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Numerical Modelling and Field Validation of Heavy Metal Transport in Rupingazi River Water Using the Advection –Diffusion Equation

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Abstract: The most important resource of life in this planet is water. With the rapid economic growth, heavy metal pollution has become a key issue in rivers as it is the most common source of drinking water in the world. Heavy metals contamination in river waters poses significant risks to both ecosystems and human health. Accurate prediction of heavy metals concentration is essential for effective water quality management and environmental protection. The objective of this study was to develop and solve a numerical model to predict the spatial and temporal distribution of heavy metal concentration in river water under varying flow conditions. The model incorporates the advection –dispersion equation. The advection diffusion equation was solved numerically to predict the spatial and temporal distribution of heavy metal concentration in a rivers system under varying environmental conditions. The equation was discretized using finite difference method (central differences). The numerical solution was obtained using python programming language and validated using the data collected from Rupingazi river. There was a high correlation between the simulated and field data values of concentration of iron in river water. The correlation coefficient was 0.899 . Sensitivity analysis was done on the model to assess how it was influenced by factors such as velocity, dispersion, sources and sinks. The model was applied to predict the spatial and temporal variations of heavy metals in Rupingazi river. The model provides variable insights for managing pollution and can inform regulatory decisions on water quality control particularly in areas with industrial and agricultural runoff.

Keywords: *Heavy Metal, Spatial, Temporal, Discretization, Validation.*

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I. INTRODUCTION

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 to notify findings, assessment of the harmful results that a factor is able to induce, strategy survey, state governance resolve and execution exercise. 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 [1].Computer simulations have contributed to finer comprehension and assessment of the water resources by use of all-inclusive numerical model simulations and evaluation of various schemes or alternatives[2].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 complexness and hazards in future. A number of models that have discrete stability and weaknesses have been in use in the water quality sector [3,4] 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 [5]. 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 [6]. This

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equation is useful 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 determine the transfer of matter like heavy metals and organic compounds in riverine habitats. Use computers aids in finer understanding of water resources through wide differing 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 in river water as well as 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 predict the 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 [7]. Numerical solution is a vital tool for environmental engineers and researchers working to control pollution and protect water resources. Many existing models are complex and difficult for non-experts to use effectively limiting their utility in decision making. A model that has the ability to predict and manage the impact of heavy metal pollution in river systems has been developed in this study

II. LITERATURE SURVEY

Numerical solution is a vital tool for environmental engineers and researchers working to control pollution and protect water resources. The Advection-Diffusion Equation (ADE) was used by the researchers as the main mathematical model for studies of pollutants dispersal in water bodies. This equation included the processes of advection (the movement caused by a water current) and diffusion (the dispersion caused by concentration differences). They focused on the parameters such as water velocity, the concentration of pollutants, and diffusion coefficients, and demonstrated how small perturbations in these parameters caused incorrect prediction of results obtained. Additionally, they focused on boundary conditions, which were the restrictions for a particle's motion which in this case was complex fluid motion modifying the advection [8]. Using Dirichlet and Neumann boundary conditions, the researchers examined the problem of pollution control as well as influencing deposits along the banks of rivers. The results also showed that there was a great potential in applying the ADE for the pollutant dispersion as it provided useful insights for further development of numerical procedures.

The physical mechanisms of advection and diffusion processes, which are significant in the transport of pollutants in water bodies were investigated [9]. They concluded that advection, which is the transportation of pollutants by water flow, is typical for rivers and coastal regions, where contaminants can easily travel over long distances in a very short period of time. The slow process of molecular diffusion, although less effective in a short span, had its time in assisting the processes of dilution of the caused contamination During the study, the difficulty of advection-diffusion modeling processes, that usually do not follow such order in real life, was pointed out. Advanced numerical methods were used by the researchers to find a compromise between these processes for the models developed, so that the displacement of the pollutants in the simulation corresponded to the actual displacement of the pollutants in the system. Thus, these results brought into focus the necessity of comprehending the said mechanisms in making credible forecasts.

Javadi *et al*., 2014 compared different numerical approaches that include Finite Difference Method (FDM) and Finite Element Method (FEM) in solving Advection-Diffusion Equation. FDM drew positive feedback due to its ease of application and effectiveness making it ideal for primary pollution models. Its scope, however, was limited due to its challenges with complex boundary conditions. The analysis indicated that since the environmental conditions were not regular, the use of FEM provided better results but at a cost of increased computational time. The study also discussed the use of implicit and explicit schemes within these methods. Implicit schemes provided more stability for wider time steps whereas explicit steps were less advanced but more tedious in time cost while small time steps were employed. The researchers claimed that the choice of methods is contingent upon the complexity of the environment and model requirements but also noted how flexible the use of FEM is in the changing environment. [10]

Iqtadar *et al*.,2022 modeled the transport of heavy metals in mining regions, analyzing risks to downstream communities. They simulated pollutant dispersion under various conditions, finding rapid contamination over extensive areas. Their recommendations included stricter regulations and community awareness programs to address toxicity risks. The study provided predictive tools for managing contamination and protecting against affected populations.

