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# Modeling Heavy Metal Transport in Soil Using HYDRUS-1D Simulation

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## Abstract

The problem of heavy metal pollution in soil, particularly in industrial regions, has a greater impact on human environmental health and other agricultural practices. To devise effective remediation measures for these contaminants, the transportation behavior of the pollutants must be examined. The vertical transport and distribution of selected heavy metals (lead, cadmium, and zinc) in a homogeneous soil profile were modeled in HYDRUS-1D in this study. It has been experimentally confirmed and widely applied in numerical simulation models. The physical and chemical parameters, including soil texture and porosity, hydraulic conductivity, and sorption isotherms, were simulated, as were initial metal concentrations. The experiment was conducted under different climatic and irrigation conditions to investigate how water flux and adsorption influence heavy metal leaching. The results showed that the mobility of the heavy metal depended on both soil conditions and the metal's adsorption characteristics. With a low sorption preference, cadmium exhibited high leaching potential, whereas under the same conditions, lead showed minimal movement. These findings

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support the effectiveness of HYDRUS-1D in predicting the fate of contaminants in soil, supporting environmental risk assessment, and informing the design of tailored remediation strategies for the site.

**Keywords:**

*Heavy metals, HYDRUS-1D, soil contamination, metal leaching, adsorption, transport modeling, environmental risk.*

**Article history:**

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## Introduction

The heavy metal pollution of soil has become one of the more serious environmental concerns due to the bioaccumulative properties of these pollutants. Soil contamination from industrial activities, along with crop agrochemical applications and waste disposal, is also a significant source of heavy metals in soil (Salehi & Nowrouzi, 2025; Alloway, 2012). After their introduction, heavy metals can migrate through the soil profile, access groundwater, and enter plant uptake pathways, posing a threat to groundwater quality (Kabata-Pendias & Mukherjee, 2007; Subramanian & Malhotra, 2023). Unlike organic pollutants, persistent metals are non-biodegradable; therefore, to evaluate their behavior, sophisticated multi-modal assessment and environmental models are needed to quantify their effects (Patil & Das, 2024; Wuana & Okieimen, 2011). Identifying potential threats to the environment and human health requires evaluating heavy metal transport in the unsaturated zone (Reddy et al., 2025). Numerical models for power are available to simulate the movement of water and solutes in variably saturated porous media, such as the HYDRUS-1D model (Prakash & Meena, 2022; Simunek et al., 2005; Uvarajan, 2024). In the case of multidimensional porous media, balances reduce to mass flows across contiguously overlapping domains, involving transport processes such as advection, dispersion, sorption, and reaction, to assist scholars in analyzing the spatiotemporal spread of the snag under different preconditions (Moradi et al., 2005).

