DISSIPATION KINETICS OF CONTAMINANTS IN SOIL

I. V. Kumpanenko*, N. A. Ivanova, V. V. Usin,
***I. D. Epinatiev, and* A. V. Roshchin,**

Semenov Institute of Chemical Physics, Russian Academy of Sciences, Moscow, Russia,
*e-mail: ivkumpan@chph.ras.ru

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Abstract – A series of compartmental mathematical models describing dissipation kinetics of contaminants in soil is discussed. These models take into account a spatial variability and heterogeneity of soil. A two-compartment first-order double-exponential decay model is found to be the most suitable for description of dissipation kinetics in soil for O-isobutyl methyl phosphonate and O,O'-diisobutyl methyl phosphonate both of which are known to be the main and much less toxic degradation products of chemical warfare agent V_x, (when compared to the toxicity of V_x itself). In accordance with this model, the dependence of contaminant concentration C on time t can be described by the following equation $C(t) = C_p + C_1 \cdot \exp(-k_1 t) + C_2 \cdot \exp(-k_2 t)$, where C_p, C_1, C_2, k_1, k_2 are fitting parameters. Comparison of coefficients of determination R^2 has revealed that approximation of experimental data using first-order double-exponential formula is more exact than approximation using simple exponential equation $C(t) = C_p + C_1 \cdot \exp(-k_1 t)$. The calculated fitting constants make it possible to estimate periods of time required for dissipation of 50% and 90% of the contaminants. O-isobutyl methyl phosphonate is found be more stable in soil with moderate moisture levels (50 mass %) whereas O,O'-diisobuthyl methyl phosphonate demonstrates higher stability in soil with an increased moisture levels (70 mass %).

Keywords: contaminants in soil, dissipation kinetics, O-isobutyl methyl phosphonate, O,O'-diisobutyl methyl phosphonate, two-compartment first-order double-exponential decay model.