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Mathematical modelling of soil phytoremediation efficiency from Pb, Cu and Ni

Oleksandra Sydorenko*
Master's Student
National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute"
03056, 37 Beresteiskyi Ave., Kyiv, Ukraine
https://orcid.org/0009-0004-5890-7630

Nataliia Golub
Doctor of Technical Sciences, Professor
National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute"
03056, 37 Beresteiskyi Ave., Kyiv, Ukraine
https://orcid.org/0000-0003-1448-1872

Abstract. The study aimed at a quantitative comparative assessment of lead, copper, and nickel removal dynamics from soil by the "metal-plant" system based on mathematical modelling to predict the cleaning timelines of contaminated areas. Soil contamination with heavy metals (Pb, Cu, Ni) due to intensive anthropogenic activities and large-scale military operations in Ukraine posed a critical threat to environmental safety and public health. Phytoremediation using hyperaccumulator plants, such as *Brassica juncea*, was considered a promising and environmentally friendly method for ecosystem restoration. However, the planning of such measures was complicated by the varying rates of element removal and their toxic effects on biomass, which necessitated the development of accurate predictive models. An exponential model of metal uptake kinetics was used to predict the cleaning timelines of contaminated areas. It was established that the soil cleaning efficiency for one vegetative period (180 days) was 92.9% for copper, 80.6% for nickel, and only 53.5% for lead. The findings revealed that the high remediation efficiency of copper was due to its high mobility and low phytotoxicity. Conversely, lead exhibited the strongest inhibitory effect, significantly limiting its extraction rate. Based on the multi-metal model, an additive toxic effect of pollutant mixtures was demonstrated, leading to a 78% reduction in the overall productivity of phytoremediators compared to monometallic contamination. The obtained results allowed for the optimisation of restoration strategies for anthropogenically

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*Corresponding author

stressed territories and lands affected by military conflicts. The developed model can be used to assess the economic feasibility of phytoremediation measures

Keywords: heavy metals; phytoextraction; toxic stress; multi-metal model; soil recovery; environmental safety

Introduction

Soil contamination with heavy metals, such as lead (Pb), copper (Cu), and nickel (Ni), remained one of the most critical environmental challenges globally, posing a severe threat to ecological safety and human health. In the context of Ukraine, this issue had acquired unprecedented urgency due to large-scale military operations and intensive industrial activities. Military-related pollution was characterised by high concentrations of metal complexes originating from ammunition fragments and destroyed infrastructure, which required immediate and effective remediation strategies. Among various decontamination methods, phytoremediation – the use of hyperaccumulator plants to extract pollutants – was recognised as a sustainable, cost-effective, and ecologically safe approach. As noted by X. Shen *et al.* (2022), who conducted a critical review on the performance and challenges of heavy metal removal, this method offered significant environmental benefits and minimised secondary ecological impact. G.A. Bortoloti & D. Baron (2022) explored the biochemical and physiological mechanisms of *Brassica* plants, highlighting their inherent potential for the phytoremediation of toxic elements. *Brassica juncea* (Indian mustard) was widely regarded as an ideal biological object for these purposes. For instance, I. Ali *et al.* (2022) screened various *Brassica* species for the phytoremediation of contaminated soils and confirmed that Indian mustard provided the highest extraction rates under complex geochemical conditions. The selection of this plant as a model was justified by its ability to rapidly generate significant above-ground biomass, its robust root system, and its documented tolerance to toxic stress. Supporting this, M. Sut-Lohmann *et al.* (2023) demonstrated that *Brassica juncea* remained a feasible hyperaccumulator of potentially toxic metals even under the extreme environmental conditions typical of anthropogenically disturbed zones. Understanding the dynamics of soil cleaning required an integrated assessment of the physiological response of the plant to toxic stress. S. Maher *et al.* (2025) provided a comparative assessment of *Brassica juncea* for efficient phytoremediation, emphasising that the mobility of metals within the soil matrix was a decisive factor for extraction kinetics.

Elements like copper and nickel often exhibited relatively higher mobility, making them more accessible for plant uptake. In contrast, lead was frequently characterised by low mobility and a strong tendency for fixation within the soil structure. Researcher P. Rani *et al.* (2023) highlighted *Brassica juncea* as a potential crop for the simultaneous phytoremediation of various heavy metals, which was crucial, when dealing with complex multi-vector pollution rather than simple ions. The chemical complexity of soil pollution in areas of active military conflict presented a unique challenge for ecological restoration. The "chemical fingerprint" of war involved a heterogeneous mixture of heavy metal complexes. The transition from monometallic to multi-metal modelling was essential for creating realistic environmental management plans. P. Cârdei *et al.* (2021) developed a mathematical model to simulate the transfer of heavy metals from soil to plant, which had become a fundamental basis for modern predictive systems. Scientists T. Leonavičienė *et al.* (2023) focused on the modelling of environmental processes and management, providing a methodological framework for assessing large-scale decontamination projects. A.M. Kamal & A.F. Alali (2025) applied kinetic modelling of heavy metal uptake and translocation in *Brassica juncea*, proving that such analytical frameworks allowed for accurate forecasting of remediation outcomes before field implementation. Dynamic models based on systems of ordinary differential equations allowed researchers to simulate temporal changes in plant biomass, calculate metal accumulation in tissues, and forecast the reduction of concentrations in the soil solution over a vegetative period (Cârdei *et al*., 2021). Such predictive tools were essential for optimising remediation parameters and assessing the feasibility of decontamination projects before their field implementation. Despite the progress in single-metal modelling, there remained a significant gap in understanding the combined toxic effects of metal mixtures, which were typical for war-affected soils. Most existing frameworks do not fully account for the additive inhibitory pressure that multiple pollutants exert on plant growth. The aim of this research was to provide a quantitative comparative assessment of Pb, Cu, and Ni removal dynamics from contaminated soils using *Brassica juncea* based on a unified nonlinear dynamic model. The scientific novelty of this work lain in the implementation of an extended multi-metal model that quantified the additive toxic effect of pollutant mixtures, specifically adapted to initial concentrations corresponding to the anthropogenic pressure found in military conflict zones in Ukraine.

