# Numerical Simulation and Field-Validated Predictive Modelling of Sediment-Bound Heavy Metal Transport and Accumulation in the Rupingazi River Fluvial System

**Sophy Njoki***

**Kenyatta University, Physics Department, P. O. Box 43844-00100, Nairobi, Kenya**

***Corresponding Author**

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## ABSTRACT

With the rapid economic growth, heavy metal pollution has become a key issue in rivers as they are the most common source of drinking water in the world. The metals in the dissolved state are found either in the water column or sediment pore water whereas those that are accumulated on the suspended and bed sediments are the ones in particulate state. Metals found in the sediments can be suspended back to the water column. A Numerical model that predicted the spatial and temporal concentration of heavy metals in river sediments under varying conditions was developed using python programming language. The model that predicted concentration of heavy metal in bed sediments incorporated the advection, diffusion, absorption, desorption, resuspension, deposition, removal and rate of chemical or biological reactions. The equations were discretized using finite difference method. The numerical solution was obtained using python programming language and validated using field data. There was a high correlation between the simulated and field data values of concentration of zinc in sediments. The correlation coefficients was 0.8296. Sensitivity analysis was done on the models to assess how they were influenced by diffusion coefficient, velocity, settling velocity, resuspension rate, adsorption and desorption. The model was applied to predict the spatial and temporal variations of heavy metals in sediments of river Rupingazi.

**Keywords:** Sediments, Heavy metals, Model, Discretization, Validation

## INTRODUCTION

Pollution of river water and their sediments with heavy metals has become an international issue which has interested law makers and researchers due to the poisoning linked with them and their bioaccumulation capability (Li, 2014). Heavy metal pollution of river water and sediments is associated with man-made influences that take place near and far too such as settlements, farms, game reserves, car wash, mining activities, storm water run-off (Chaves *et. al* 2016, De Melo *et al*.,2016; Turatsinze *et al*.,2024).

In underwater environment as observed by Ahamad *et al., (*2024) heavy metals can be found in either dissolved or particle-bound forms. Metals in the dissolved state are found either in the water column or sediment pore water whereas those that are accumulated on suspended and bed sediments are the ones in particulate state. Continuous assessment of sediment-bound heavy metals is necessary, since crucial facts in regard to their distribution and level of contamination is obtained Wang *et al*., (2022) and Nwagbara (2025) observed that heavy metals in rivers tend to build more in sediments than in water. The analysis of the metal pollution of a river gives a foundation of the connection linking the metals divided between sediment-bound and dissolved forms in aquatic systems. The sediment - water interchange could also be liable for the deposition of metal in the sediments (Jia *et al*., 2021; Singh *et al*., 2005; Silva *et al*.,2014). When sediments are polluted with heavy metals, they pose an environmental problem due to the fact that they are toxic, non-degradable and easily accumulate in biota and food chain (Chakraborty *et al*.,2023; Sundaray *et al*., 2014). Sediments are considered major pointers of water pollution since they are principal sources and sinks of the heavy metals (Sojka *et al.,* 2022; Zhang *et*

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*al*.,2015). Heavy metals are released from sediments through the process of resuspension of particulates at the boundary between sediment and water. When pollution of river water is being considered in any study, sediments should also be considered as they are environmental pointers for evaluation criteria of environmental water quality degradation.

Models give descriptions of a process in the actual world. Models can predict the destiny of contaminants and their effect on the quality of water and aid in comprehending their consequences on human health and environment. Models are adapted in communication of findings, assessment of harmful effects, policy and strategy analysis, decision-making in governance and implementation of management practices. The procedures associated with the movement of pollutants are mostly not even in space and time. Therefore they are simply manipulated using comprehensive model that not only looks into the process and dissemination of a pollutant, but in addition speculates its changing trends with time (Jampani *et al*., 2024).Computer simulations have contributed to finer comprehension and assessment of the water resources by use of all-inclusive numerical model simulations and evaluation of multiple schemes or alternatives (Singh, 2022).Numerical models are essential when the prediction of the transport of a pollutant is being considered in a body of water. Monitoring and modelling are activities that are carried out together. Monitoring helps in evaluating the contaminants that get into the water body while modelling is crucial for indicating their complexity and hazards in future. A number of models that have discrete stability and weaknesses have been in use in the water quality sector (Wang *et al*.,2013) for supporting planning and policy making in design of feasible actions with regard to pollution of water in agriculture.