Many existing models are complex and difficult for non-experts to use effectively limiting their utility in decision making. A model which has been validated and has the ability to predict and manage the impact of heavy metal pollution in river systems has been developed in this study [11]

- *Objective of Research*

Preparation, validation and application of computer program to solve transport equation of heavy metal pollutants in water.

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III. RESEARCH METHODOLOGY

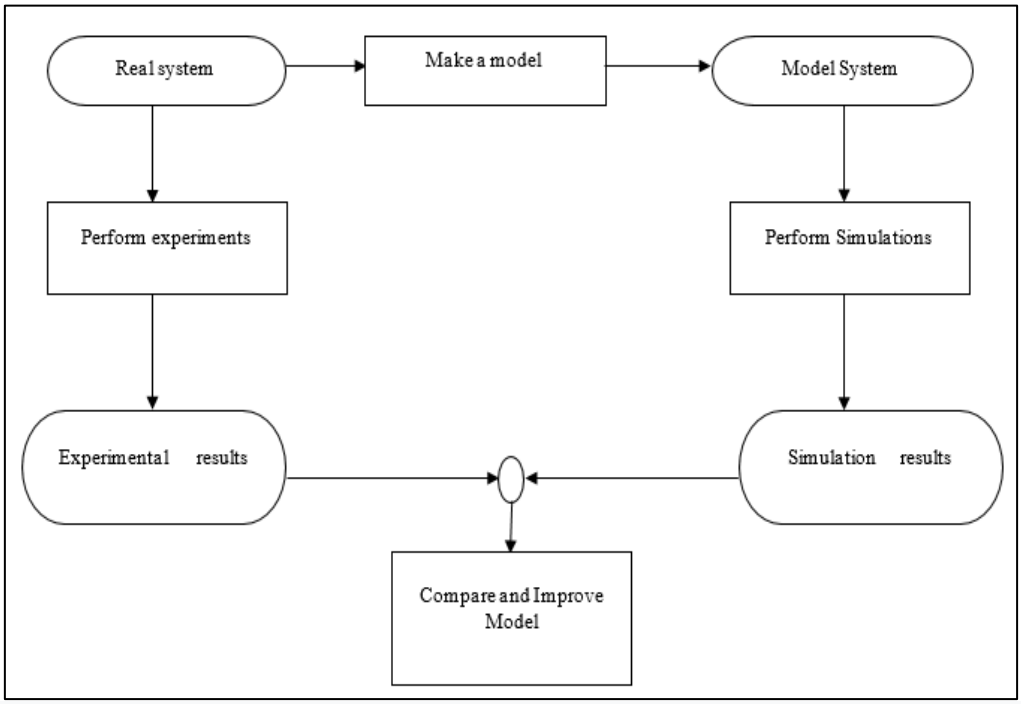


Fig 1 Process of Building a Computer Model, and the Interplay Between Experiment, Simulation

➢ *Mathematical Model*

The mathematical model describing heavy metal transport must comprise equations governing all the processes involved [12,13]. The understanding of how a contaminant moves is fundamental in control and prediction of water quality in rivers. For the evaluation of the change in concentration of a contaminant t, an advection-dispersion equation is often used [14]. This equation provides a very practice and principal mathematical model which has been widely applied in the fields of natural sciences and engineering. A mathematical model describes a particular physical problem in form of mathematical expressions (that involves making a lot of assumptions) which can be worked out. In most circumstances mathematical modeling comprises of first step in any numerical simulation, The advection-diffusion equation [15]

$$\frac{\partial c}{\partial t} = \frac{-\partial(uc)}{\partial x} + \frac{D\partial^2 c}{\partial x^2} - Ws + R \quad \text{..... 1}$$

c heavy metal concentration in river water(mg/L)

U for advection velocity(m/s)

D longitudinal diffusion coefficient (. m^2 /s

x distance along the river(m)

t time(s)

R resuspension rate(mg/L.s)

Ws Settling rate(mg/L.s)

In order to use the advection diffusion equation some assumptions were made: River is one dimension, Advection velocity and diffusion coefficient are constant, Initial concentration is a known distribution, Boundary conditions are Dirichlet and Uniform mixing distribution.