Materials and Methods

Parameter justification and physical meaning used model

To ensure a rigorous comparative analysis of the phytoremediation efficiency of various heavy metal complexes (rather than simple ions), a unified nonlinear dynamic model of the "metal-plant" system was applied. The system was described by three interrelated state variables: plant biomass (*B*), normalised metal concentration in plant tissues (*Me*), and metal concentration in the soil (*S*). The system of nonlinear ordinary differential equations was formulated as follows:

$$\frac{dPB}{dt} = PB\,(a - b\,PB) - PB\,\frac{d\,Me}{e+Me}; \qquad (1)$$

$$\frac{dMe}{dt} = \alpha\,S\,(1 - Me) - \beta\,Me; \qquad (2)$$

$$\frac{dS}{dt} = -\alpha\,PB\,S + \beta\,PB\,Me + \phi\,(S_0 - S). \qquad (3)$$

The first equation described the dynamics of biomass growth. The term *B(a - bB)* represented standard logistic growth, where *a* – specific growth rate and *b* defined the carrying capacity of the environment. The term *B(d · Me) / (e + Me)* introduced the inhibitory toxic effect caused by the accumulation of heavy metal complexes, where *d* represented the maximum toxicity coefficient and *e* – half-saturation constant for toxicity. The second equation modelled the kinetics of metal uptake by the hyperaccumulator *Brassica juncea*. The absorption was driven by the soil concentration (*S*) and the specific absorption coefficient (α), bounded by a biological saturation effect *(1 - Me)*. The partial excretion or return of metals was governed by the coefficient β. The third equation defined the mass balance in the soil, accounting for the depletion due to plant extraction ($-\alpha BS$), the return from decaying tissues ($\beta B \cdot Me$), and natural soil recovery processes driven by the coefficient φ towards an equilibrium concentration S_0 (Cârdei *et al*., 2021).

Experimental scenarios, computational setup and software implementation

The numerical simulation was strictly conducted for a vegetative period of 180 days, accurately representing the growth cycle of herbaceous hyperaccumulators in a temperate climate. To determine the base system parameters, it was utilised the mathematical modelling methodology for environmental processes proposed by T. Leonavičienė *et al.* (2023). Based on this methodology, base parameters for the overall system were standardised as follows: $a = 0.10$, $b = 0.01$, $e = 1.0$, $\beta = 0.0005$ day^{-1}, $\varphi = 0.0001$ day^{-1}, and an equilibrium concentration $S_0 = 100$ mg/kg. Differences between the metal complexes were implemented exclusively through the metal-specific absorption coefficients (α) and toxicity constants (d) to ensure a controlled comparative baseline. The values for these specific parameters were adapted based on the phytoextraction assessment methodology presented by J. Suman *et al*. (2018). The established values were: lead (Pb): $\alpha = 0{,}0010$ day^{-1}, $d = 0{,}07$; copper (Cu): $\alpha = 0{,}0025$ day^{-1}, $d = 0{,}03$; nickel (Ni): $\alpha = 0{,}0018$ day^{-1}, $d = 0{,}05$. Unlike base scenarios with a fixed *S0*, this study investigated varied initial soil pollution levels reflecting the anthropogenic impact of military actions in Ukraine: Cu (100, 150, 300 mg/kg), Pb (70, 125, 150 mg/kg), and Ni (50, 100, 150 mg/kg). Furthermore, an advanced multi-metal model was implemented to simulate the simultaneous presence of multiple pollutants. In this model, the total toxic effect (T_{total}) was integrated into the system of differential equations as a linear combination (additive contribution) of individual metal complexes inhibiting biomass growth. Mathematically, this factor was expressed as:

$$T_{total} = \sum_{i=1}^{n} (d_i \cdot C_i), \quad (4)$$

where d_i – toxicity constant of the i-th metal, and C_i – current concentration in plant tissues. The mathematical modelling was executed in the Python programming environment. The NumPy library was utilised for efficient multidimensional array operations and data structuring. The SciPy library, specifically the *odeint* integrator from the *scipy.integrate* module, was employed for the robust numerical resolution of the stiff system of non-linear differential equations. Time-series data visualisations were generated using Matplotlib.

Results and Discussion

Analysis of biomass growth under toxic stress

The simulation of *Brassica juncea* growth over a 180-day period provided a detailed view of how complex compounds of heavy metals influence primary productivity. In the control scenario (Fig. 1), where concentrations remained at background levels, the biomass accumulation followed an ideal sigmoidal trajectory. The absence of significant inhibitory pressure allowed the plant to reach its maximum carrying capacity by approximately the 100th day of vegetation. The graph clearly distinguished an intensive exponential growth phase between days 20 and 60, after which the growth rate gradually slowed down, stabilising at a level of approximately 10.0 kg/m^2. This indicated the optimal functioning of the plant's enzymatic systems in the absence of toxic stress.

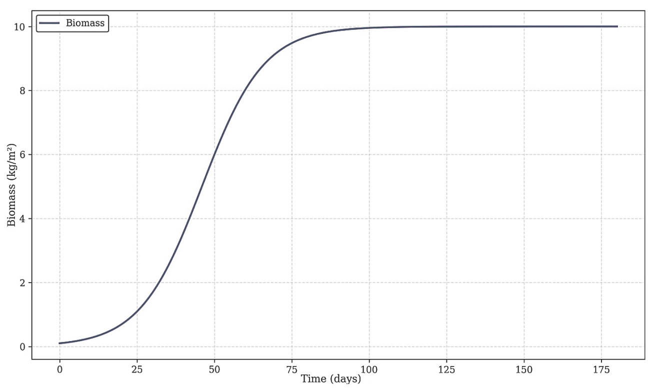

Figure 1. *Dynamics of mustard biomass growth at standard (background) soil metal concentrations*
Note: Cu – 25 mg/kg, Pb – 20 mg/kg, Ni – 20 mg/kg (control)
Source: developed by the authors

However, the introduction of copper complexes (Fig. 2) shifted this equilibrium. Even at the maximum tested concentration of 300 mg/kg, the biomass reduction remained minimal.