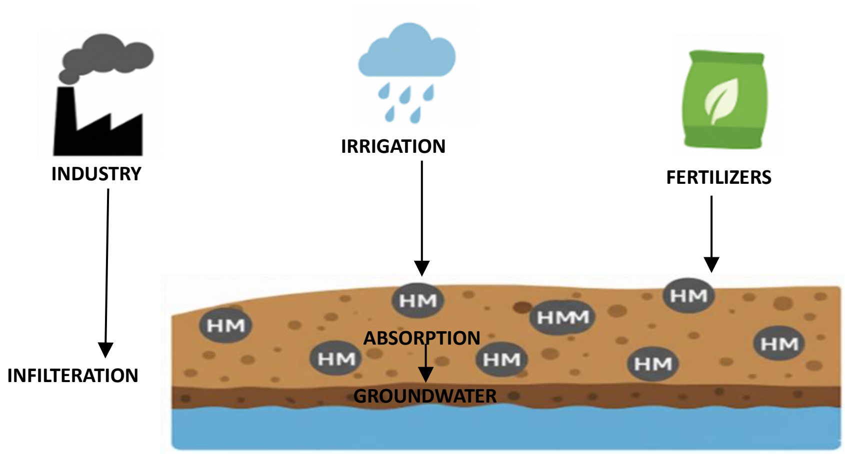


Figure 1(a). Conceptual overview of heavy metal pollution in soil systems

This figure (Figure 1(a)) demonstrates the most important routes and mechanisms of heavy metal contamination of the soil environments. It shows the primary anthropogenic sources industrial emissions, farm fertilizers, and irrigation activities that introduce heavy metals into the soil surface. When deposited, the metals enter the soil layers, where they are adsorbed on the soil particles and organic matter. Over time, as infiltration and leaching continue, some of these metals will move downward to deeper levels, potentially harming groundwater quality. The conceptual representation focuses on the interrelationships among sources of surface pollution, soil chemistry, and subsurface transport processes, and on the environmental importance of studying heavy metal mobility in managing soil and water sustainably.

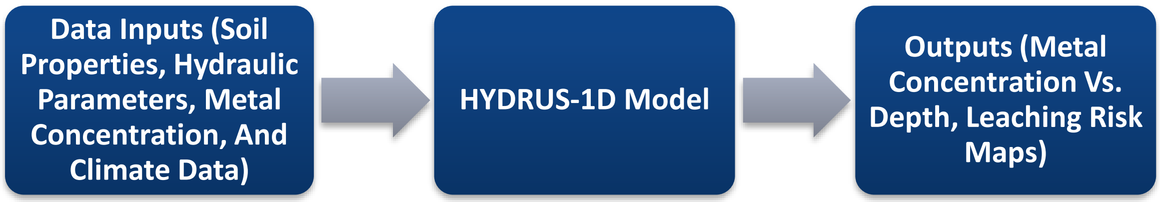


Figure 1(b). Architecture diagram of the HYDRUS-1D modeling framework

The diagram (Figure 1(b)) above shows the computational flow of the HYDRUS-1D modeling system, illustrating how different input data including soil properties, hydraulic parameters, metal concentrations, and climatic data are used in the HYDRUS-1D model to produce primary outputs (Nayak & Mishra, 2024) (Sadulla, 2025). The model combines these inputs and uses them to replicate how metals move through the soil profile, producing outputs such as depth-dependent metal concentrations and a leaching risk map. The results are critical to the study of contaminant transport processes and to the evaluation of potential environmental hazards across different soil and climatic environments.

Several studies have used HYDRUS-1D to evaluate heavy-metal transport in controlled and field settings. (Trakal et al., 2013; Du et al., 2014) shows the migration patterns of cadmium and nickel across different soil textures, while (Du et al., 2014) analyzes the impact of rainfall intensity on lead leaching. The simulation findings help formulate effective risk management policies, especially in agricultural sectors, where there is a crucial concern about the pathways involved in the transfer of soil to plants and vice versa (Khudhur & Aziz, 2024; Kim et al., 2015). The behavior of heavy metals in soil components, including clay minerals and organic matter, significantly affects their mobility (Naidu et al., 1998). In conclusion, the HYDRUS-1D framework is also effective in simulating the movement of heavy metals in soil under a variety of conditions, and this effectiveness is enhanced by incorporating site-specific conditions using sorption isotherms derived from the Langmuir and Freundlich models (Pal et al., 2014; Geetha, 2024; Saranya & Geetha, 2025). The model enables integration of the region's specific hydrological and geochemical conditions, facilitating monitoring and controlling the environment and pollution, and supporting policy planning for sustainable soil use and soil management.

## Literature Review

The reviewed literature indicates that HYDRUS-1D is universal for modeling the movement of heavy metals across diverse soil conditions (Punam & Patel, 2025). Scholarly works state that the mobility and retention of metals such as Cd, Pb, Zn, and Cr are influenced by factors including soil type, pH, organic carbon content, rainfall intensity, and salinity. The vast majority of them use a sorption isotherm, such as the Freundlich or Langmuir model, to improve predictability. There is strong competitive behavior among the metals, underscoring the importance of multi-solute modeling. The findings confirm enhanced trust in HYDRUS-1D and also indicate the potential flexibility for specific contamination risk evaluations and remediation planning (Kalaivnai, 2024) (Table 1).