A contaminant that is present in river water moves as the water flows (Zhou and Huang 2022). The flow of river water and transportation of contaminants within itself are problems that are tackled by means of analytic problem solving methods, computer simulations and data obtained from experimental work that is needed for calibration of simulations of the critical processes and results. The transportation of a contaminant in solute state is represented with a partial differential equation commonly referred to as advection-dispersion equation (Vaganor *et al*.,2024). This equation is applicable in several areas such as aquifer circulation, engineering science (petroleum and chemical), biomedical science and sciences of the environment to illustrate the nature of soluble concentration. Also, it is ordinarily employed to evaluate the transport of matter like heavy metals and organic compounds in riverine habitats. Computer aided models enhance the understanding of water resources through a wide range of numerical simulations. Models allow the end users to form a concept of the situation in the river basin that one can use to predict the concentration and transportation of heavy metals found in river water and their sediments. When using a model, the quality of water can be projected and explained. Various variables such as length, width and depth can be fed into the model. The evolution of computer models that can forecast dispersion of pollutants in natural waters has become very urgent. These models when compared to physical models are cost effective and can easily adapt to new situations (Shen *et al*., 2023; Wang *et al*.,2013).

## METHODOLOGY

Fick's second law applies to diffusion of metals distributed between the sediment and the water column above. A metal trapped in sediment can diffuse back into the water column following a concentration gradient.

Pollutants are transported by both advection (bulk flow movement) and dispersion (spreading due to turbulence and molecular diffusion). This leads to

$$\frac{\partial C}{\partial t} + V\frac{\partial C}{\partial x} D\frac{\partial^2 C}{\partial x^2} \quad \text{..... (1)}$$

$$\frac{\partial c}{\partial t} = \frac{-\partial(uc)}{\partial x} + \frac{D\partial^2 c}{\partial x^2} + K_{ads}C_w - K_{des}C_s + R - R_{esuspension} + S_{depositon} - S_{removal} \quad \text{..... (2)}$$

Equation 2 describes the temporal variation of contaminant concentration in a river accounting for the major physical, chemical and sediment interaction processes affecting pollutant transport. The term $\frac{\partial c}{\partial t}$ represents the rate of change of contaminant concentration at a given location. The advection term $\frac{-\partial(uc)}{\partial x}$ describes the transport

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of the contaminant by the bulk movement of the flowing water, where u is the flow velocity and x is the longitudinal distance along the river. The dispersion term $\frac{D\partial^2 c}{\partial x^2}$ accounts for the spreading and mixing of the contaminant due to turbulent diffusion and velocity variations within the flow, with D representing the dispersion coefficient. The term$K_{ads}C_w$ represents the adsorption of dissolved contaminants from the water column onto sediment particles where$K_{ads}$ the adsorption coefficient and $C_w$is the heavy metal concentration in water. The term $K_{des}C_s$ represents desorption which is the release of heavy metals from sediments back into the water column where$K_{des}$ is the desorption coefficient and$C_s$ is the heavy metal concentration in the sediments. The reaction term R accounts for chemical and biological processes and other transformations that may alter heavy metal concentration. The resuspension $R_{esuspension}$ term represents the re-entry of contaminated sediments into the water column due to turbulence or increased flow conditions. The deposition $S_{depositon}$ term accounts for the settling of heavy metal –laden particles from the water column onto the river bed. The removal term $S_{removal}$ represents processes that permanentlyremove heavy metals from the system such as dredging or long term burial within the sediments.-.The assumptions made when using the mathematical model represented by equation (2) are; Concentration of heavy metals occur mainly along the spatial dimension, vertical processes like dispersion and advection are more dominant as compared to transport along the horizontal direction, Characteristics of sediments such as porosity, density and particle size are uniform, boundary conditions are contant.Lateral sinks and sources have negligible effects, dispersion coefficient is depth dependent, external factors like variation due to seasons, anthropogenic activities do not cause significant changes in the system.

