АКТУАЛЬНІ ПИТАННЯ УПРАВЛІННЯ РІВНЕМ ЕКОЛОГІЧНОЇ БЕЗПЕКИ ТЕХНОГЕННИХ ОБ'ЄКТІВ

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MODELING OF THE PROCESS OF MIGRATION OF CHEMICAL ELEMENTS IN COAL DUMPS

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Introduction: The use of natural resources has increased, which in turn increases the anthropogenic pressure on the environment. One of the sectors of use of natural resources is mining. Coal is one of the sources of electricity. The production of electricity based around the coal industry in Ukraine reaches 25-30% [1]. One of the negative factors of the impact of the coal industry, during coal mining, is the formation of coal dumps. Coal waste is empty rock that accumulates in specially designated areas and has a negative impact on the atmosphere, lithosphere and hydrosphere. About 60 million tons of rock is accumulated in Ukraine annually [2]. The coal dumps of Western Donbass are characterized by low pH values, low electrical conductivity, low nutrient content, and a high concentration of heavy metals, which is several times higher than the maximum allowable concentrations (MPC) [3].

Purpose: As a result of the obtained data, try to create a model of the migration of chemical elements in the substrate.

Literature review: The migration of metals and their concentration in soil as a heterogeneous system with variable composition is controversial due to the complexity of these highly interconnected processes and the huge amount of input data required for these models. In general, the migration of metals depends on several conditions, including the granulometric composition of the soil, its filtering capacity, pH, metal sorption, composition of soil phases (percentage of clay, organic matter, iron, etc.), climatic conditions (e.g., moisture), and the geochemical structure of the terrain. Given that these parameters are not easy to determine, yet are necessary to characterize metal migration, basic parameters for modeling metal migration in soil are often insufficient. Therefore, the application of mathematical models for a comprehensive description of the migration of metals should take into account the complete, complex nature of these processes. Several mathematical algorithms have already been implemented as tools to improve phytoremediation efficiency and to better understand specific soil processes. One example is the implementation of a system dynamic approach (SDA), which provides a set of differential equations defined by specific models for specific physiological responses of plants. One example is a study where a system dynamics approach was used to predict the uptake of cadmium, lead, copper, and zinc in rice shoots grown on a contaminated site near an abandoned lead and zinc mine [4]. In this study, six different chelating agents were applied in experimental fields and NH_4OAc and $CaCl_2$ chelating agents were found to be the most suitable extractants for predicting the bioavailability of heavy metals for rice grown on a ground cover with several problems causing plant abiotic stress, including mixed contamination with metals. In another study, SDA was successfully used to predict the time required for uptake of 2,4,6-trinitrotoluene (TNT) by Populus fastigiate. However, this study was conducted under artificial conditions of eared soil and not on a large scale [5]. Another model that can be used for phytoremediation planning is the PLANTX model, which takes into account the dynamic transport of compounds from soil to plants and air, as well as the metabolism of pollutants, including their final accumulation in stems, leaves or fruits. It is mostly useful for organic contaminants. In general, the model is based on the diffusion of pollutants through the soil solution and soil pores, the transport of pollutants into roots, and the total distribution of pollutants in plant tissues [6]. The Freundlich model can be used to estimate the absorption of heavy metals from contaminated soil characterized by significantly different concentrations of pollutants. The model is based on both the total and the available concentration of the pollutant. This method supports the non-linearity of absorption and takes into account the differences between plant species, which helps in the process of selecting the most suitable plants for a given area. A positive feature of a Freundlich-like model is that it is easy to operate and can be used to predict field phytoremediation performance. With this model, a more realistic prediction of the potential of the technology can be obtained, as the use of linear transfer functions from soil to plant may overestimate absorption [7].

Materials and methods. The object of the study was a coal waste heap in the Western Donbass, Ukraine. The Western Donbass is a coal basin within the Dnipropetrovsk region, part of the Donetsk coal basin. The research methodology consists in a comprehensive analysis of such physical and chemical parameters of substrate as: pH, specific electrical conductivity of the soil (EC), the total content of heavy metals, other toxic and rare-earth elements. For an intact soil sample, the quantitative content of nutrients for plants was additionally determined, namely, NO^{3-}, NH_4^+, PO_4^{3-} ions (spectrophotometrically) and the concentration of mobile forms of elements obtained by water extraction and extraction with ammonium acetate buffer (pH = 7) and ammonium acetate solution with the addition of citric acid (pH=4).

Results. According to the analysis of physical and chemical indicators, there was determined that the pH of the soil from the site where accumulated coal dump is 7.68, the value of specific electrical conductivity is 1200 µS/cm. Results of mine rock research with regard to plant nutrients, they testify about insufficient amount of nitrate (from 0.007 mg/kg) and ammonium (0.11 mg/kg) forms of nitrogen, as well as phosphates (0.016 mg/kg) [8]. The analysis of the physical-chemical properties of coal waste is presented in Table 1.

Table 1 – Physical-chemical parameters of the coal dump

pH	EC µS/cm	Nutrients		
		NO^-_3, mg/kg	NH^+_4, mg/kg	PO^{3-}_4, mg/kg
7.68	1200	0.007	0.11	0.016

Table 2 shows the concentration of potentially active and mobile forms of heavy metals and other toxic elements.

Table 2 – Concentration of potentially active and mobile forms of heavy metals and other toxic elements in the substrate

Elements	Co	As	Cu	Pb	Mn	Zn
C mg/kg	296.8	76.6	140.9	122.5	3740	572.3

The water-soluble content of chemical elements was determined based on the inductively coupled plasma mass spectrometry (ICP-MS) method. During the analysis of potentially dangerous elements that can be leached from this rock, it was found that with an aqueous solution of ammonium acetate (pH=7 and pH=5), dangerous forms that can enter the environment were not detected.

Conclusion. The results of the physical and chemical analysis of the substrate taken from the coal mining dump are given, which indicate a low content of nutrients and a high concentration of potentially active heavy metals and other toxic elements.

Discussion. The use of mathematical models in environmental studies can improve the evaluation of various outcomes in order to make an objective decision about the most suitable process for a selected contaminated site. Models of contaminant uptake and accumulation can play a key role in understanding the processes occurring in soils and plants, which may subsequently allow for the management of contaminated sites. Many existing models have been tested with limited data and may only apply to certain described soil and plant conditions. In order to achieve the desired effectiveness of remediation, the main direction is the combination of physical and chemical properties of contaminated land with mathematical models and programming tools.

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