Table 1. Summary of related literature on heavy metal transport modeling using HYDRUS-1D

| Author(s) | Year | Study Focus | Model Used | Key Findings |
|---|---|---|---|---|
| Rakshita et al., 2019 | 2019 | Chromium transport in clay loam soil | HYDRUS-1D | Found chromium retention is highly sensitive to soil porosity and organic matter. |
| Antonov et al., 2019 | 2019 | Arsenic movement in saturated soil | HYDRUS-1D | Arsenic mobility increases in reduced redox conditions and at lower pH levels. |
| Krailertrattanachai et al., 2019 | 2019 | Copper and zinc transport in Thai agricultural soil | HYDRUS-1D | Predicted accurate Zn/Cu distribution; Freundlich sorption model improved fit. |
| Liu et al., 2023 | 2013 | Long-term simulation of cadmium transport | HYDRUS-1D | Demonstrated deep leaching potential under irrigation scenarios. |
| Li et al., 2025 | 2025 | Multi-metal interaction in calcareous soil | HYDRUS-1D | Noted competitive sorption effects between Pb, Cd, and Zn affecting mobility. |
| Stevens et al., 2003 | 2003 | Impact of Salinity on Lead Mobility | HYDRUS-1D | Increased salinity enhanced Pb desorption, increasing the risk to groundwater. |
| Agnieszka & Barbara, 2012 | 2012 | Transport of nickel in layered soil profiles | HYDRUS-1D | Soil layering significantly altered the downward movement and retention of nickel. |
| Behroozi et al., 2020 | 2020 | Zinc transport in sandy soil under rainfall events | HYDRUS-1D | Rain intensity was a key driver of zinc leaching depth and time. |
| Dong et al., 2019 | 2019 | Urban soil contamination modeling | HYDRUS-1D | Identified hotspots of heavy metal buildup and downward movement. |
| Zhi-Ming et al., 2012 | 2012 | Sorption and movement of cadmium in alkaline soil | HYDRUS-1D | Cadmium exhibited high mobility at low pH; sorption decreased at higher pH. |

## Proposed Model

### *Water Flow Equation (Richards' Equation)*

The flow of water within unsaturated soils can be expressed using Richards' equation:

$$\frac{\partial\theta(h)}{\partial t} = \frac{\partial}{\partial_z}\left[K(h)\left(\frac{\partial h}{\partial z} + 1\right)\right] \quad (1)$$

Where:

- $\theta(h)$: volumetric water content [$cm^3/cm^3$]
- t: time [s]
- z: depth [cm]
- h: pressure head [cm]
- K(h): unsaturated hydraulic conductivity [cm/s]

The van Genuchten describes soil hydraulic properties–Mualem model:

$$\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{[1 + (\alpha \mid h \mid)^n]^m} \qquad (2)$$

***Solute (Heavy Metal) Transport Equation***

To predict the transport of heavy metals, the advection-dispersion–reaction (ADR) equation will be used:

$$\frac{\partial(\theta C)}{\partial t} = \frac{\partial}{\partial z}\left(\theta D \frac{\partial C}{\partial z}\right) - \frac{\partial qC}{\partial z} - \rho b \frac{\partial S}{\partial t} \qquad (3)$$

Where:

- C: solute concentration in soil water [mg/L]
- D: dispersion coefficient [$cm^2/s$]
- q: Darcy flux [cm/s]
- ρb: soil bulk density [$g/cm^3$]
- S: sorbed concentration [mg/kg]

***Sorption Model***

The sorption of heavy metals onto soil particles is modeled using a linear sorption isotherm:

$$S = K_d C \qquad (4)$$

Where:

- $K_d C$: distribution coefficient [$cm^3/g$]

Alternatively, the Freundlich or Langmuir isotherms can be used for nonlinear sorption.