Discretization of the Mathematical Models

Forward difference is used or time derivative

This is used for discretization of time in problems that depend on it.

$\frac{\partial C}{\partial t}= \frac{C_j^{n+1}-c_j^n}{\Delta t}$……(3)

$C_j^n$ is the solution of the current time interval

$C_J^{n+1}$represents solution of the next time interval

Δt represents the magnitude of the time step

Central difference is used for space derivative

This is a numerical scheme that gives very accurate estimations of derivatives. It is used in approximation of the first and second order spatial derivatives

$\frac{\partial C}{\partial x} = \frac{C_{j+1}^n-C_{j-1}^n}{2\Delta x}$ …… (4)

The equation governing the heavy metal concentration in sediments (3.10) was discretized as follows

$\frac{C_j^{n+1}-C_j^n}{\Delta t} = -U[\frac{C_{j+1}^n-C_{j-1}^n}{2\Delta x}]$+D$[\frac{C_{j+1}^n-2C_j^n+C_{j-1}^n}{(\Delta x)^2}]$+$K_{ads}C_w - K_{des}C_s + R - R_{esuspension} + S_{depositon} - S_{removal}$……(5)

Multiplying all the terms by $\Delta t$

$\frac{C_j^{n+1}-C_j^n}{} = -U[\frac{\Delta t\, C_{j+1}^n-C\Delta t_{j-1}^n}{2\Delta x}]$+D$[\frac{\Delta tC_{j+1}^n-2\Delta tC_j^n+\Delta tC_{j-1}^n}{(\Delta x)^2}]$ $+\Delta tK_{ads}C_w - \Delta tK_{des}C_s + \Delta tR - \Delta tR_{esuspension} + \Delta tS_{depositon} - \Delta tS_{removal}$……(6)

- Collecting all the terms n + 1 on the left and n terms on the right we get

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$$C_j^{n+1} = -\frac{U\Delta t\, C_{j+1}^n}{2\Delta x} + \frac{U\Delta t\, C_{j-1}^n}{2\Delta x} + \frac{D\,\Delta t C_{j+1}^n}{(\Delta x)^2} - \frac{2D\,\Delta t C_j^n}{(\Delta x)^2} + \frac{D\,\Delta t C_{j-1}^n}{(\Delta x)^2} +$$

$$\Delta t K_{ads} C_w - \Delta t K_{des} C_s + \Delta t R - \Delta t R_{esuspension} + \Delta t S_{depositon} - \Delta t\ S_{removal} \quad (7)$$

$$C_j^{n+1} = C_j^n - \frac{U\Delta t}{2\Delta x}(C_{j+1}^n - C_{j-1}^n) + \frac{D\Delta t}{(\Delta x)^2}(C_{j+1}^n - 2C_j^n + C_{j-1}^n) + \Delta t\, K_{ads} C_w - \Delta t K_{des} C_s + \Delta t R - \Delta t R_{esuspension} + \Delta t \Delta t\, S_{removal} \quad (8)$$

Let $\frac{U\Delta t}{2\Delta x} = p_1$ and $\frac{D\Delta t}{(\Delta x)^2} = p_2$

The equation 8 therefore become

$$C_j^{n+1} = C_j^n - p1(C_{j+1}^n - C_{j-1}^n) + p2\ (C_{j+1}^n - 2C_j^n + C_{j-1}^n) + \Delta t\, K_{ads} C_w - \Delta t K_{des} C_s + \Delta t R - \Delta t R_{esuspension} + \Delta t S_{depositon} - \Delta t\, S_{removal} \quad (9)$$

