTION

According to [3], some of the substances that form the crust of the Earth are elements that cannot be decomposed into simpler substances. Some of these elements are poisonous, even if these are present in a low concentration. These elements are known as heavy metals. Among heavy metals, [3] includes mercury, cadmium, arsenic, chromium, talc and lead.

More generally, according to [5], bioaccumulation is defined as the accumulation of substances (eg pesticides) in organisms of various types. It also states that bioaccumulation occurs in organisms when absorption occurs at a faster rate than elimination of the same substances by catabolism or excretion. According to [1], the longer the half-life of a toxic substance, the greater the risk of chronic poisoning, even if the levels of the toxin are not very high. According to [8], bioaccumulation in fish can be predicted by mathematical models. Expanding the bioaccumulation of heavy metals into other categories of biological material is currently a normal phenomenon. The importance of the consequences of the use of mathematical models in this field will be clear from the results of this article and from the resulting conclusions.

In order to better understand the phenomena related to the propagation of heavy metals in the environment (both in the mineral world and in the world of life), we should know the following definitions:

- Accumulation of substances: Process or phenomenon[1] that involves retaining or increasing the concentration[2] (partial or total) of substances entering an environmental entity through contact with these substances and entities in any possible way.
- Bioaccumulation: If the accumulation is in a living (biological) entity of the environment, then it is called bioaccumulation[3].
- Bio concentration: It is a particular case of bioaccumulation, where the substance that is bio accumulated has as its source only water.
- Bio magnification: The term refers to the monotonous increase of the concentration of a substance in the biological tissues in a food chain. [9]. [4].

2. MATERIAL AND METHOD

The mathematical models of heavy metal bioaccumulation are part of the general category of mathematical models describing biology phenomena. These models are included in that branch of biology called biomathematics, [4] which is the branch of biology that deals with the application of mathematical principles in biology and medicine. Biomathematics has multiple applications in the well-known branch of biology: Comparative Genetics, Population Genetics, Neurobiology, Cytology, Pharmacokinetics, Epidemiology, Oncology, or Biomedicine.

— Biodynamic bioaccumulation model

This model is presented in [6], being one of the simplest possible and obviously easier to use in the proposed investigations. The author [3] shows that the complexity of the metal accumulation process in plants and animals, as well as the multitude of internal and external factors that influence this process, require the

[1] Substance sequestration results in increased concentration of contaminant in the considered environmental entity (biological or not) at a value higher than normal in the same entity or than the normal environmental concentration.
[2] According to [7].
[3] It is also shown in [2] that the level (intensity or magnitude) of bioaccumulation depends on the absorption rate, the absorption mode and the rate of elimination, as well as on processes of transformation of the substance accumulated through metabolic processes, as well as other factors environment. All these dependencies are essential in shaping the bioaccumulation phenomenon.

introduction of unifying principles and simplifying hypotheses that allow the solving of mathematical models, using a small number of parameters. Obviously, the introduced simplifications must not remove the model from the real process. The model proposed by [6] is a biodynamic model based on the principle of conserving the mass. Mathematical models of bioaccumulation can be used according to [8], in double sense: a) to provide information on the degree of environmental pollution, if the bio-indicator concentration is known; b) creates the possibility of estimating the concentration at the biotic receptor level when the concentration is known in the external environment. Several useful properties are retained in the construction of model, according to [6]:

- ≡ The bioavailability of metals depends on the environment and the chemical composition of the environment;
- ≡ Only certain metal compounds are bioavailable;
- ≡ Animals and plants possess mechanisms to regulate accumulation and elimination of heavy metals in the body;
- ≡ Information about the process of bioaccumulation of a form of metal in a particular pathway cannot be transferred to another form or other path of accumulation;
- ≡ The metals are neither created nor destroyed by the body, they may, only, pass from one form to another;
- ≡ Accumulation capacity varies from organism to body and even for the same specie varies with age, sex, and route of exposure.

— Unifying concepts and principles

According to [8], the main ideas of the model are:

- ≡ the principle of conserving the mass[4];
- ≡ the existence of multiple accumulation paths;
- ≡ the existence of an internal disposal mechanism.