This resilience was mathematically represented by the toxicity constant d = 0.03. From a biological perspective, this indicated that, while Cu was a heavy metal, its role as an essential micronutrient allowed the plant to maintain high metabolic activity even under elevated loads. The "zoom-in" area in Figure 2 clearly demonstrated that the difference between 100 mg/kg and 300 mg/kg variants was less than 5%, confirming the low sensitivity of the hyperaccumulator to this specific pollutant. Throughout the entire vegetative cycle, the growth curves for different Cu concentrations nearly duplicated the trajectory of the control, suggesting highly effective internal copper detoxification mechanisms in *B. juncea* tissues.

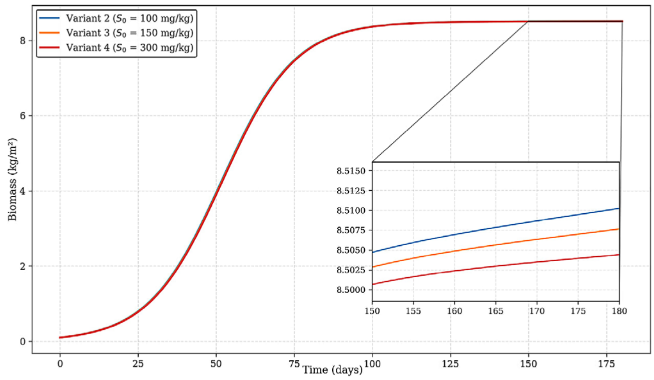

***Figure 2.** Dynamics of Brassica juncea biomass growth at different initial Cu concentrations in the soil*
Source: developed by the authors

In stark contrast, the modelling of lead (Pb) contamination (Fig. 3) revealed a critical suppression of growth. With a toxicity coefficient of d = 0.07, lead complexes exert more than double the inhibitory pressure compared to copper. The biomass curve for the 150 mg/kg variant failed to reach the 7.0 kg/m^2 mark, showing a significant "lag phase" in the middle of the vegetative cycle. This suggested that the energy resources of *B. juncea* were redirected from growth to detoxification and structural sequestration within the root tissues, which aligned with the phytostabilisation strategy. The graph showed that with increasing Pb concentrations, the plateau was reached much earlier but at significantly lower biomass levels, indicating irreversible physiological disruptions upon reaching a critical threshold.

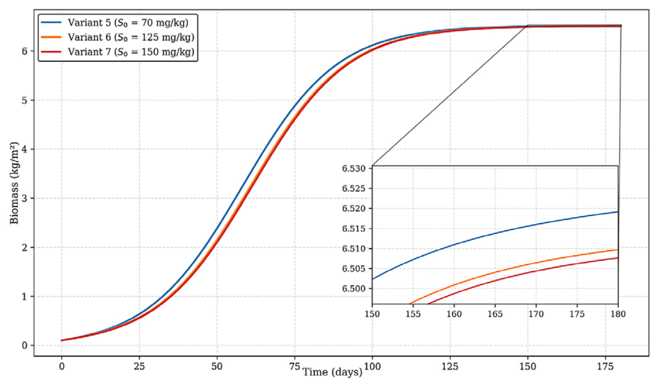

***Figure 3.** Dynamics of Brassica juncea biomass growth at different initial Pb concentrations in the soil*
Source: developed by the authors

Nickel (Ni) represented an intermediate case (Fig. 4). With d = 0.05, the biomass stabilisation occurs around 7.5 kg/m^2 for the highest dose. The transition from the active growth phase to the plateau was smoother than that of lead, indicating a more balanced interaction between the metal complex and the plant's enzymatic systems. Analysis of the charts showed that at a concentration of 50 mg/kg, the effect of nickel was moderate; however, at 150 mg/kg, there was a clear 25% reduction in productivity compared to the control. This confirmed nickel's status as an element with moderate phytotoxicity, where accumulation capacity was limited by the gradual depletion of the plant's adaptive reserves.

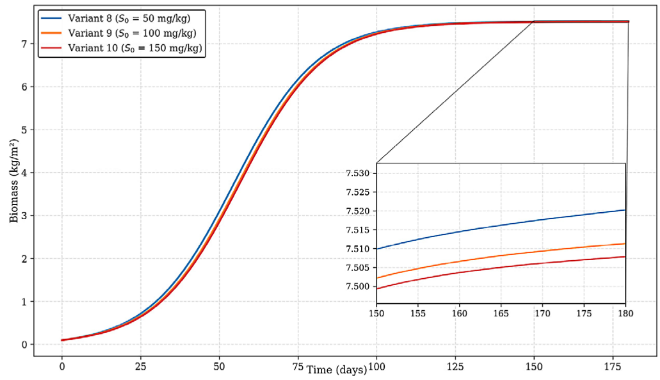

Figure 4. *Dynamics of Brassica juncea biomass growth at different initial Ni concentrations in the soil*

Source: developed by the authors

So, the dynamics of biomass accumulation served as an integrated indicator of the phytoremediation system's stability. A comparative analysis of the modelling results confirmed a toxicity hierarchy of Pb > Ni > Cu. The established mathematical relationships allowed for both the confirmation of growth inhibition and the quantitative prediction of biomass loss, which was crucial for calculating the total efficiency of metal removal from the soil. The results obtained regarding the selective toxicity of heavy metals were consistent with several foundational studies in the field. B.V. Tangahu *et al.* (2011) emphasised that the efficiency of phytoremediation was intrinsically linked to the plant's ability to maintain biomass production under chemical stress, noting that lead consistently exhibited the highest inhibitory potential among common industrial pollutants. Finding of this research that copper acted as a less toxic stressor aligned with the observations of P.C. Nagajyoti *et al.* (2010), who highlighted the dual role of Cu as both a nutrient and a potential toxicant depending on the concentration threshold.

