

Modelling the Transport of Heavy Metal Contaminant in Soil Media

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ABSTRACT

Contaminants on soil surface spread downward into the soil overtime, leading to pollution of the soil and groundwater. Hence, this study applied mathematical model to predict the transport of heavy metals in soil subsurface. The heavy metals considered include iron (Fe), lead (Pb), chromium (Cr) and cadmium (Cd). The results revealed that the rate of heavy metal transfer from the pollution source into soil depth decreased exponentially with time. Nevertheless, within 96 hours (4 days), the concentration of the heavy metals from the soil surface had reached up to 2 m depth. The predicted concentration after 4 days at 2 m depth are 0.1098 mg/l for Fe, 0.1054 mg/l for Pb, 0.0269 for Cr and 0.0085 mg/l. Generally, predicted heavy metals fit well with the measured values. Ultimately, the application of model can help the implementation of effective management strategies and control of heavy metal contamination.

KEYWORDS: Modelling, Prediction, Heavy Metals, Transport, Soil

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I. INTRODUCTION

Soil contamination by heavy metals is a serious environmental concern due to their implications on groundwater quality and ecosystem health. High level of heavy metals in soil, which often originate from anthropogenic sources, such as industrial activities, agricultural wastes, and urban runoff, poses serious risks to both human health and environmental integrity, particularly when groundwater is utilized as drinking water source. Most heavy metals have serious health issues, such as neurological disorders and renal damage (Alloway, 2013; Siyar et al., 2022).

There are various mechanisms of heavy metal transfer in soils, which are influenced by several factors. Heavy metal transport in soil occurs through molecular diffusion and convective transport. Molecular diffusion is driven by concentration gradients, where heavy metals migrate from regions of higher concentration to areas of lower concentration. This process is influenced by soil properties such as porosity and particle size (Gong et al., 2023). Convective transport, on the other hand, occurs when water movement through the soil matrix carries heavy metals with it, particularly in saturated conditions (Gao et al., 2020). This dual mechanism highlights the complexity of contaminant transport in soil.

Moreover, the diffusion coefficient of heavy metal and seepage velocity determine are important variables in modelling of heavy metals transfer rate in soil media. Therefore, this study utilised the diffusion coefficient and seepage velocity determined from an experimental investigation of iron transport in soil media to predict the concentration of iron at a given depth in the soil for a specified time.

II. MATERIALS AND METHODS

Experiment was conducted to determine the diffusion coefficient and seepage velocity of heavy metal in soil. The average estimated diffusion coefficient and seepage velocity were used to model the transport of the heavy metal in soil media.

2.1 Materials

The materials used include soil sample, PVC pipe, measuring cylinder, graduated beaker, distilled water, funnels, test tubes, sieve, weighing balance, filter papers, conical flasks, spatula, pH meter, stop watch, Atomic

Absorption Spectrophotometer (AAS) and iron(II) compound ($\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$), lead(II) nitrate ($\text{Pb}(\text{NO}_3)_2$), potassium dichromate ($\text{K}_2\text{Cr}_2\text{O}_7$) and cadmium chloride (CdCl_2).

2.2 Procedures for Measurement of Heavy Metal Concentration

Soil sample was collected in layers of 0.25 m thickness from the surface to 2.00 m soil depth. Initial concentration of iron (Fe) was prepared and added to the soil. Thus, 1 litre of distilled water was mixed with $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$. The mixture was poured into PVC column loaded with the soil sample. 2 m high and 4 inches (0.10 m) diameter cylindrical column was divided into 8 equal parts with 0.25 m (25 cm) apart. The cross-sectional area of the column was determined as 0.007857m^2 . A hole was carefully bored at these division marks and sealed firmly with tape to prevent leakage. Soil sample was collected through these holes. The collected soil sample was packed and compacted into the cylindrical column to simulate the natural soil texture. The prepared $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$, $\text{Pb}(\text{NO}_3)_2$, $\text{K}_2\text{Cr}_2\text{O}_7$ and CdCl_2 solutions, with known concentrations, were introduced into the column. Every day (24 hours), the seals at the various holes were carefully removed to collect soil sample from the column. The sampling was done for a total of 4 days (96 hours). The collected soil samples were analysed in the laboratory to measure the heavy metals concentration at each depth using Atomic Absorption Spectrophotometer (AAS).