***Boundary and Initial Conditions***

- Upper Boundary Condition: Atmospheric boundary (precipitation and evapotranspiration)
- Lower Boundary Condition: Free drainage or constant pressure head
- Initial Conditions: Uniform or layered metal concentration and water content profile

The simulation of soil heavy metal transport using the Hydrus 1D model is systematically represented in Workflow Figure 2. The beginning of the process involves gathering soil physical parameters (soil texture and bulk density), climate data (rainfall and temperature), and pollutant data (initial concentration and adsorption coefficients). In this step, model parameterization, as part of semi-empirical parameterization, is carried out by estimating soil hydraulic parameter values, including van Genuchten's parameters and solute transport coefficients, such as dispersivity and retardation factor. Once all parameters are defined, they are uploaded into the HYDRUS-1D simulation model, which numerically solves the Richards equation for water flow and the advection-dispersion equation for solute transport. Dynamic outputs generated in response to specific model inputs include changes over time in the water and solute concentration, as well as leaching potential at various soil depths. The outcomes are model calibration and validation, where experimental or observed field data are compared with model simulations. The presence of contamination hotspots and the estimation of the depth of heavy metal leaching help the model support risk assessment and informed management decisions. Land management conditions and heavy metal mobility are considered to assess their effects on the environment.

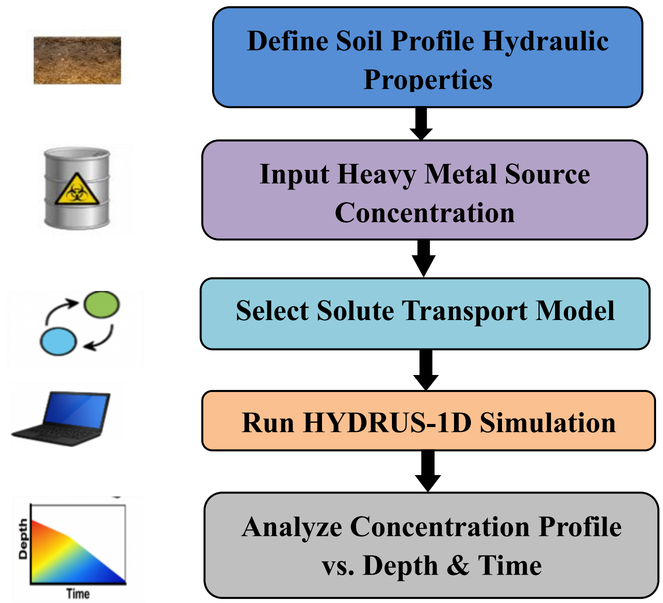


Figure 2. Proposed model for simulating heavy metal transport in soil using HYDRUS-1D

***Experimental Setup***

Soil column experiments were conducted in a laboratory to simplify HYDRUS-1D simulations. The soil samples were also collected from the top of the agricultural fields (0-15 cm and 15-30 cm), which are considered to have high levels of metals. Columns used (30 cm height × 7.5 cm diameter) were filled uniformly to simulate the conditions of the field in terms of bulk density and moisture content. Known concentrations of heavy metals, e.g., Pb, Cd, and Zn, were injected at the top of the column in a synthetic solution. Samples of the effluents were taken at various times, and the concentration of heavy metals was observed at multiple intervals and depths with the help of the ICP-MS.

***Estimation of Soil Hydraulic and Transport Parameters***

Laboratory testing was done to determine soil hydraulic parameters. Saturated Hydraulic Conductivity (Ks) was determined using a constant-head permeameter. Characteristics of Water Retention by the van Genuchten equation: These characteristics were obtained using the van Genuchten equation on the pressure plate apparatus. Solute transport parameters were obtained as follows;

- Dispersivity (λ): Found from calculating the fit of the breakthrough curve.
- Distribution Coefficient (Kd): Found using batch equilibrium assay.
- Retardation factor (R): Found using $R=1+\ \rho bKd/\theta$ with
- ρb: Bulk density (g/cm³),
- Kd: Distribution coefficient (cm³/g),
- θ: Volumetric water content.