For time derivative

Forward difference

$$\frac{\partial C}{\partial t} = \frac{C_j^{n+1} - C_j^n}{\Delta t} \quad \text{..... 2}$$

For space derivative

Central difference

$$\frac{\partial C}{\partial X} = \frac{C_{j+1}^n - C_{j-1}^n}{2\Delta x} \quad \text{..... 3}$$

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

$$\frac{C_j^{n+1} - C_j^n}{\Delta t} = -U\left[\frac{C_{j+1}^n - C_{j-1}^n}{2\Delta x}\right] + D\left[\frac{C_{j+1}^n - 2C_j^n + C_{j-1}^n}{(\Delta x)^2}\right] - Ws] + R \quad \text{.... 5}$$

Multiplying all the terms by Δt

$$\frac{C_j^{n+1} - C_j^n}{} = -U\left[\frac{\Delta t\, C_{j+1}^n - C\Delta t_{j-1}^n}{2\Delta x}\right] + D\left[\frac{\Delta t C_{j+1}^n - 2\Delta t C_j^n + \Delta t C_{j-1}^n}{(\Delta x)^2}\right] - Ws\Delta t + \Delta t\ R + \quad \text{..... 6}$$

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

$$C_j^{n+1} = -\frac{U\Delta t\, C_{j+1}^n}{2\Delta X} + \frac{U\Delta t\, C_{j-1}^n}{2\Delta X} + \frac{D\Delta t C_{j+1}^n}{(\Delta x)^2} - \frac{2D\Delta t C_j^n}{(\Delta x)^2} + \frac{D\Delta t C_{j-1}^n}{(\Delta x)^2} - Ws\Delta t + \Delta t\, R + C_j^n \quad \ldots\ldots 7$$

$$C_j^{n+1} = C_j^n - \frac{U\Delta t}{2\Delta X}(C_{j+1}^n - C_{j-1}^n) + \frac{D\Delta t}{(\Delta x)^2}(C_{j+1}^n - 2C_j^n + C_{j-1}^n) - Ws\Delta t + R\Delta t \quad \ldots\ldots 8$$

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

$$C_j^{n+1} = C_j^n - p1(C_{j+1}^n - C_{j-1}^n) + p2(C_{j+1}^n - 2C_j^n + C_{j-1}^n) - Ws\Delta t + R\Delta t \quad \ldots\ldots 9$$

$$C_j^{n+1} = C_j^n - p1(C_{j+1}^n - C_{j-1}^n) + p2(C_{j+1}^n - 2C_j^n + C_{j-1}^n) + \Delta ts \quad \ldots\ldots 10$$

The mathematical model represented by equation 10 was validated using field data obtained from river Rupingazi.

IV. RESULTS AND DISCUSSIONS

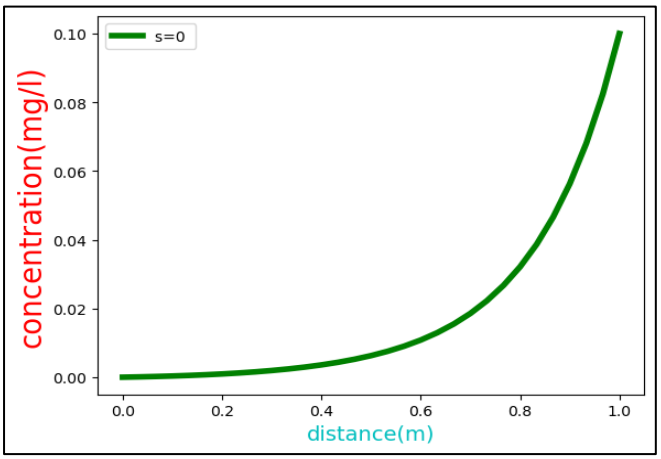


Fig 2 Spatial Variation in Concentration

The graph 2 indicated that heavy metal spreadsout from the source location due of diffusion and was advected by the flow velocity (flows in direction of flow) The concentration increased from zero as substance was injected near the boundary

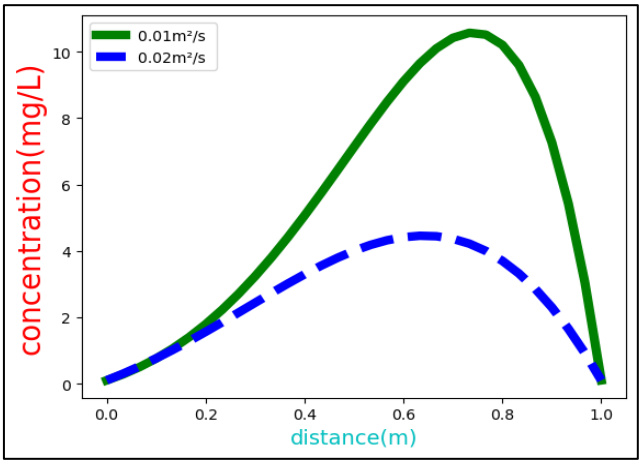


Fig 3 Influence of Diffusion Coefficient on Concentration

Diffusion coefficient controls the degree at spreading of the substance in the system. These results indicate that high diffusion coefficient led to wider concentration profile and lower peak concentrations indicating that the substance spread more quickly in space. Concentration spreads out more symmetrically and evenly in both directions. Low diffusion coefficient resulted in narrower, sharper profiles with higher concentration peaks as the substance is primary advected with limited spreading. As distance increases from the source, the concentration rapidly dropped off. There was less dispersion.