Plate 1: Set-up of columns diffusion coefficient measurement



Plate 2: Preparation of samples for AAS analysis



Plate 3: Transferring samples to instrument for heavy metals analysis

2.3 Model for Prediction of Heavy Metals Transport

The heavy metal transport into soil media was modelled using the advection-diffusion equation stated in Equation (1), according to a previous study by Ujile and Owhor (2018) with slight modifications.

$$\frac{\partial C}{\partial t} = -D_x \frac{\partial^2 C}{\partial x^2} - D_z \frac{\partial^2 C}{\partial z^2} - v_x \frac{\partial C}{\partial x} - v_z \frac{\partial C}{\partial z} \tag{1}$$

where:

- C = Concentration of contaminants
- t = Duration of contaminant transport (day)
- x, z = Direction of transport in x- and z-directions along soil depth (m)
- D_x, D_z = Diffusion coefficient in x- and z-directions (m²/day)
- v_x, v_z = Diffusion coefficient (m²/day)

Boundary conditions:

$$t = 0 \quad 0 < X < \infty; \quad C = 0 \tag{2}$$

$$t > 0 \quad X = \infty; \quad C = 0 \tag{3}$$

$$t > 0 \quad X = 0; \quad C = C_o \tag{4}$$

The analytical solution to Equation (1) is given by Equation (5).

$$C(x, z, t) = \frac{C_o}{2} \left\{ \operatorname{erfc} \left[\frac{z+x\sqrt{D_x/D_z}-v_z t}{2\sqrt{D_z[1+(D_x/D_z)^2]}t} \right] + \operatorname{erfc} \left[\frac{z+x\sqrt{D_x/D_z}+v_z t}{2\sqrt{D_z[1+(D_x/D_z)^2]}t} \right] \right\} \exp \left(\frac{v_z [2(z+x\sqrt{D_x/D_z})-v_z t]}{4D_z [1+(D_x/D_z)^2]} \right) \tag{5}$$

The concentrations of the heavy metal were measured only in vertical direction during the experimental study. Hence, the following assumptions were considered:

- i. The transport of heavy metals into the soil media is most effective in the vertical or downward direction (z-direction) in the column.
- ii. Seepage velocity is negligible in horizontal direction (x-direction).

Thus, equation (5) reduces to:

$$C(z, t) = \frac{C_o}{2} \left[\operatorname{erfc} \left(\frac{z-v_z t}{2\sqrt{D_z[1+(D_x/D_z)^2]}t} \right) + \operatorname{erfc} \left(\frac{z+v_z t}{2\sqrt{D_z[1+(D_x/D_z)^2]}t} \right) \right] \exp \left(\frac{2z v_z - v_z^2 t}{4D_z [1+(D_x/D_z)^2]} \right) \tag{6}$$

Therefore, equation (6) was used to predict the concentration of heavy metal along the soil depth after substituting the average determined diffusion coefficient and seepage velocity. The predicted concentrations were compared with the experimental results (measured).

III. RESULTS AND DISCUSSION

The average diffusion coefficients determined from the experiment are shown in Table 1, while the seepage velocity is 0.0025±0.019 m/day. The compared results of the predicted heavy metal concentrations with the experimentally measured concentration are shown in Figures 1 to 4.