Kinetics features of metal accumulation and soil decontamination

The dynamics of metal uptake showed that the saturation of plant tissues occurred much faster than the depletion of the soil reservoir. In the control scenario (Fig. 5), the accumulation of Cu, Pb, and Ni in plant tissues remained minimal, reflecting standard background levels. The plotted curves demonstrated a near-zero slope throughout the 180-day period, confirming the baseline state of the plant without induced phytoextraction. For copper (Fig. 6), the normalised concentration in the plant reached 90% of its maximum within the first 40 days. The visual trajectory of the graphs demonstrated a sharp exponential rise followed by an early and stable plateau, indicating rapid tissue saturation. This rapid "loading" phase was driven by the high absorption coefficient α = 0.0025. The specific absorption coefficient (α) used in this study represented the combined influence of soil pH, organic matter content, and the plant's genetic potential for uptake. Comparative analysis revealed that the high α for copper allowed for a rapid saturation of plant tissues, creating a "pull effect" that continuously drawn the metal from the soil solution. This was mathematically evidenced by the steep decline in soil concentration (S) during the first half of the vegetative period.

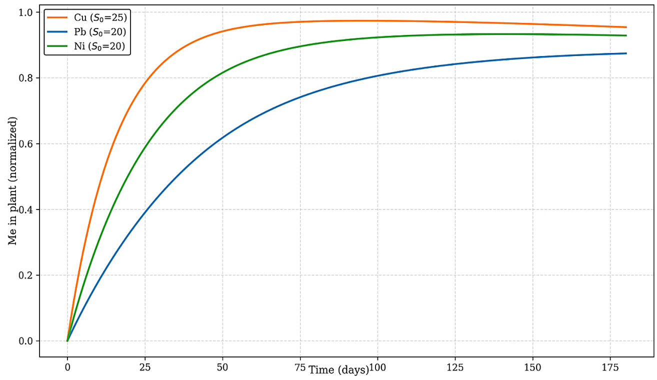

Figure 5. *Dynamics of Cu, Pb, and Ni accumulation in plant tissues (control)*
Source: developed by the authors

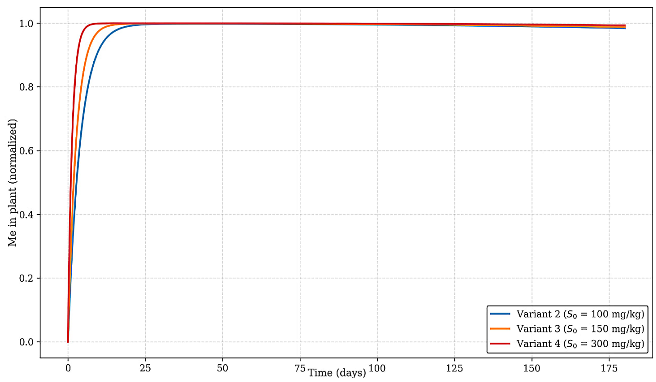

Figure 6. *Dynamics of Cu accumulation in plant tissues at different initial concentrations*
Source: developed by the authors

In contrast, lead (Fig. 7) was characterised by a detrimental combination of low mobility and high toxicity. The corresponding curves exhibited a prolonged, gentle slope without a distinct early peak, reflecting the slow and limited translocation of the metal into the tissues. The low absorption of lead (α = 0.0010) was compounded by its high toxicity constant (d = 0.07). This created a negative synergy: the metal was absorbed slowly, but the small amount that was absorbed causes disproportionately large damage to the metabolic machinery of *B. juncea*. This feedback loop – where the metal inhibits the very biomass needed to remove it – was a central finding of this modelling exercise. This confirmed the thesis that the majority of absorbed Pb was typically retained in the root system rather than translocated to the shoots, confirming the necessity of long-term monitoring for Pb-polluted sites.

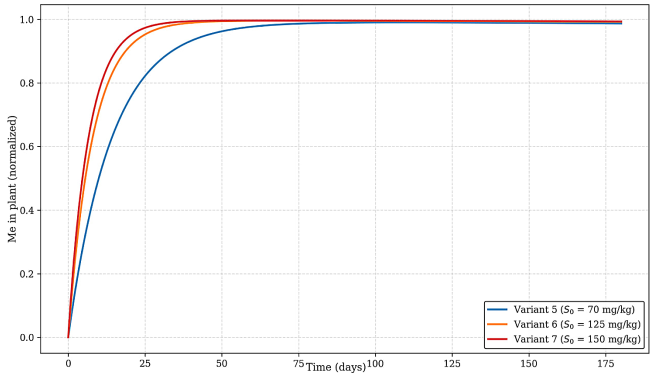

Figure 7. *Dynamics of Pb accumulation in plant tissues at different initial concentrations*
Source: developed by the authors

For nickel (Fig. 8), the model recorded intensive accumulation kinetics, positioned between the rapid uptake of copper and the slow absorption of lead. Visually, the accumulation curves lack the steep initial surge seen with copper but reach higher final concentration levels than lead, achieving dynamic equilibrium closer to the end of the 180-day cycle. The steady increased in normalised concentration confirmed its moderate mobility.

