Acta Mechanica Slovaca 16 (1): 26 - 29, 2012

* Corresponding author
Phone +421 55 602 2223
E-mail address: dusan.knezo@tuke.sk
(prof. RNDr. Dušan Knežo, CSc.)

Article information
Article history: AMS-Volume16-No.1-00139-12
Received 15 January 2012
Accepted 15 March 2012

Mathematical Model of Harmful Substance Amount in Soil

Dušan Knežo
Department of Applied Mathematics and Informatics, Faculty of Mechanical Engineering, Letná 9, 042 00 Košice, Slovak Republic

BIOGRAPHICAL NOTES

prof. RNDr. Dušan Knežo, CSc. is head of the Department of Applied Mathematics and Informatics He graduated at the Faculty of Natural Sciences, University of P.J. Šafarik in Košice. He received the PhD.-degree at the Mathematic-Physics Faculty, University of J.A. Comenius in Bratislava, and he was habilitated at the Faculty of Mechanical Engineering, University of Žilina, in the scientific branch of applied mathematics. His scientific focus is oriented to the modelling of processes in the biomedical engineering, to the research of materials, as well as to the measurement and diagnostic equipment, prognostics and evaluation of medical proceed. He is a co-author of one monograph, one academic textbook and author of several textbooks. He has published more than 60 papers in the scientific journals and in the proceedings of the conferences and he has more than 80 quotations concerning his professional works. He was also incorporated in various grant research projects and industrial projects.

KEY WORDS

Degradation of substances, soil, mathematical model

ABSTRACT

There are brought into soil various chemical substances as a result of human activity with a positive or negative impact on the soil characteristics. Concentration of the added substances is changing over time and it is important due to many reasons to know the relation between the substance concentration and the time. One of important factors with an impact on the substance concentration in the soil is the natural degradation of materials. That is why there is presented in this paper a mathematical model of substance degradation process during a simple and repeated application of the given substance.

1. Introduction

Human activity is resulting in bringing of various chemical substances into the soil, namely intentionally or randomly, such as herbicides, pesticides and oil materials. These materials have also negative impacts on the environment or on the human health directly. Therefore it is important to know the time changes of substance concentration in the contaminated soil. We will investigate a thin layer of soil on the assumption that the substance concentration in the whole layer is homogenous immediately after application of the chemical substance into this layer or after contamination of this layer by a chemical matter. Another condition is that the concentration of the substance in the soil will be changing only due to the natural degradation of this substance and all other impacts on change of the concentration will be neglected. We want to find out a mathematical model describing the time behaviour of the substance concentration in the soil in the case of a simple application of the substance, as well as during a repeated application. The term "application of substance" means not only the intended application of matter into the soil, but also a random and unintended contamination of soil by the chemical substance.

2. Model of Substance Degradation in the Case of Simple Application

Let in the time $t = 0$ was implemented into the soil such amount of chemical substance that its concentration in the soil is the C_0, thus:

$$C(0) = C_0; \tag{1}$$

whereas the $C(t)$ is the substance concentration in the time t. If we are supposing that reduction of the substance concentration due to natural degradation is proportional directly to the concentration and so the change of concentration ΔC during the time interval Δt is:

$$\Delta C = -kC\Delta t.$$

From the last equation follows the differential equation

$$\frac{dC}{dt} = -kC, \tag{2}$$

where the constant k, $k \in R$, $k > 0$, is a parameter of substance degradation velocity. Solution of the linear differential equation of the 1st order (2), which fulfils the initial condition (1), is

$$C(t) = C_0.e^{-kt}. \tag{3}$$

The next relation defines the time behaviour of the concentration:

$$C(t)\begin{cases} 0 & \text{for } t < 0 \\ C_0.e^{-kt} & \text{for } t \geq 0, \end{cases} \tag{4}$$