Table 1: Diffusion Coefficient of Heavy Metals

Diffusion Coefficient, D (m ² /day)			
Fe	Pb	Cr	Cd
1.2719 x 10 ⁻³	1.0517 x 10 ⁻³	8.9003 x 10 ⁻⁴	7.4480 x 10 ⁻⁴

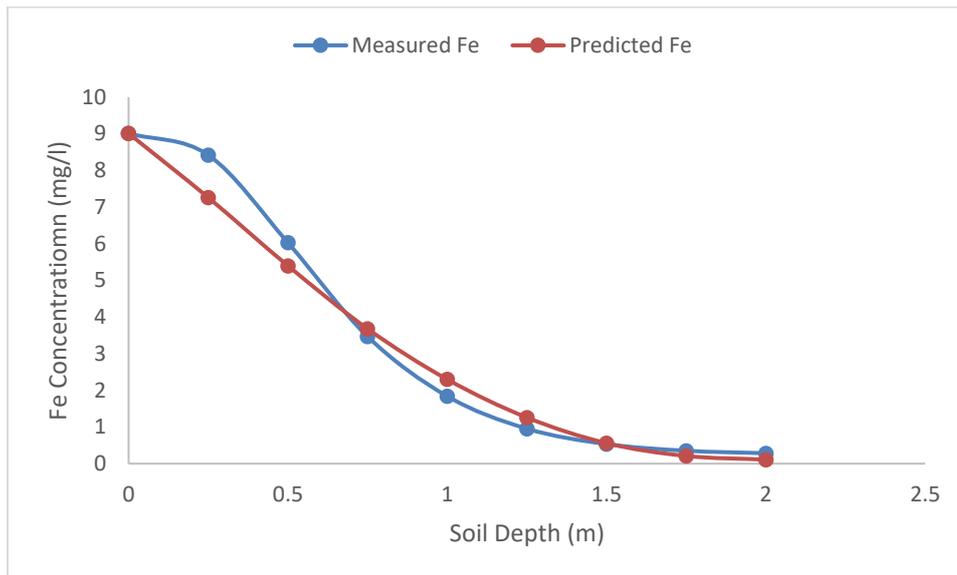


Figure 1: Predicted and measured Fe concentration along soil depth

Figure 1 shows the trends of predicted and measured of Fe concentrations along soil depth. The profiles indicate that Fe concentration for both measured and predicted decreases with increase in soil depth. The results show that the predicted concentration of Fe decreases from 7.2595 mg/l at 0.25m depth to 0.1098 mg/l at 2m depth after 96 hours (4 days). The predicted Fe concentrations are comparatively good at all the sampling depths, with estimated Root Mean Square Error (RMSE) value between the predicted and measured given as 0.4876. Therefore, the closeness of the predicted and measured values validates the capability of the model to simulate heavy metal distribution in soils. The Fe concentration level at 2 m depth after 4 days is slightly below the WHO standard specified for drinking water quality (0.3 mg/l). This implies that Fe can migrate into soil media to levels that can constitute pollution to the soil overtime.