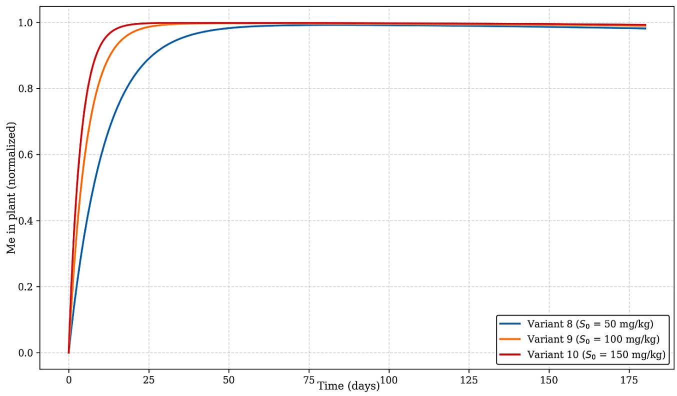

Figure 8. *Dynamics of Ni accumulation in plant tissues at different initial concentrations*
Source: developed by the authors

The model's ability to decouple growth dynamics from uptake kinetics allowed to identify that the primary limitation in remediation was not just the chemistry of the soil, but the physiological vulnerability of the plant's growth mechanisms to metal complexes. Ultimately, the overall efficiency of phytoextraction was determined not solely by the specific absorption coefficient but by the total formed biomass capable of storing these elements.

The additive effect in multi-metal systems

The temporal decrease in heavy metal complex concentrations within the soil matrix occurred significantly more intensively at higher initial baseline values of S_0. This dynamic was physically explained by the larger concentration gradient established between the soil solution and the root surface. A steeper concentration gradient thermodynamically driven more active plant uptake, forcing the physiological transport mechanisms to operate at maximum capacity. Figure 9 illustrated this process under control conditions. The graph showed that at background pollution levels, the reduction in soil metal concentrations was minimal and followed a nearly linear trajectory, as the low concentration gradient does not trigger maximum uptake rates.

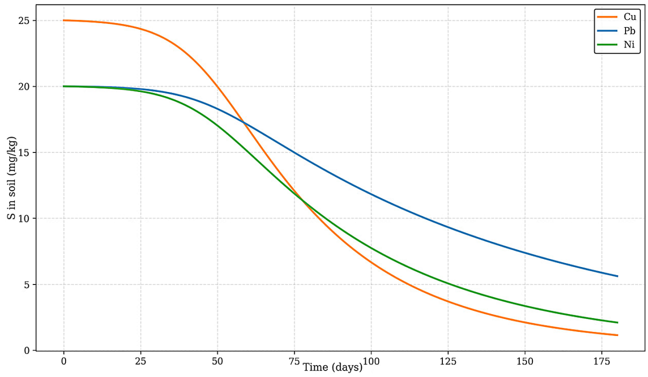

Figure 9. *Changes in Cu, Pb, and Ni concentrations in the soil (control)*
Source: developed by the authors

According to the model's numerical outputs, the most effective soil cleaning over a single vegetative period was recorded for copper, achieving an exceptional decontamination efficiency of 92.9% (Fig. 10). This metric was visually represented by the significant vertical gap between the initial starting point on the Y-axis (S_0 = 300 mg/kg) and the final residual concentration at day 180, which dropped to approximately 21.3 mg/kg. The steep downward slope of the curves in Figure 10 indicated that the most intensive cleaning occurred during the first 60-80 days of growth. This remarkably high metric was directly associated with copper's high bioavailability and the robust biomass growth it permits. The plant was able to generate a massive biological "sink" (maximum root and shoot biomass), which continuously pulled the metal from the soil without succumbing to severe growth inhibition.

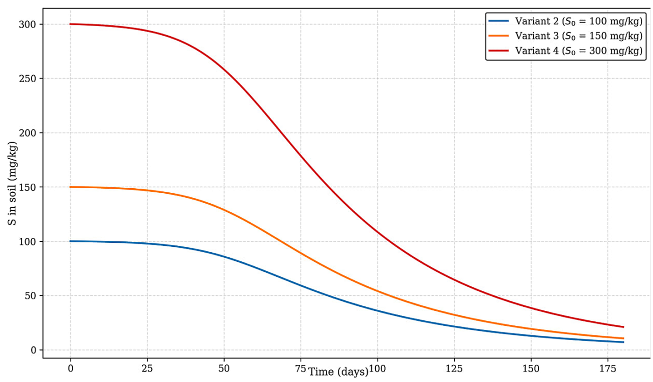

Figure 10. *Decrease in Cu concentration in the soil at different initial pollution levels*
Source: developed by the authors

In contrast, lead demonstrated the lowest removal rate, peaking at only 53.5% efficiency (Fig. 11). On the graph, this limited efficiency was evidenced by the much shallower slope of the curves compared to copper. Even after 180 days, the final concentration for the 150 mg/kg scenario remained high (above 69 mg/kg), which was clearly visible as the curve failed to approach the lower portion of the Y-axis. The severe limitation in Pb extraction was a direct consequence of the smaller "biological sponge" (reduced biomass) available to soak up the pollutant due to its high toxicity. These computational results were in agreement with the empirical conclusions drawn by A. Pruteanu *et al.* (2026), who pointed to the strict dependence of purification intensity on the initial dose of elements in the substrate.