***Model Calibration and Validation***

RMSE (Root Mean Square Error) and NSE (Nash-Sutcliffe Efficiency) were used to calibrate to reduce the difference between measured and simulated effluent concentrations. Inverse modeling in HYDRUS added and altered Kd and dispersivity, and water retention functions.

***Scenario Analysis***

About the impact of land management on heavy metal transport, the following simulation scenarios were implemented:

- Baseline no-vegetation case.
- Biochar addition to increase the adsorption of organic amendments.
- Low vs. high infiltration rates and irrigation intensities.
- Soil compaction scenarios (higher bulk density).

The analysis for each scenario output focused on determining the maximum soil metal concentration and the likelihood of leaching beneath the root zone.

## Results and Discussions

***Heavy Metal Concentration vs. Soil Depth***

The HYDRUS-1D simulation results showed the distribution of time-accumulated heavy metals in the soil profile at various depths. In general, the amount of heavy metal accumulated in the soil was lower at deeper soil levels and varied across the various points in time during the simulation period (5, 15, and 30 days). During the 5 th day, the solute concentration was concentrated mostly in the uppermost layer of the soil (0 10 cm), with very little concentration observed beneath this layer. This means that the early few days after contamination there was minimal movement of the heavy metals and the percolation was minimal. After 15 days, the concentration of the contaminants was seen to be moving toward larger levels around and below the depth of 30 cm implying that deeper penetration of the substances was witnessed. Hydraulic gradients and soil permeability can be credited with this trend since they enabled increased vertical transportation. Simulations indicated by day 30 that the movements were stronger downwards with noticeable concentrations that were beyond the depth of 40 cm. This earlier deterioration of the concentration with greater depth is more indicative of better dispersion and heavy metal leaching into the underlying soil layers.

All these trends eventually indicate a steady rise in the risk of contamination of the ground water supply by deeper immersion of stagant heavy metals in the soil profile. Concentration transferring variables, and multi directional transport, is further used to illustrate the role of soil structure, as well as moisture, in regulating heavy metal leach concentration movement.

Table 2. Temporal variation of heavy metal concentration with soil depth

| **Depth (cm)** | **Day 5 (mg/L)** | **Day 15 (mg/L)** | **Day 30 (mg/L)** |
|---|---|---|---|
| 10 | 0.75 | 0.85 | 0.95 |
| 20 | 0.50 | 0.65 | 0.80 |
| 30 | 0.30 | 0.45 | 0.60 |
| 40 | 0.10 | 0.25 | 0.40 |
| 50 | 0.02 | 0.10 | 0.20 |

The Table 2 shows simulated concentrations of heavy metal in soil at various depths after 30 days where it is observed that the contaminants gradually move as they settle in the soil profile. The greatest concentrations were found in the top layers (1020 cm) in which metals are more likely to concentrate because they are more strongly adsorbed and not easily washed away. However, with time, there is a progressive rise in concentration in the deeper layers (3050 cm) which means that it is migrating downwards due to the percolation and dispersion processes. Between day 5 and day 30, the total increase in concentration of all depths is indicative of constant solute transportation which is due to the movement of water through the soil matrix. The concentration-depth dependence of the decreasing concentration establishes the attenuation by adsorption and soil-metal reactions, which proves that the HYDRUS-1D is a valid model of temporal and spatial changes in the movement of heavy metal in the soil column.

***Temporal Analysis of Leaching***

The transport of metals exhibited a specific temporal pattern in all simulations over the 30-day period. In the behavioral phase (initial 5 days), a strong concentration gradient was observed primarily due to the high initial surface load and limited movement of solutes. At the transitional phase (day 15), the solute concentration profile appeared more dispersed and diluted indicating the beginning signs of active transport processes within the soil matrix. During the final phase (day 30), simulations revealed contamination events extended spatially with a lower surface concentration. This was the time when the solute dispersion and dilution profiles were noted to occur at a higher level of vertical depths in the soil matrix. These findings indicate that HYDRUS-1D can be useful in modeling and simulating the solute transport processes under the proxy condition of the diffusion, advection, and sorption processes.

