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MATHEMATICAL MODELLING TECHNIQUE TO ASSESS SOIL CONDITIONS

Abstract: *This paper analyzes the results of studying contaminated soil samples from a combat zone (Sumy region, Ukraine). The authors proposed a mathematical model for simulating and assessing the impact of military operations on soil and groundwater. The mathematical model will make it possible to predict the occurrence of environmental emergencies and reduce the frequency of expensive experimental studies of soils contaminated with heavy metals.*

Keywords: *heavy metals, soil, groundwater, mathematical model.*

Introduction

The armed conflict that broke out in Ukraine in 2014 caused environmental problems associated with the accumulation of pollutants in soil and water bodies. Between 2014 and 2021, about 50,000 square kilometres have been affected in Ukraine due to hostilities. A study of the soil surface in the conflict zone was conducted in 2014 under OSCE support. The study found a 1.2–12-fold increase compared to the background levels in heavy metals content in most of the soil samples taken from the areas of hostilities. Mercury, vanadium and cadmium concentrations were consistently 1.1–1.3 times higher than the normal levels. The highest content of heavy metals was found in the areas of shell bursts. Since the beginning of Russia's full-scale invasion of Ukraine (February 24, 2022), these areas have grown significantly (up to 150–180 thousand sq km) with an significant increase in the consequences for the ecosystems.

According to open sources, the armed aggression has polluted more than 3% and contaminated up to 10% of Ukrainian land, causing up to UAH 500 billion in damage. Landmines represent a separate type of contamination. According to the Ukrainian Deminers Association, an area of more than 80.5 thousand sq km (14%) of Ukraine's territory is mined. Such lands (soils) have been removed from economic use, in part or whole, until complete mine clearance [1].

As the international experience shows, armed conflicts significantly impact properties of soil health, disrupting some of its physical and chemical properties and causing contamination, which is especially dangerous for agricultural lands. Direct hits by shells, burnt-out military equipment and oil products, destroy ecosystems and cause soil and water to become contaminated with heavy metals and toxic elements. The most hazardous soil pollutants are lead, mercury, arsenic, cadmium, copper, nickel and zinc. During military operations, these and other heavy metals are released into the surrounding environment from firearms remnants with mixtures of metal-containing particles. Metal residues are one of the most dangerous consequences of military actions, and they generally persist for the longest time in the areas of hostilities.

Potentially toxic elements in the war-affected areas include lead and related contaminants – antimony, chromium, arsenic, mercury, nickel, zinc and cadmium. The explosives also contain large amounts of mercury. Zinc, copper, nickel, lead and chromium are used to coat bullets, missiles, gun barrels and military vehicles. Barium, stibium, bismuth, and boron are standard charging compounds in weapons, and tungsten is used in aerial bombs. Once released into the environment, potentially toxic elements of the ammunition get oxidised upon contact with air, and their residues enter the soil, where various chemical processes occur.

To determine the impact of hostilities on the soil surface after the liberation of Sumy Oblast in 2022, experts took samples at the sites of bomb drops and in demined areas. The results showed that the contents of the following metals exceeded the maximum allowable concentrations: lead – in 60% of soil samples (1.4 to 10.6-fold); copper – in 50% of samples (1.1 to 6.1-fold); zinc – in 20% (1.3 to 3.4-fold); manganese – in 20% (2.3 to 2.4-fold). The soil samples' total content of heavy metals exceeded the background levels by 1.1–5.4 times. The study revealed the highest levels of lead and the lowest levels of iron [2].

The global experience of post-war territory clearance shows long-term demining, reclamation and decontamination of such lands. Given the particular density of mining and artillery shelling, such processes will require significant workforce and financial resources.

Since extensive soil and water chemical contamination is expected, ensuring an effective environmental monitoring system after the war is essential. Such monitoring will make it possible to determine the actual degree of ecological damage and implement timely and effective measures to prevent further deterioration and restore safe ecosystems for both people and animals.

Purpose and research goals

Currently, experimental research methods cannot be used because of the ongoing shelling throughout the country. A possible solution to this problem is to develop a method for predicting potential soil and groundwater contamination levels using mathematical models.