The statement on the preservation principle on which the simple model presented in this chapter is based, is the following: the variation in time of the amount of metal accumulated in the body is equal to the difference between the quantity taken and the amount eliminated.

The list of the parameters used in the presented model is given in Table 1.

Table 1. List of parameters used in the biodynamic model of the bioaccumulation process

Name	Notation	Unit
denotes the total of the concentrations in the bio receptor system; c_i is the metal concentration in the bioreactor indexed with i	c	(%)
the mass flow entering the bio receptor i	F_i	s^{-1} (%/s)
the mass flow coming out of the bio receptor i	G_i	s^{-1} (%/s)
time	t	s
the set of parameters on which contaminant absorbs (receipt) depends	u	
the set of parameters on which contaminant loss (the elimination). depends	w	
equilibrium concentration in the system	c^e	(%)
the direct absorption rate[5] of the contaminant from the external environment	k_i^u	s^{-1} (%/s)
concentration of the contaminant in the external environment	c_W	%
food preference factor	p_i^j	
efficiency of chemical assimilation	α_i^j	
diet rate	k_i^j	
elimination rate	k_i^e	

For a system of interconnected bioreceptors and a single contaminant, the mathematical model of metal accumulation in organisms is given (proposed) by the system of ordinary differential equations:

$$\frac{dc_i}{dt} = \mathfrak{F}_i(c,u) - \mathcal{G}_i(c,w)), i = 1,\ldots,n \qquad (1)$$

When the system is in equilibrium, the input flow is equal to the output stream. This hypothesis results in the value of the equilibrium concentration in the bio receptor system:

$$\mathfrak{F}_i(c^e,u) = \mathcal{G}_i(c^e,w)), i = 1,\ldots,n\,. \qquad (2)$$

The value of the equilibrium concentration resulting from (2) includes the contribution of the assimilation and elimination mechanisms. Also, as a principle of model construction, is retained from [6], the hypothesis of hierarchical indexing of bio receptors. By hierarchical indexing, it is understood that if $i<j$. then the bio receptor i can be the source of feed for the bio receptor j. In addition, the following assumptions are made:

[4] This principle must be applied with great care. On the one hand we refer to biological entities that are either growing or not, so that can have mass variations, regardless of the process being pursued. On the other hand, depending on the time interval between the measurements, although the amount of contaminant increases in the bioreceptor, due to an appreciable increase in its mass, the concentration may decrease!

[5] The rate of a chemical, physical or other process, designates what needles in mechanics means the speed of the process. Thus, the direct take-up rate of the contaminant from the external environment is measured in percent per unit of time. Percentage measurements are made in the percentage concentration of the contaminant in the bioreceptor. At the same time, the external environment of the bioreactor loses contaminant, and its elimination rate must be measured in percent of the contaminant lost per unit of time, but referring to the contaminant concentration of this bioreactor external environment. Obviously, for clarity, the transfer rate of the contaminant from the external environment to the bioreactor should be expressed in mass units per unit time and then converted to bioreactor concentrations, respectively, for the outside of the bioreactor.

≡ for all *j* and *i*. with $i \le j$. the bio receptor *j* cannot be the source of feed for the bio receptor i;
≡ mass flow depends linearly on mass concentrations;
≡ the elimination flux depends only on the internal mass concentration of the bio reactor.

The author [6] asserts that, based on the I_a, I_b and I_c assumptions, F and G flows can be explained as:

$$\mathfrak{F}_i = k_i^u c_w + \sum_{j=1}^{n} p_i^j \alpha_i^j K_i^j c_j,\ \mathfrak{G}_i = k_i^e c_i,\ i = 1,\dots,n \cdot \quad (3)$$