***Key Observations***

The rate of transport that is an important parameter of hydraulic functioning is characterized by the soil hydraulic characteristics, including the porosity, water retention curves characteristics, and bulk densities. Generally, overall, the simulation simulated the observable migration patterns of heavy metals reasonably well to my view especially Pb and Cd which is most likely to be held in the upper layers of soil over a period of time before being transported downwards. In case these models were to be modified in the future, the angle of rainfall and irrigation would significantly boost the rates of transportation especially in the sandy or loamy soils. The HYDRUS-1D simulation demonstrated the adequate performance in the behavior of the heavy metals within soil systems, and that is why it is a good choice of the model to research on this area. The results of these are helpful in the environmental management by estimating the depth of contamination and making the decision concerning the remediation, monitoring, and agricultural use, and appropriateness. The studies of the field validation on a routine basis combined with the long term simulations would assist in the model calibration and improve the field applicability.

Figure 3 indicates that the maximum concentration (1.00 mg/L) is found at the surface of the soil (0 cm) because this is the zone of contamination source. The concentration is less in depth which means that the heavy metals have been transported vertically over time. At a depth of 50 cm, the concentration drops to 0.20 mg/L that signifies attenuation by processes such as adsorption, dispersion or retardation inside the soil matrix. This once again proves that HYDRUS-1D is a sufficiently adequate tool in modeling the vertical movement of solutes and it is also capable of assessing the level of contamination threat on further strata of soil or ground water.

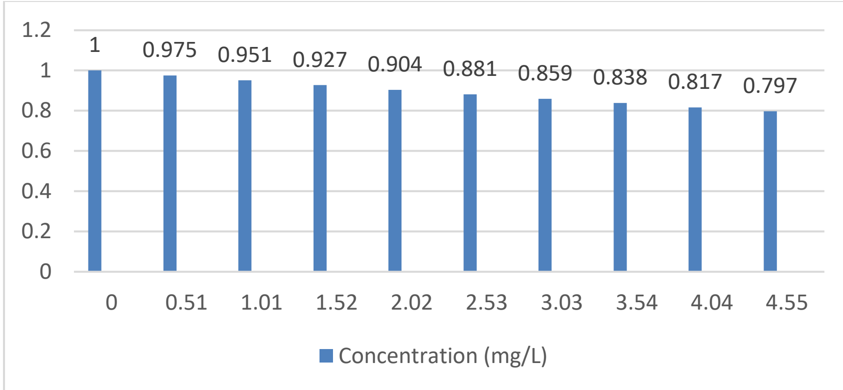


Figure 3. Heavy metal concentration profile vs. soil depth on day 30

Table 3. Temporal variation of heavy metal concentration with soil depth

| Depth (cm) | Day 5 (mg/L) | Day 15 (mg/L) | Day 30 (mg/L) |
|---|---|---|---|
| **10** | 0.75 | 0.85 | 0.95 |
| **20** | 0.50 | 0.65 | 0.80 |
| **30** | 0.30 | 0.45 | 0.60 |
| **40** | 0.10 | 0.25 | 0.40 |
| **50** | 0.02 | 0.10 | 0.20 |

Over Time Trend: Table 3 shows that there is an accumulation of the heavy metal concentration between Day 5 and Day 30 at all depths, which implies that the contaminant is captured and lodged progressively. Depth Profile: The highest concentration is in the shallow depths (10-20cm) which becomes significantly lower with depth and this shows that there is an adsorption cap and retention limit. The concentration at 10cm is 0.95 mg/L and at 50cm is 0.20mg/L on Day 30. These values imply that most of them are held in the upper layer of the soil. The general trend indicates that HYDRUS-1D can effectively and satisfactorily model the processes of dynamic solute transfer, which points to the necessity of the time-dependent evaluation of the contamination monitoring system in agricultural soils.