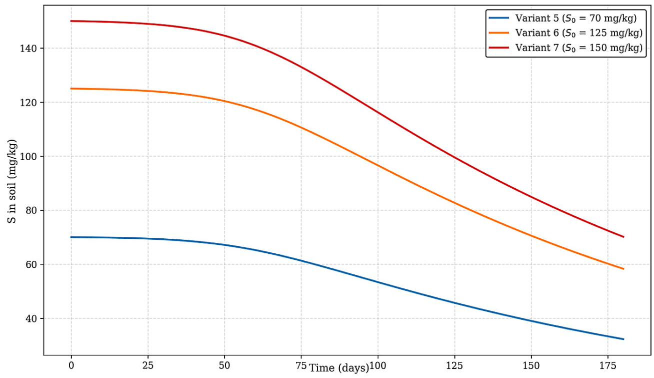

Figure 11. *Decrease in Pb concentration in the soil at different initial pollution levels*
Source: developed by the authors

For nickel, the extraction rate reached a highly effective 80.6% (Fig. 12). This efficiency was indicated on the figure by the final convergence of the concentration curves toward lower values, representing a substantial reduction from the initial levels. The trajectory showed a steady decline throughout the period, meaning the "cleaning" process for Ni was more prolonged and consistent than for Cu. This robust computational result was supported by the experimental findings of K. Selvaraj *et al.* (2021), who emphasised the significant potential of mustard plants for active Ni accumulation.

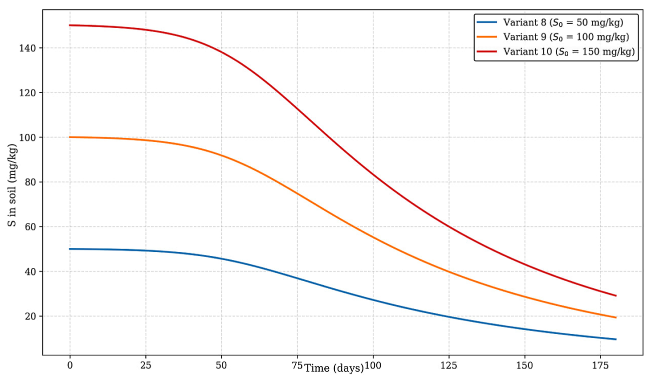

Figure 12. *Decrease in Ni concentration in the soil at different initial pollution levels*
Source: developed by the authors

So, the comparative analysis of soil decontamination dynamics confirmed that the cleaning efficiency was determined by the synergy between metal mobility and the resulting plant biomass.

While the model predicted high success for copper and nickel remediation, the persistent nature of lead concentrations highlighted the limitations of using *B. juncea* as a sole remediator for Pb-heavy sites. These findings emphasised the necessity of accounting for metal-specific toxicity, when planning long-term ecological restoration projects.

Multi-metal contamination and additive toxic stress dynamics. Practical implications and environmental risk assessment

A critical and highly innovative component of this mathematical research was the numerical simulation of simultaneous soil contamination by a "cocktail" of all three heavy metal complexes (Pb, Cu, and Ni). This scenario was not merely a theoretical exercise but a high-fidelity representation of the complex anthropogenic pressure characteristic of industrial zones and territories significantly affected by modern military actions in Ukraine. In such environments, soil was rarely contaminated by a single element; rather, it faced a multi-vector assault from various metal species originating from shell fragments, propellants, and destroyed infrastructure. In the case of a multi-metal mixture, the model established that the combined toxic effect led to a drastically more pronounced and non-linear inhibition of *Brassica juncea* biomass growth compared to any single-element system (Fig. 13). Specifically, while the control variant reached a stable biomass of 10.0 kg/m^2, the multi-metal scenario results in a dramatic stagnation of growth, with the final biomass barely reaching 2.2 kg/m^2 by the end of the 180-day vegetative period. This represented nearly 78% reduction in biological productivity. Mathematically, this was the result of the additive nature of the toxicity constants S. Sharma & B. Singh (2024) recently demonstrated through similar numerical simulations that multi-metal interactions led to a non-linear surge in oxidative stress, which validated the growth stagnation observed in model.

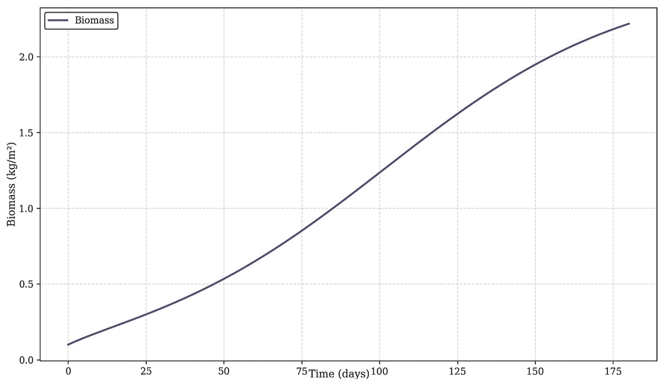

***Figure 13.** Dynamics of mustard biomass growth at elevated concentrations of three metals simultaneously (mixture)*

Source: developed by the authors

This severe suppression of biological productivity directly created a "biomass bottleneck", which significantly impaired the overall efficiency of the remediation process. As shown in Figure 14, while the normalised concentration of each metal within the surviving plant tissues remained relatively high, the total mass of pollutants extracted from the soil was much lower than in monometallic variants. The visual trajectory of the accumulation curves demonstrated a rapid initial spike followed by an early, compressed plateau. This rapid saturation, evident within the first 30 days, was not indicative of efficient extraction; rather, it visually confirmed that the stunted plant cannot safely distribute the toxic load across new growing tissues, leading to premature physiological gridlock.