The food preference matrix satisfies the following properties:

$$p_i^j = 0 \text{ for } j \ge i \quad (4)$$

and if there is j, so $p_i^j \ne 0$, then:

$$\sum_{j=1}^{n} p_i^j = 1 \cdot \quad (5)$$

For the following statements. we use a partial order relationship on $\mathbb{R}^n$. defined by the formula:

$$x \ge y \text{ if } x_i \ge y_j \ \ \forall i = 1,\dots,n \quad (6)$$

The author [8] lists two important properties of the mathematical model defined by (1) and (3):

≡ Independent of the initial state of the system, the solution tends asymptotically to the state of equilibrium when time tends to infinite:

$$c(t) \to c^e \text{ for } t \to \infty \quad (7)$$

≡ The steady state monotically increasing depends on the accumulation rate in the external environment and the concentration of the contaminant in the external environment:

$$c_1^e \ge c_2^e \text{ if } c_{w1} \ge c_{w2} \quad (8)$$

$$c_1^e \ge c_2^e \text{ if } k_1^u \ge k_2^u \quad (9)$$

≡ The equilibrium point is monotonically decreasing relative to the elimination rate:

$$c_1^e \ge c_2^e \text{ if } k_1^e \le k_2^e. \quad (10)$$

Using the assumptions (3), which give the forms of input and output flows in the system, the system (1) can be written in compact form:

$$\frac{dc}{dt} = Ac + k^u \quad (11)$$

with the initial conditions:

$$c(0) = c_0 \cdot \quad (12)$$

Matrix A is a triangular inferior matrix due to hypothesis Ia. In these conditions, after [8].,the general solution of the equation (11) with the initial conditions (12) is of the form:

$$c(t) = \exp(At)c_0 + \int_0^t \exp(A(t-s))k^u ds \ . \quad (13)$$

3. RESULTS

A first category of results that will be used in the elaboration of the experimental plan forms the sketch of a set of process parameters. Among these parameters, will be select those who need to be directly or indirectly measured. The list of important parameters of the accumulation process is given in Table 1.

A second category of results consists of exploring various types of environmental phenomena that can cause bioaccumulation or, why not, bio-drain. The author [8] gives the classical solutions for the phenomena of attenuation of a shock initially applied to the model through the initial conditions.

The solution for attenuating an initial shock is a simple analytic solution and can be used to predict the time to return to balance and to predict equilibrium concentrations (in the environment and in the plant). A numerical solution for three different cases of plant structure is given in Figure 1.

The use of numerical solutions opens the perspective of building simulators that can create complex environmental events. They can also simulate bioaccumulation phenomena for plants with a more complex structure. The effect of a contaminant wave on a plant with an initial concentration zero of the contaminant is described for the three plant structure cases in Figure 2.

This second category of results opens multiple perspectives for modelling the bioaccumulation phenomenon and shows clearly the usefulness of the models: first the mitigation prognosis, secondly the values at which the concentration of the contaminant in the plant will stabilize.

Finally, a third result is the bioaccumulation simulator based on this model. This simulator can be developed in different directions by completing with additional relationships, restrictions, or even new parameters.