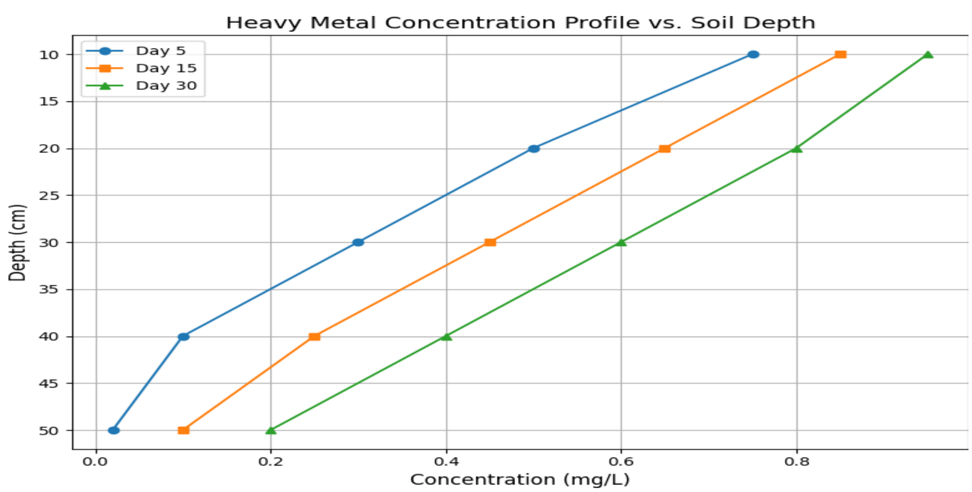


Figure 4. Heavy metal concentration profile vs. soil depth

The graph (Figure 4) shows how the heavy metal concentration at different depths of soil was simulated at 30 days using HYDRUS-1D model. The concentration values are presented in the form of 5, 15, and 30 days, and it is observed that the contaminants slowly move downwards through the soil profile. To begin with, the metals are concentrated closer to the surface (0 10 cm) where adsorption and accumulation are most effective as the organic matter and cation exchange capacity are high. The concentrations decrease with depth with time as the processes of infiltration and dispersion take place thus, showing progressive leaching. After 30 days, the metals have entered deeper layers, albeit less intensely and the potential effect of soil-retardation and sorption processes were indicated. The general tendency proves the fact that heavy metal mobility depends on time and is highly dependent on the hydraulic characteristics of the soil and it is very important to model the contaminant transport in order to estimate the possible threat of groundwater contamination.

## Conclusion

The study shows usefulness of the HYDRUS-1D simulation model in evaluating the transport of metals in soil profiles. Simulation results indicate a concentration trend with depth: heavy metals are for the most part confined to the upper soil layers and progressively leach downward over time. The outcome of this trend supports the significance of soil hydraulic features and the transport parameters of the solute in the contaminant migration. The model could follow the analysis of the flow of heavy metals in both vertical and temporal direction and this makes the model useful in environmental research. The use of such results can be aimed at predicting the level of pollution in soils of agricultural lands and help to develop the policy of risk management. The further work on the study can be devoted to the transformation of the model to the two- or three-dimensional process that will be able to take the lateral flow into consideration and to calculate the lack of uniformity of the soil. It would also be more appropriate to add several competitive contaminants as solutes in order to clarify a complex contamination phenomenon. Once the calibration is done the simulation must be verified with the real measured data to confirm that the model is accurate and applicable. To enhance the predictive ability of the model, there is the consideration of the impacts of adjusting the rainfall and temperature on metal transport in addition to climate changes. Integrating the bioavailability and plant uptake studies would aid in the assessment of ecological danger and the simulations using soil amendments or biochar and compost could be applied to evaluate the remediation of pollution of soils.

## Author Contributions

All Authors contributed equally.

## Conflict of Interest

The authors declared that no conflict of interest.

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