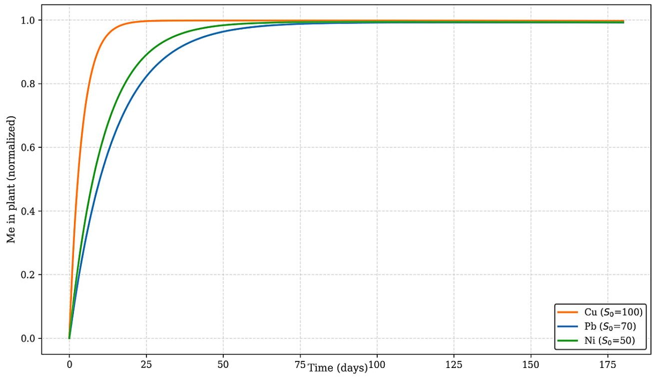

Figure 14. *Dynamics of Cu, Pb, and Ni accumulation in plant tissues at elevated concentrations of three metals simultaneously*

Source: developed by the authors

This occurred because there was simply not enough physical plant tissue (the "biological sponge") available to store the absorbed complexes. Consequently, it was observed a marked deceleration of the overall soil cleaning process (Fig. 15). The soil concentration curves for all three metals in the mixture showed a much flatter trajectory compared to their respective single-metal scenarios, indicating that the time required for complete decontamination would increase by several vegetative cycles. This highlighted the absolute necessity of accounting for the combined influence of metals, when forecasting phytoremediation efficiency for real-world environmental restoration projects.

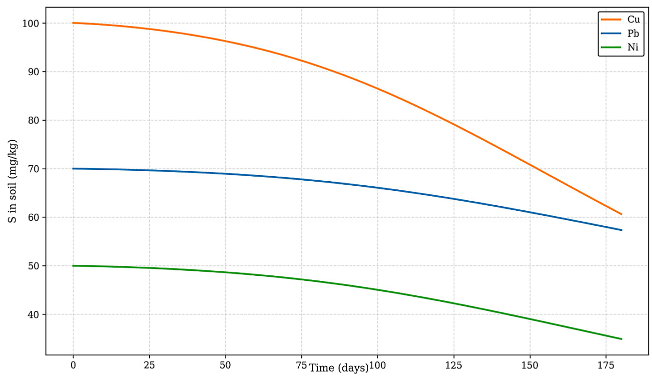

Figure 15. *Changes in Cu, Pb, and Ni concentrations in the soil at elevated concentrations of three metals simultaneously*

Source: developed by the authors

The observed decrease in process intensity during mixed contamination point to complex biological competition between different metal complexes for root absorption mechanisms (ion transporters) and subsequent antagonistic intracellular effects. This phenomenon was thoroughly described in the seminal work of A. Małecka *et al.* (2019). Researchers established that *B. juncea* (v. Malopolska) effectively activated antioxidant enzyme systems, such as SOD and APX, to combat oxidative stress during metal accumulation. The authors' results proved that, while the plant was a robust hyperaccumulator, extreme multi-metal loads can eventually overwhelm these defense mechanisms, redirecting energy from growth to survival. The consistency of our numerical outputs – showing the predictable 92.9% efficiency for Cu and 80.6% for Ni in isolation, but a systemic failure to reach these metrics in the mixture – robustly confirmed the adequacy and predictive power of the developed dynamic model. Findings of this research suggested that for military-polluted sites, remediation strategies must be adjusted to account for this synergistic inhibition, potentially requiring lower planting densities or the introduction of microbial bio-stimulants to support biomass resilience under extreme multi-vector stress. One of the most significant findings was the extreme sensitivity of the remediation timeline to the initial pollutant "cocktail". For lands affected by heavy artillery fire, where Cu and Pb concentrations often exceeded baseline levels by several orders of magnitude, a single vegetative cycle was clearly insufficient for full decontamination. Based on model of this study, the 53.5% efficiency for lead indicated that at least three consecutive 180-day cycles would be required to reach safe thresholds in highly polluted soils. Furthermore, the model highlighted a critical "toxic threshold" identified by the parameter e = 1.0 (half-saturation constant). When plant tissue concentrations exceeded this value, the growth inhibition became non-linear and accelerates rapidly. For practitioners, this meant that phytoremediation efforts must be carefully monitored: if initial biomass growth was severely stunted within the first 30-45 days, the system had likely entered a "toxic spiral", where extraction cannot keep pace with biomass degradation.

The obtained simulation results regarding selective toxicity and accumulation patterns were consistent with several foundational and contemporary studies. Specifically, the critical physiological disruptions and growth inhibition observed under lead stress align with the findings of A. Ado *et al.* (2015). Scientists recorded that high lead concentrations significantly decreased root and shoot length, as well as the total chlorophyll content in *B. juncea*. This corresponded to the research of G. DalCorso *et al.* (2019), who demonstrated that heavy metal stress triggers complex molecular signalling pathways that regulated metal transporters. Researchers' work highlighted that the genetic potential of the plant to sequester metals in vacuoles was the primary driver of tolerance. The efficiency of *Brassica juncea* as a versatile hyperaccumulator in model of this study supported the empirical observations of H. Ali *et al.* (2013). The authors established that phytoextraction was the most commercially viable technique for large-scale soil recovery due to its low cost and environmental compatibility. Scientists' study confirmed that the success of the process was fundamentally dependent on the plant's ability to produce high biomass in the presence of bioavailable metal ions. Furthermore, the synergistic toxic effects in multi-metal mixtures demonstrated in this research correlate with the recent numerical simulations by S. Sharma & B. Singh (2024). The authors proved that the interaction between different heavy metals led to a non-linear increase in phytotoxicity, which cannot be predicted by studying metals in isolation. Scientists' findings emphasised that Pb specifically acted as a strong inhibitor of the translocation of other essential and non-essential elements. This was further supported by the comprehensive remediation frameworks proposed by A. Yan *et al.* (2020), who demonstrated that revegetation with hyperaccumulators not only removed toxins but also restored soil microbial health. L. Liu *et al.* (2018) established that the choice of remediation technique must be strictly aligned with the chemical speciation of metals and the target clean up level. Researchers concluded that phytoextraction remained the most effective strategy for managing low-to-medium pollution in industrial substrates.