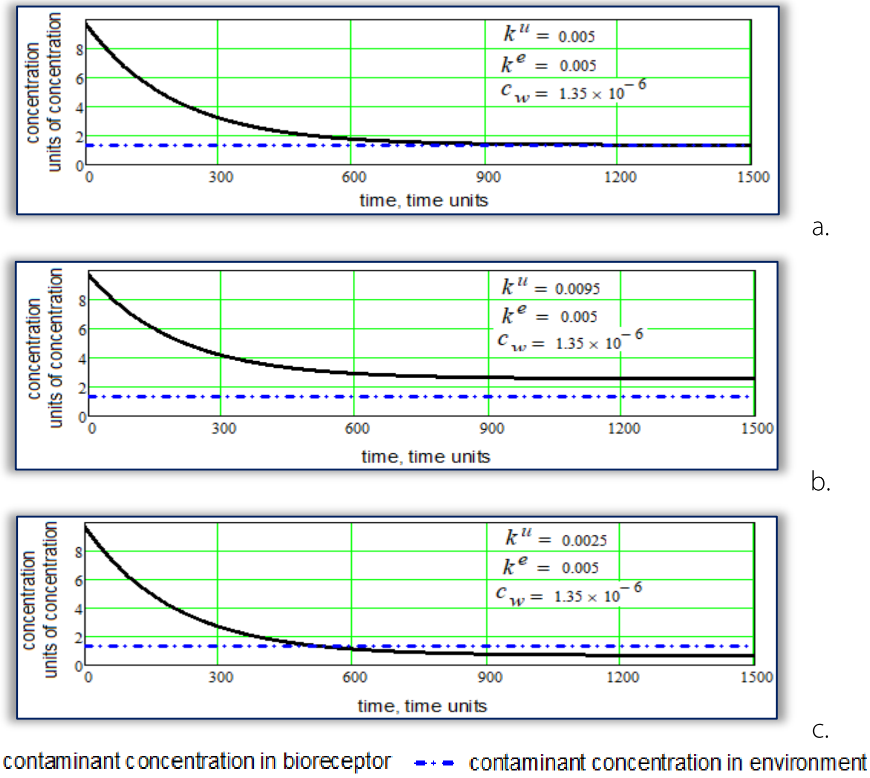

Figure 1 - Variation of contaminant concentration in the receiver in the case of initial pollution simulated by an initial non-zero value of the concentration in the bio receptor. The initial value of the concentration in the bio receptor was assumed c_0 = 0.00000975 units of concentration, higher than that of the contaminant in the medium

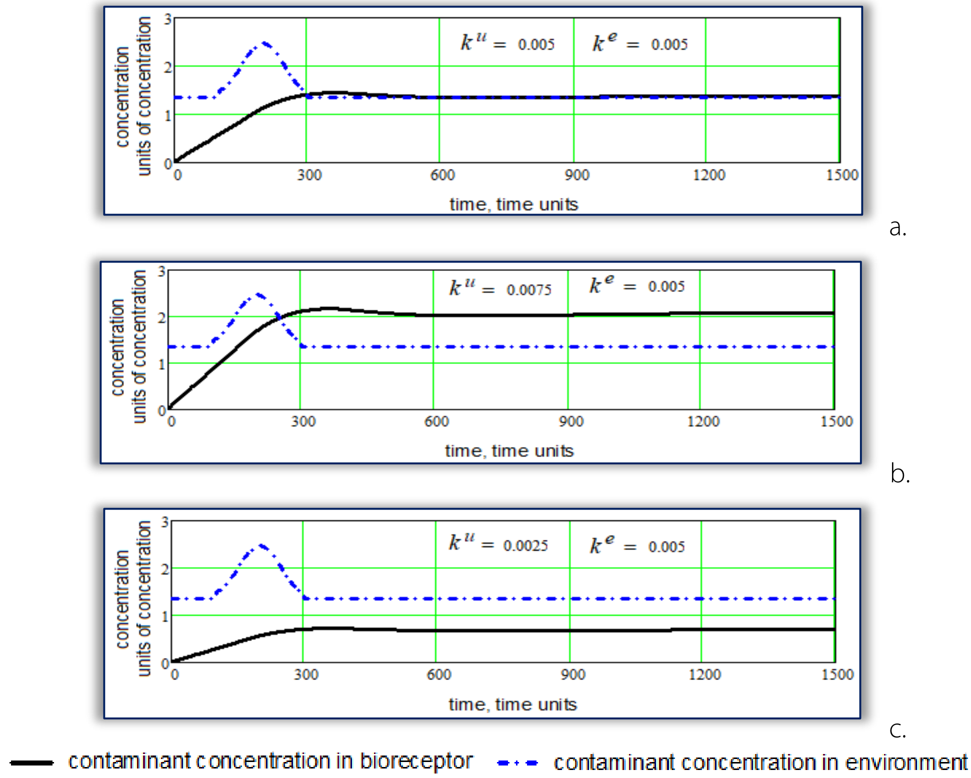

Figure 2 - Variation of the contaminant concentration in the receiver in the case of environmental pollution with a contaminant stream that alters the concentration of the contaminant environment in a continuous, increasing sense. The baseline concentration in the bio receptor was assumed to be c_0=0.00 units of concentration to observe the description of the impact of the pure contaminant wave.