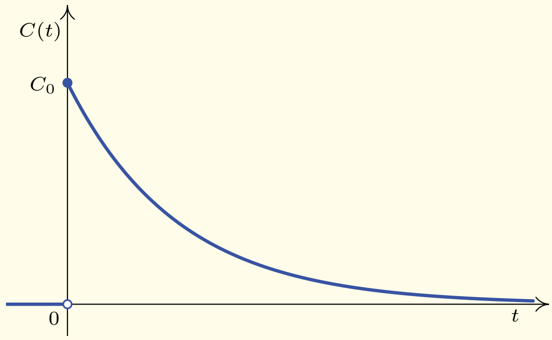

Fig. 1: *Time behaviour of concentration.*

If there is known the halftime of substance degradation DT_{50}, i.e. the time interval, which is necessary for reduction of 50% of the substance amount due to the natural degradation, so the relation (4) can be written in the form

$$C(t)\begin{cases} 0 & \text{for } t < 0 \\ C_0.e^{-\frac{\ln 2}{DT_{50}}t} & \text{for } t \geq 0, \end{cases} \tag{5}$$

because

$$k = \frac{\ln 2}{DT_{50}}.$$

Sometimes it is necessary to calculate the time point tcr with the defined critical concentration level C_{cr}, $0 < C_{cr} \leq C_0$. Such situation is typical, for example, if we want to determine time of the reduced contamination under the given level or if there are applied chemical protective substances and their concentration mustn't be reduced under a certain value and it is necessary to determine the time for a next repeated application. According to the relation (5) we obtain:

$$t_{cr} = \frac{DT_{50}}{\ln 2}\ln\frac{C_0}{C_{cr}}.$$

We note that if the mentioned amount of substance is applied not in the time $t = 0$, but in the time point $t = \tau$, $\tau > 0$, so for the time behaviour of the concentration is valid (see Fig. 2)

$$C(t)\begin{cases} 0 & \text{for } t < \tau \\ C_0.e^{-k.(t-\tau)} & \text{for } t \geq \tau. \end{cases} \tag{6}$$

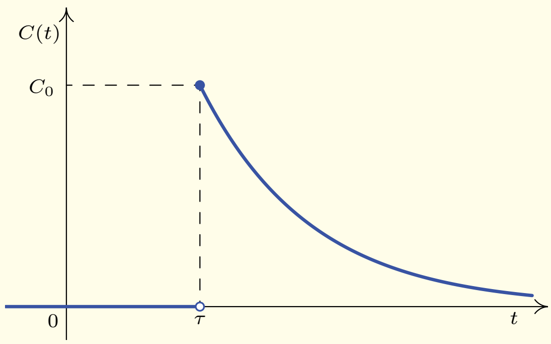

Fig. 2: *Concentration at shifted application.*

3. Model of Substance Degradation in the Case of Repeated Application

We are supposing that there was applied the substance repeatedly in the time points T_0, T_1, T_2, ..., T_{n-1}, $0 = T_0 < T_1 < T_2 < \ ... \ < T_{n-1}$, in this way that during the i-th application, i.e. during application in the time T_{i-1}, was applied into the soil such amount of substance, which is able to create in the pure soil the concentration level C_{i-1}, i=1;2; ... ;n. In this case there can be used relations (4) and (6) repeatedly and according to this method it is possible to demonstrate that for the time behaviour of the concentration is valid:

$$C(t) = \begin{cases} 0, & t \in (-\infty; 0), \\ C_0 . e^{-kt} & t \in \langle 0; T_1 \rangle, \\ \vdots & \\ \sum_{j=0}^{i-1} C_j . e^{-k(t-Tj)}, & t \in \left(T_{i-1}; T_i\right) \\ \vdots & \\ \sum_{j=0}^{n-1} C_j . e^{-k(t-Tj)}, & t \in \langle T_{n-1}; \infty \rangle, \end{cases} \qquad (7)$$

$$C(t) = \begin{cases} 0, & t \in (-\infty; 0), \\ e^{-kt} . C_0 & t \in \langle 0; T_1 \rangle, \\ \vdots & \\ e^{-kt} . \sum_{j=0}^{i-1} C_j . e^{kTj}, & t \in \left(T_{i-1}; T_i\right) \\ \vdots & \\ e^{-kt} \sum_{j=0}^{n-1} C_j . e^{kTj}, & t \in \langle T_{n-1}; \infty \rangle, \end{cases} \qquad (8)$$

The Fig. 3 illustrates the time behaviour of concentration.