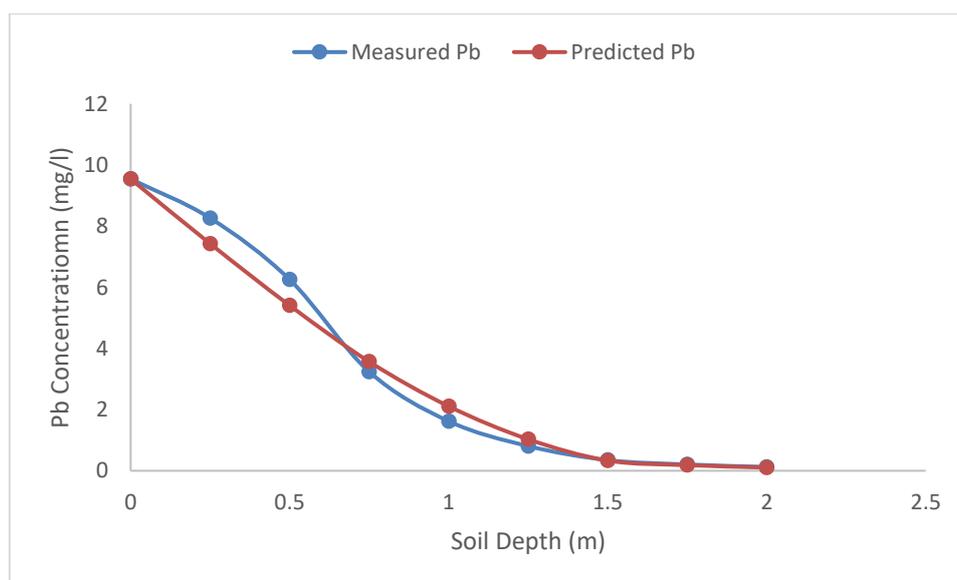


Figure 2: Predicted and measured Pb concentration along soil depth

Figure 2 shows the profiles of predicted and measured of lead (Pb) concentrations along soil depth. Like iron, the trends indicate that Pb concentrations for both measured and predicted decrease with increase in soil depth. Thus, the predicted concentration of Pb decreases from the initial concentration of 9.5429 mg/l to 0.1054 mg/l at 2m depth after 4 days, as against 0.1235 mg/l recorded in the measured sample at 2 m soil depth. The predicted Pb concentrations at the sampling depths are comparative with measured Pb concentrations. Further analysis revealed that the RMSE value between the predicted and measured concentration of Pb is 0.5494. This signifies that the predicted and measured Pb are close, implying that the model has capability to

simulate and predict the transport of Pb in the soil. However, the concentration level of Pb at 2 m depth after 4 days implies that it can migrate into soil and groundwater media overtime to levels that can compromise water quality.

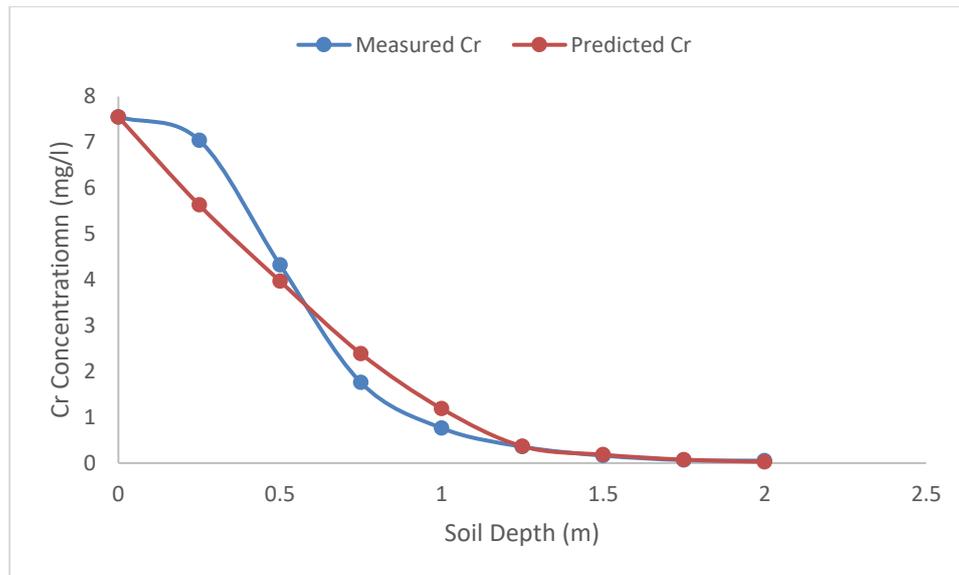


Figure 3: Predicted and measured Cr concentration along soil depth

Figure 3 shows the profiles of predicted and measured of Cr concentrations along soil the depth. Again, the profiles also indicate that Cr concentrations for both measured and predicted decreases with increase in soil depth. The result shows that the predicted concentration of Cr decreases from its initial concentration of 7.5556 mg/l to 0.0269 mg/l at 2m depth after 4 days, as against 0.0519 mg/l measured from the experiment at 2 m soil depth. The predicted Cr concentrations is slightly below that obtained from the experiment at 2 m depth. Nevertheless, the predicted concentration fitted well with the measured Cr concentration. The error analysis shows that the RMSE value between the predicted and measured concentration of Cr is 0.6714. Generally, the model has high prediction accuracy. Moreover, the concentration level of Cr at 2 m depth after 4 days implies that it can migrate into soil and groundwater media overtime to levels that can compromise water quality.