Materials and Methods

When developing a general algorithm for assessing the environmental impact of hostilities, it is recommended to collect the following information in advance:

- on the use of certain types and kinds of ammunition, shells, missiles, and aerial bombs on the studied territory;
- on the mining of the territory and the possibility or impossibility of its complete clearance;
- on the impact on local features from the destruction of unexploded ordnance that cannot be neutralised and can only be eliminated in situ by detonation;
- on the surface condition, as explosions can alter the topography of the territory and move soil layers.

A method has been proposed for modelling the spread of heavy metal salts deep into the soil in contaminated areas. Such modelling aims to estimate the likelihood and timing of emergencies.

Heavy metals from ammunition and military equipment end up in the soil and groundwater. The first type of emergency occurs with deep soil salinisation. The second type of emergency arises when molecules of heavy metals enter the water table. The modelling of the movement of heavy metal molecules in multilayer soils involves several stages. The initial prerequisite for developing the mathematical model field is the presence of chemical compounds of heavy metals in the surface soil at concentrations exceeding the allowable levels.

$$\rho_i^d\left(x_0, y_0, z_0, t\right) \geq PC_i \quad (1)$$

where:

ρ_i^d – concentration of the dangerous substance;

x_0, y_0, z_0 – initial coordinates of the source of pollution;

PC – permissible concentration;

i – chemically dangerous compound that has reached its limit (permissible concentration).

The movement of heavy metals occurs in the aeration zone, and different territories will have different rates of contamination spread.

The nonlinear nonstationary model uses an equation from the theory of physicochemical fluid dynamics in porous media [3].

$$D_m(\theta)\frac{d^2C}{dX^2} = \theta\frac{dC}{dT} \tag{2}$$

where:

$D_m(\theta)$ – molecular diffusion coefficient, m^2/s;

C – salinity of the soil (rocks), %;

Θ – volumetric humidity, %;

X – spatial coordinate, m;

T – time coordinate, s.

It should be noted that these values are probabilistic and depend on the structure of the aeration zone, the properties of metal molecules, temperature, pressure, humidity and substance concentration.

The analytical solution of equation (2) has the form:

$$C_{hx} = \left(C_s - C_0\right) erfc\left[\frac{1}{2}\cdot\frac{h_x}{\sqrt{\frac{D_m(\theta)\cdot t}{\theta}}}\right] \tag{3}$$

where:

C_{hx} – predicted salinity level at h_x depth, %;

C_s – surface salinity of the aeration zone at (x_0, y_0, z_0) surface points at $h = 0$;

C_0 – the initial level of salinity at (x_0, y_0, z_0) points on the surface of the soil before storage at $t = 0$;

h_x – distance of the calculation points from the (x_0, y_0, z_0) surface points, i.e. from the earth's surface, m;

t – term of prediction calculation, day;

erfc – tabulated function.

The risk of emergencies and assessment of potential consequences are provided as additional boundary conditions in the model:

- an emergency caused by an increased deep soil salinisation

$$C_x < q\left(C_x, t, h_x\right) < 0.35 \tag{5}$$

- an emergency caused by the penetration of a chemically hazardous compound containing heavy metals into subsurface or groundwater

$$h_0 \le q\left(C_x, t, h_x\right) \le H \tag{6}$$

where:

h_x – depth of penetration of chemically hazardous compounds into the soil;

$q(C_x, t)$ – an indicator that further determines the nature of the spread of danger and is a reflection of the sources of danger;

H – depth of the aquifer within the territory of possible distribution.

The model is based on the following assumptions: metal accumulation is cumulative; salt transfer occurs during free penetration and normal infiltration; soil humidity is characterised by seasonal fluctuations (winter-spring and summer-autumn).

To apply the modelling method, it is necessary firstly to assess experimentally the concentration of hazardous substances, the depth of their penetration and the structure of the aeration zone, which may have changed due to shelling and explosions. The values of other variables used in the formulas can be obtained from the literature.

Conclusion

A mathematical model has been proposed for modelling and assessing the impact of hostilities on soil and groundwater. Based on the modelling results, predicting the time of environmental emergency occurrence is possible. This method can significantly reduce the need for expensive experimental research and determine the priority of land revegetation in different parts of the country.

References

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