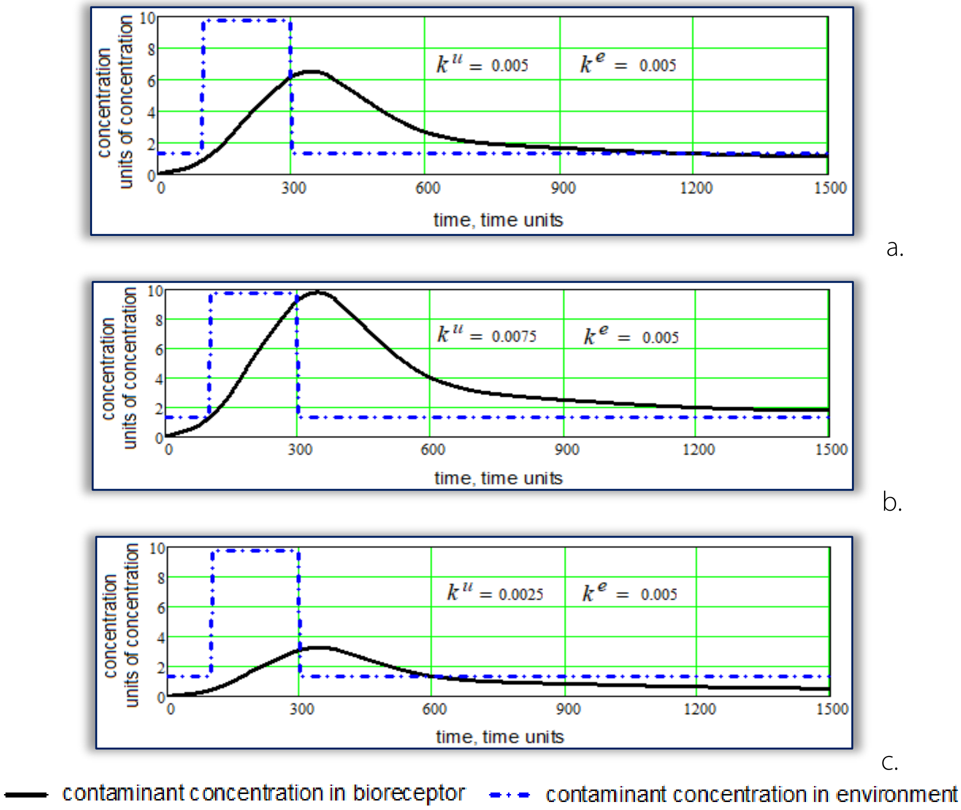

Figure 3 - Variation of contaminant concentration in the bio receptor in case of environmental pollution with a rectangular wave contaminant that alters the concentration of the environment in the contaminant. The initial value of the concentration in the bio receptor was assumed to be c0=0.00 units of concentration to observe the description of the impact of a pure contaminant.

4. CONCLUSIONS

The conclusions of this study refer to two problems: the value of the model and its perspectives. Respectively, specifying by the terminology of the mathematical model the parameter list that will be the subject of the experiments.

As for the model, at least intuitively, its behaviour or relatively short duration is in line with reality. The attenuation of environmental pollution phenomena, the prediction of stabilization of high concentrations over time, confirm our general observations and intuition.

From the experimental point of view, the model shows that the concentrations of contaminant in the environment and in the plant at a significant number of moments, as well as the determination of the accumulation and elimination rates, are the most important parameters in performing the experiments and rewriting the models.

A number of development perspectives poses more difficult issues, but they will be explained and modelling will be attempted at the right time.

The model presented is not yet sufficient for an isolation pattern of a plant in a pot, because if the soil is considered the environment then, in the case of a strict initial load, the concentration of the contaminant in the medium should decrease. The model presented cannot simulate satisfactory this phenomenon. Therefore, to solve this problem, it is recommended to use a mathematical model with two biodynamic components.

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