Python Programming Language

Python is a high-level object oriented programming language. It is widely used in numerical modelling due to its simplicity and extensive collection of libraries. Its syntax is concise and allows researchers to develop, test and implement computational models efficiently. Python language provides libraries that allow numerical computations, data manipulation, visualization and simulations. Numpy enables efficient numerical operations on large data. Matplotlib allows graphical visualization of data allowing presentation of model outputs and trends effectively. Python efficiently solves ordinary and partial differential equations used to describe physical processes. Finite difference, finite element and finite volume numerical schemes can be implemented in python in simulation of pollutant, water quality and sediment interactions. Python programming language is flexible and enables researchers to customize a model to specific objectives of a study and environmental conditions.

In the present study Python was used to develop and implement a numerical model for simulating heavy metal concentrations in water and sediments of Rupingazi River. The language facilitated the discretization and solution of the Advection-Dispersion Equation that described the transport and concentration of heavy metal in aquatic systems. The python language allowed efficient implementation of model parameters, calibration processes and validation against field data.

Main Functions in the Numerical Solution.

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Figure 1 shows an overview of computational functions used in this study.

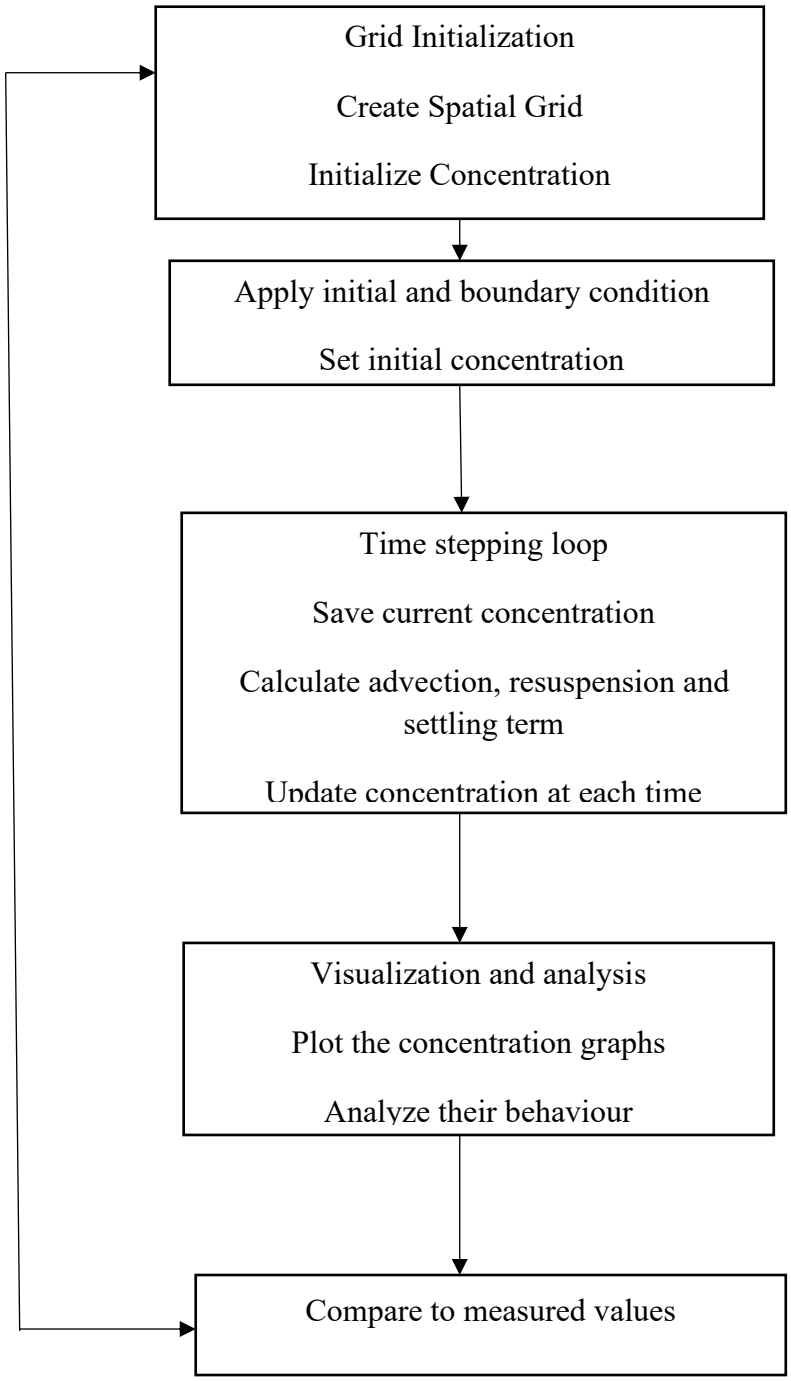


Figure 1 Overview of Computational Routines

**Model Validation**

Model validation is a process of determining whether a model can accurately give results similar to real-world observations. Validation is important in order to test the ability of the model to simulate pollutant transport and concentration levels in natural systems like rivers. It also helps in identification of weaknesses in assumptions and parameters used. The models were calibrated by adjusting parameters such as dispersion coefficient, flow velocity, adsorption coefficient, desorption coefficient, settling and resuspension rate so that its output closely matched the field data. The measured concentrations of metals in water and sediments during dry and wet seasons were used for calibration and validation of the models.

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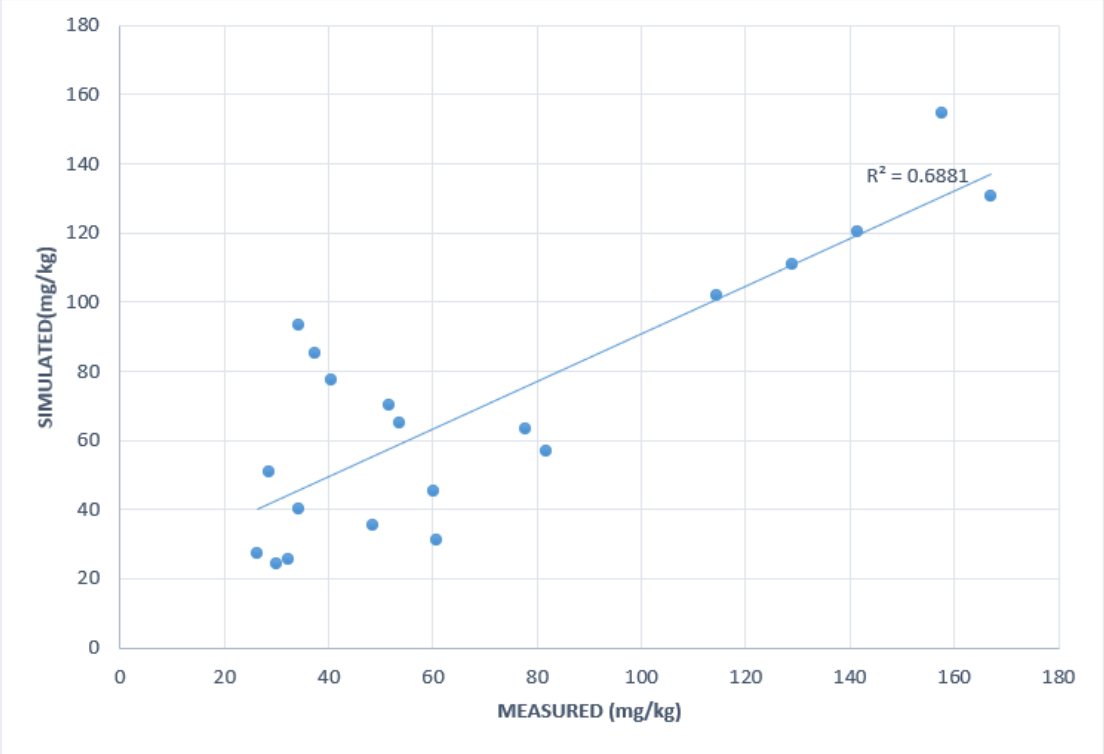


Figure 2 Comparison of Measured and Model Results of Zinc in Sediments During the Wet Season

Figure 2 indicates that there was a strong positive relationship between the measured and simulated concentrations and Zinc in sediments. The correlation coefficient was 0.8296 for Zinc in sediments confirming that the models can be considered reliable for prediction of heavy metal concentration in river water and sediments.