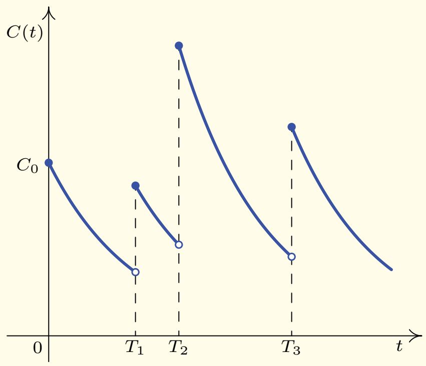

Fig. 3: *Concentration at repeated application.*

In the same way like it was performed for the simple application, we are able also in this case to determine the time point of critical concentration C_{cr}. We are thinking about intervals I_1, I_2, ... , I_n, kde I_i=<T_{i-1};T_i> for i=1;2; ... ;n−1 and I_n=<T_{n-1}; ∞>. The function C(t) is continuous, descending and limited function for each of intervals I_i. If we designate

$$C_{Li} = \inf_{t \in Ii} C(t); \qquad C_{Ui} = \max_{t \in Ii} C(t),$$

for i = 1;2;...;n, so for every C_{cr} ∈ <C_{Li};C_{Ui}> exists at interval I_i only one t_{cr} so that

$$C_{cr} = C(t_{cr}).$$

From the relation (8) we obtain

$$t_{cr} = \frac{1}{k} \ln \frac{\sum_{j=0}^{i-1} C_j . e^{kTj}}{C_{cr}}. \qquad (9)$$

$$C(t) = C_{cr},$$

It means that for every t ∈<T_{i-1};t_{cr}> is

$$C(t) \leq C_{cr},$$

and for each t ∈ <t_{cr};T_i> is

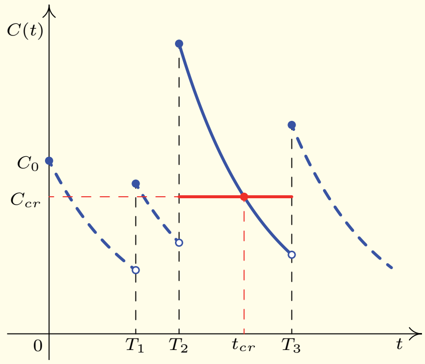

Fig. 4: *Concentration at repeated application.*

(see Fig. 4).

$C^{\star}$

In the case that the concentration mustn't exceed the defined limit value , it is necessary to

$$C_0 \leq C^{\star} \quad and \quad C_{Li} + C_i \leq C^{\star},$$

choose such application times and substance

amounts so that
for $i = 1;2;...;n-1$. If we want to $C_\star$reach a situation that for $t \in <0;T_n>$ the concentration will not be reduced under the stated limit , it is necessary

$$C_0 > C_\star \quad and \quad C_{Li} \leq C_\star,$$

to choose such application times and substance amounts so that
for $i = 1;2;...;n-1$.

In a special case, if there was applied the substance repeatedly in the time points $t = 0;T;2T;...;(n-1).T$, $T > 0$, $n \geq 2$ in the same amounts, thus $T_i = (i-1)T$ and $C_i = C_0$, for $i = 1;2;...;n-1$, it is

$$C(t) = \begin{cases} 0, & t < 0, \\ C_0.e^{-kt} & 0 \leq t \leq T, \\ \vdots & \\ C_0.\frac{1-e^{ikT}}{1-e^{kT}}.e^{-kt}, & (i-1).T \leq t < i.T \\ \vdots & \\ C_0.\frac{1-e^{nkT}}{1-e^{kT}}.e^{-kt}, & (n-1).T \leq t. \end{cases}$$

possible to present (see [1]), that for the time behaviour of concentration is valid

$$t_{cr} = \frac{1}{k}\ln\left(\frac{C_0}{C_{cr}}.\frac{1-e^{ikT}}{1-e^{kT}}\right), t = 1,2,...,n.$$

For the t_{cr} from the relation (9) we obtain in this case

4. Conclusion

It is possible to perform an estimation of the concentration of harmful chemical substances in the soil using the above-described mathematical model of the natural degradation of substances. This model is a simple model and it does not take into consideration another factors influencing reduction of concentration of chemical matters in the soil. Despite of this the presented model is applicable during a standard practice. The suggested model is theoretical, however in the case of it's experimental verification it could be defined the accuracy of the model for description of real processes. Such verification could be also important for development of a more accurate mathematical model in the future.

5. References

[1] Knežo, D., Mathematical Model of Substances Degradation, AEI Conference, in press.

[2] Kucharski, M.,Sadowski, J., Degradation of Ethofumesate in Soil under Laboratory Conditions, Polish J. of Environ. Stud. Vol. 18, No. 2 (2009), 243–247.

[3] http://focus.jrc.ec.europa.eu/dk/docs/finalreportFOCDegKin04June06linked.pdf

[4] http://www.york.ac.uk/media/environment/documents/people/brown/albrechtsen.pdf