Strategy of induced extraction discussed in this research was supported by B. Kos &

D. Leštan (2003). The authors demonstrated that using biodegradable chelating agents can increase lead solubility by several orders of magnitude, thereby significantly enhancing the uptake rate. Researchers' results also showed that the integration of permeable barriers was a necessary safety measure to prevent the leaching of mobilised lead into the groundwater. The necessity of assessing environmental risks in complex zones was further reinforced by O.O. Okedeyi *et al.* (2014). Scientists established that the enrichment of heavy metals in surface soils and local vegetation was directly proportional to the intensity of nearby industrial activities. Study of South Africa confirmed that metals like Cu and Pb showed a high bioaccumulation factor, posing a risk of entering the food chain. The application of non-linear differential equations to track these environmental dynamics followed the predictive concepts established by A. Rein *et al.* (2011). Researchers introduced dynamic plant uptake models that accounted for changes in plant growth and transpiration over time, proving that such models were more accurate than static risk assessments. It also confirmed that accounting for the time-dependency of both soil and plant tissue concentrations was vital for realistic remediation forecasting. Finally, the mathematical rigor of system evaluation conducted in this research was consistent with the methodological approaches of Y. Ouyang (2005). The author proved that principal component analysis and similar multivariate mathematical tools were essential for evaluating the performance of monitoring systems in complex ecological environments. Scientist's findings demonstrated that these models allowed for the identification of the most significant environmental variables that drive the dynamics of pollutant transfer. So, the integration of these diverse scientific findings confirmed that the efficiency of phytoremediation was a product of complex interactions between metal chemistry, plant physiology, and mathematical growth laws. The developed model provided a robust analytical tool for predicting these interactions and optimising soil restoration in anthropogenically stressed regions.

Conclusions

Based on the results of the mathematical modelling of phytoremediation processes for soils contaminated with heavy metals (Pb, Cu, Ni) using Indian mustard (*Brassica juncea*), it was determined that adapted system of nonlinear differential equations adequately described the dynamics of the "metal-plant" system over a 180-day vegetative period. The model incorporated the relationship between biomass accumulation and the inhibitory impact of metal-specific toxicity, enabling the prediction of soil cleaning efficiency without the need for prolonged field experiments A significant differentiation in phytoremediation efficiency was established depending on the pollutant type. The system demonstrated the highest self-cleaning capacity for copper (92.9% efficiency), driven by a combination of a high specific absorption coefficient ($\alpha = 0.0025$ day^{-1}) and low phytotoxicity ($d = 0.03$). For nickel, this metric was 80.6%, whereas lead proved to be the least accessible for extraction (53.5%) due to its critical suppression of biomass growth ($d = 0.07$). Furthermore, the numerical simulation of multi-metal contamination confirmed the presence of an additive toxic effect. The simultaneous presence of lead, copper, and nickel at concentrations typical for war-affected territories led to a cumulative inhibition of *B. juncea* biomass growth (down to 2.2 kg/m^2), which represented a 78% reduction in biological productivity compared to monometallic scenarios. The selection of soil restoration strategies was scientifically substantiated: Indian mustard was a highly effective tool for the complete phytoextraction of Cu and Ni. In the case of lead contamination, phytoremediation should be considered a phytostabilisation method aimed at metal immobilisation. The perspectives for further research include expanding the dynamic model to account for the impact of soil amendments, such as EDTA, and microbial biostimulants to support biomass resilience and optimise recovery timelines for agricultural lands in Ukraine affected by military conflict.

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Conflict of Interest

None.

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Математичне моделювання ефективності фіторемедіації грунтів від Pb, Cu та Ni

Олександра Сидоренко
Магістрант
Національний технічний університет України «Київський політехнічний інститут імені Ігоря Сікорського»
03056, Берестейський просп., 37, м. Київ, Україна
https://orcid.org/0009-0004-5890-7630
Наталія Голуб
Доктор технічних наук, професор
Національний технічний університет України «Київський політехнічний інститут імені Ігоря Сікорського»
03056, Берестейський просп., 37, м. Київ, Україна
https://orcid.org/0000-0003-1448-1872

Анотація. Метою дослідження була кількісна порівняльна оцінка динаміки вилучення свинцю, міді та нікелю з ґрунту системою «метал-рослина» на основі математичного моделювання для прогнозування термінів очищення забруднених територій. Забруднення ґрунтового покриву важкими металами (Pb, Cu, Ni) внаслідок інтенсивної техногенної діяльності та масштабних воєнних дій в Україні становило критичну загрозу екологічній безпеці та здоров'ю населення. Фіторемедіація із використанням рослин-гіперакуляторів, таких як *Brassica juncea*, розглядалася як перспективний та екологічно безпечний метод відновлення екосистем. Проте планування таких заходів ускладнювалося різною швидкістю вилучення елементів та їхнім токсичним впливом на біомасу, що потребувало розробки точних прогностичних моделей. У роботі було використано експоненціальну модель кінетики поглинання металів для прогнозування термінів очищення забруднених територій. Було встановлено, що ефективність очищення ґрунту за один вегетаційний період (180 днів) становила 92,9 % для міді, 80,6 % для нікелю та лише 53,5 % для свинцю. Також, у дослідженні було виявлено, що висока ефективність ремедіації міді зумовлена її високою мобільністю та низькою фітотоксичністю. Натомість свинець виявив найсильніший інгібуючий ефект, що суттєво обмежував швидкість його екстракції. На базі мультиметальної моделі було продемонстровано адитивний токсичний ефект суміші забруднювачів, що призводило до зниження загальної продуктивності фіторемедіантів на 78 % порівняно з монометалевим забрудненням. Отримані результати дозволили прогнозувати залишкову концентрацію токсикантів, оптимізувати стратегії відновлення техногенно навантажених територій та земель, що постраждали від воєнних конфліктів. Розроблена модель може бути використана для оцінки економічної доцільності фіторемедіаційних заходів

Ключові слова: важкі метали; фітоекстракція; токсичний стрес; мультиметальна модель; відновлення ґрунтів; екологічна безпека