## RESULTS AND DISCUSSIONS

Sensitivity Analysis of the Model for Heavy Metal Concentration in Sediments

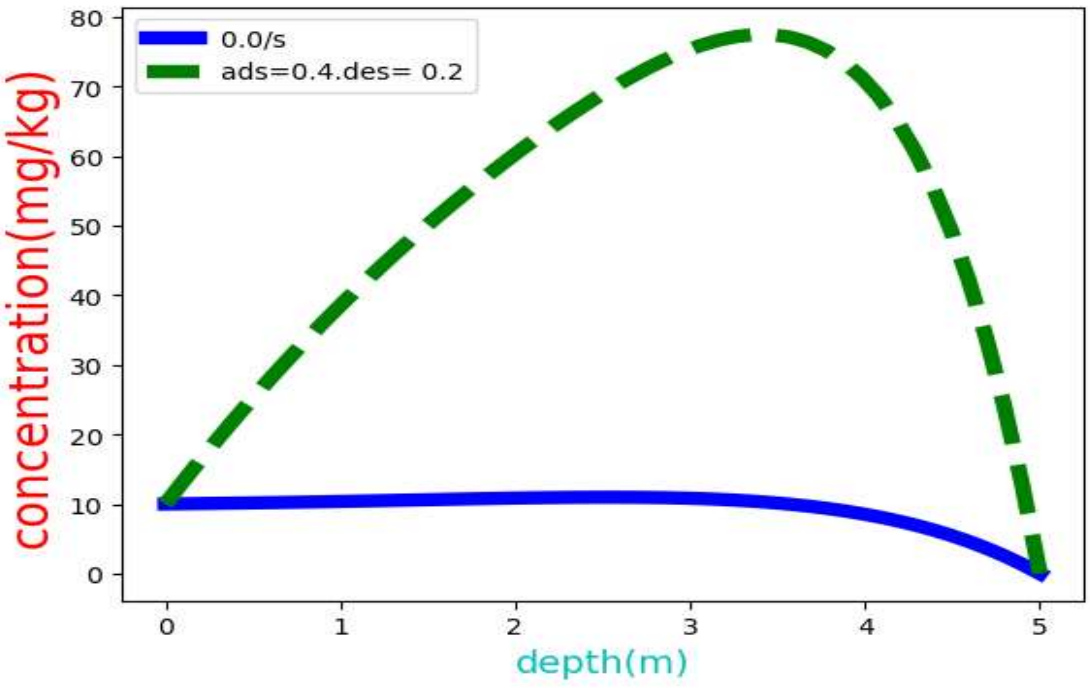


Figure 3 Influence of Adsorption and Desorption

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For the shallow depth some part of the heavy metals attaches to the sediment particle while others remain in the dissolved state. Between 2-3m there is maximum accumulation heavy metals as indicated in figure3 which may be due to an increase in the area of exposure. For greater depths adsorption and desorption lead to a decrease in concentration chemical processes like metal precipitation may also cause the lower movement. The relativity uncharged concentration gives the impression that there is very little interchange between the dissolved heavy metals and sediments. The little decrease at the bottom could have been as a result of diluting or lessened metal input over time