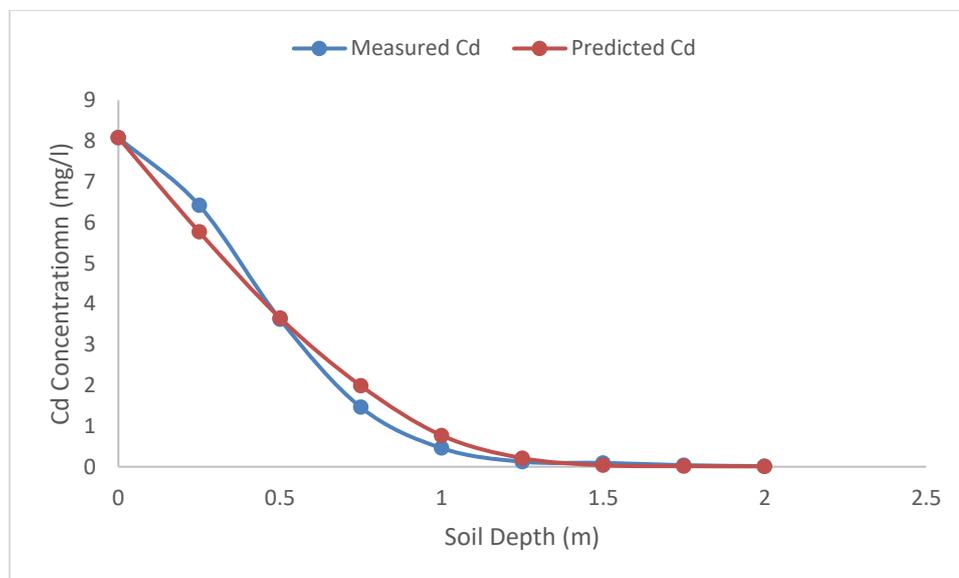


Figure 4: Predicted and measured Cd concentration along soil depth

Figure 4 shows the profiles of predicted and measured of cadmium (Cd) concentrations along soil depth. The Cd concentrations for both measured and predicted decreases with increase in soil depth. Thus, the predicted concentration of Cd decreases from the initial concentration of 8.0816 mg/l to 0.0085 mg/l at 2m

depth after 4 days, as against 0.0145 mg/l recorded in the measured sample at 2 m soil depth. The predicted Cd concentrations at the sampling depths are comparative with measured Cd concentrations. The RMSE value between the predicted and measured concentration of Cd is 0.3686. The comparative results generally show that the model has high prediction accuracy. Additionally, the concentration level of Cr at 2 m depth after 4 days also implies that it can migrate into soil and groundwater media overtime to levels that can compromise water quality.

Nevertheless, the slight deviations observed across the predicted heavy metals from the measured can be attributed to specific characteristic properties soil, such as moisture (Kroeksakul et al., 2024), colloidal redistribution and soil porosity (Wen et al., 2019), and soil particle size distribution (Zhao et al., 2024). The transport dynamics of heavy metals can also influence the deviations, as Tan et al. (2022) observed in a similar study that the rate of Pb, Cu and Cd transport in the column were faster with change in surface water intrusion. Overall, the model results show high prediction capacity for Fe, Pb, Cr and Cd and the trends matched well with the measured at the various soil depths. Therefore, the Advection-Diffusion model has good prediction accuracy and can be utilized to model and predict the transport of heavy metals in soil subsurface. The prediction accuracy of contaminants by Advection-Diffusion equation was equally reported in a previous study by Kumar et al. (2024).

IV. CONCLUSION

Contaminants from the soil surface, including heavy metals, spread into soil and compromise soil properties, as well as groundwater quality if it migrates downwards to aquifer zone. The findings from the study revealed that predicted Fe, Pb, Cr and Cd fit well with the experimentally measured values at all soil depth within 2 m depth. Therefore, the Advection-Diffusion model has good prediction accuracy and can be applied for prediction of heavy metals transport in soil subsurface, and as a management strategy for regulation and control of heavy metal contaminants in soil media.

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