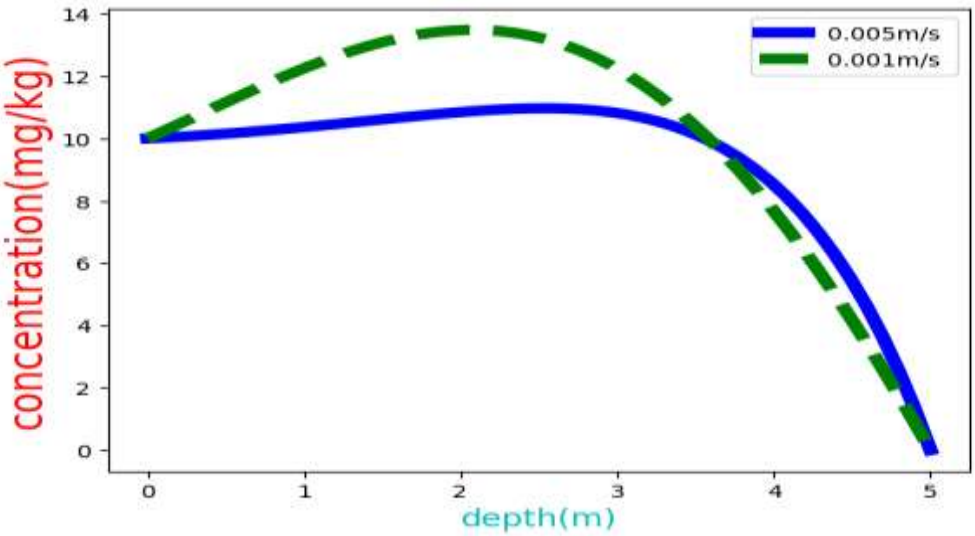


Figure 4 Influence of Velocity on Concentration

Figure 4 indicates that for shallow depths, the concentration of heavy metals increases slightly prior to arriving at the peak. This could be attributed to deposition of contaminants from discharge of industries, surface runoff and adsorption on the fine sediment particles flow of velocity 0.005m/s results in reduced peak concentration resulting from high suspension of heavy metals thus preventing them from setting at a lower velocity of 0.001m/s, the buildup of heavy metals increases owing to reduction in disturbance that allows more metals to be deposited. At greater depths there is a decrease in concentration as a result of reduction in interaction with contaminants from river water.

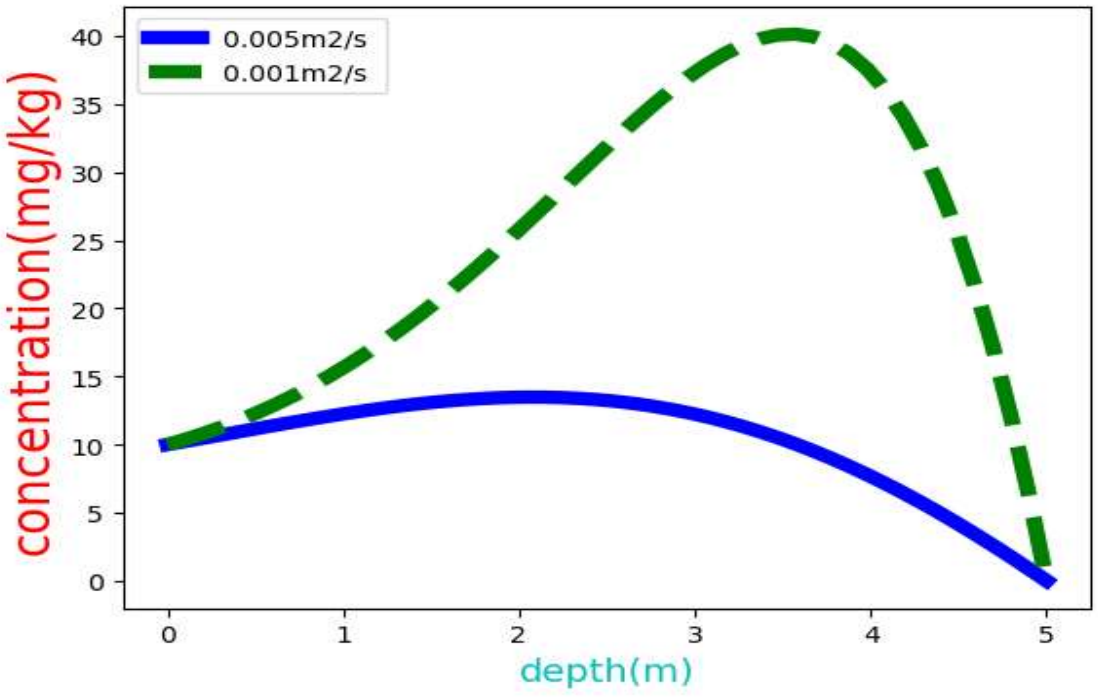


Figure 5 Influence of Diffusion on Concentration

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From figure 5. an increased in depth gives rise to a gradual rise in concentration. For a lower diffusion coefficient, the concentration rises steeply and sharply. The metals remain trapped at a particular depth as result of slow movement A higher diffusion coefficient results in a uniform distribution of a lower peak and the decline is gradual. The heavy metals spread more evenly thought the sediment depth.

Application of Numerical Model for Heavy Metal Concentration in Sediments

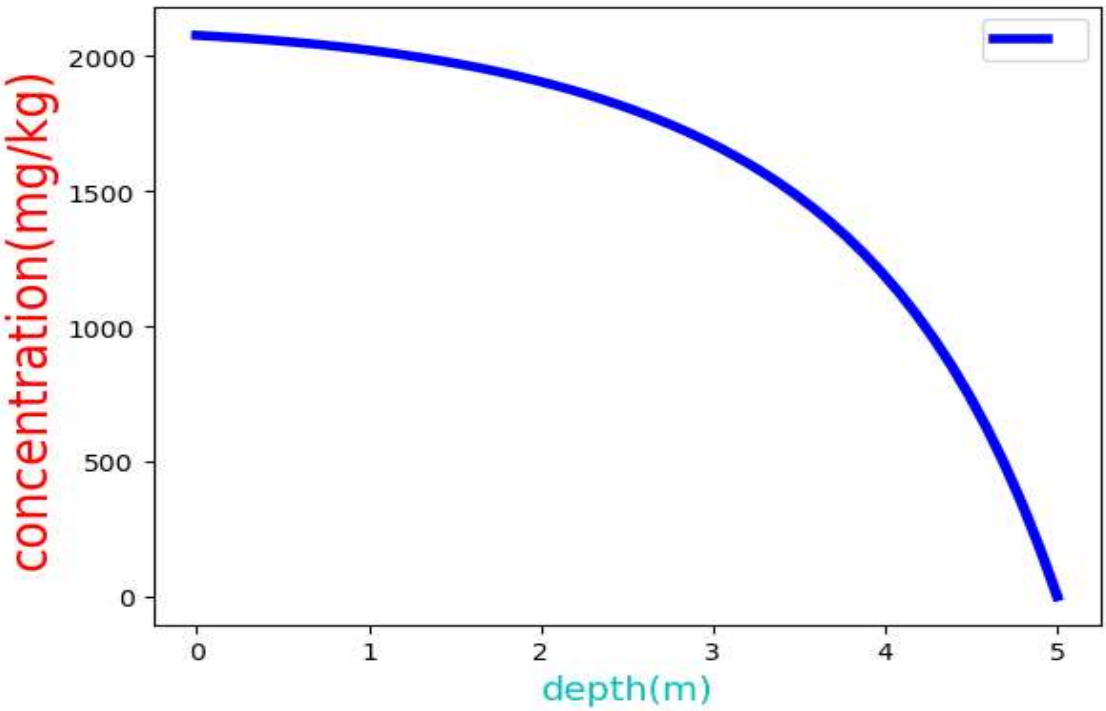


**Figure 6 Spatial Variation of Iron**

Figure 6 shows a decline in concentration of iron with greater depth. High concentration at the shallow depth could be as a result of accumulation on the surface from the surface runoff or deposition from the atmosphere. A rise in depth results to a reduction in concentration of iron that could possibly be as a result of leaching or diffusion.

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