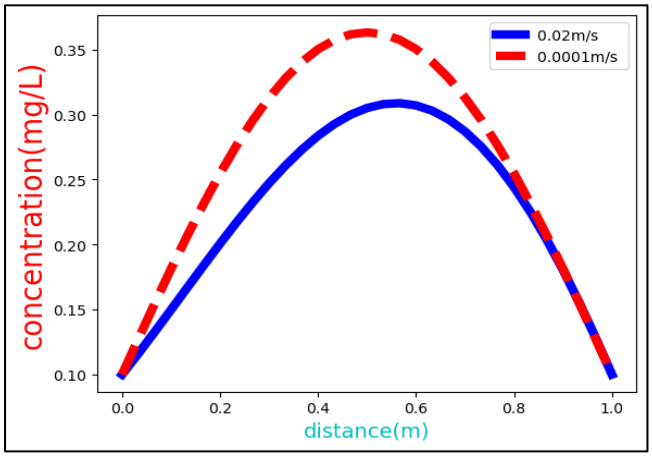


Fig 4 Influence of Velocity on Concentration

A large velocity caused the concentration profile to shift downstream with the peak concentration moving faster along the x-axis. The substance moved from the source move quickly and the peak of the concentration curve was located further from the source at a given time

When the velocity is small advection is less dominant. A small velocity meant the substance moved more slowly along the flow direction. The concentration peak was more downstream more gradually. The substance spent more time in the system allowing for more diffusion and dispersion to occur. The concentration was wider and less steep. The peak was more spread out across the flow direction because the substance is diffusing and dispersing over a larger area as it moves downstream

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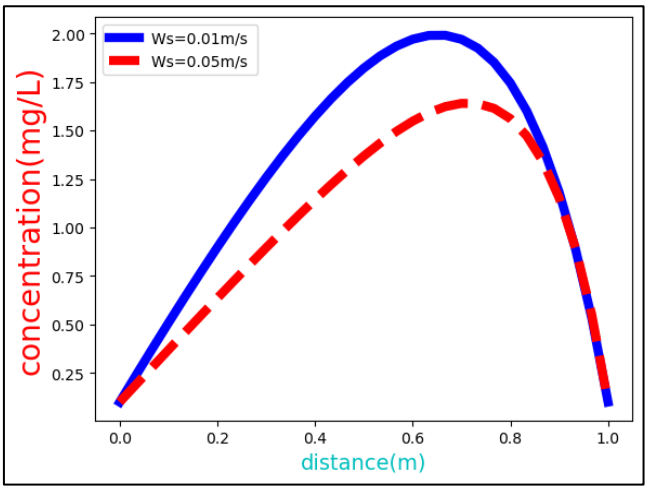


Fig 5 Influence of Settling Velocity on Concentration

Settling velocity is the rate at which particles sink through the water column due to gravity. Higher settling velocity accelerated the removal of heavy metals from the water column as they deposited onto the river bed. From the graphs, higher settling velocity acted as a sink term reducing the heavy load in the water column but concentrating it in the sediments. Lower settling velocity enhanced transport and distribution, increasing the exposure of aquatic organisms to heavy metals over larger areas. It allowed particles to remain suspended longer leading to greater transport downstream and higher concentration in the water column.

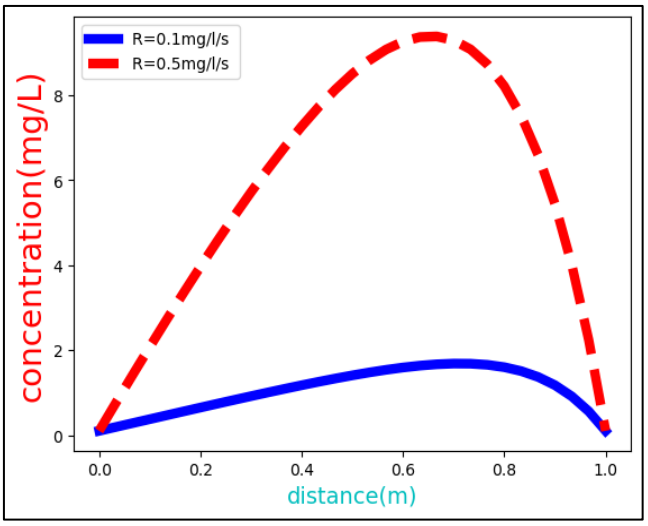


Fig 6 Influence of Resuspension Rate on Concentration

Figure 6 shows that high resuspension rate led to increase in heavy metal concentration in water column

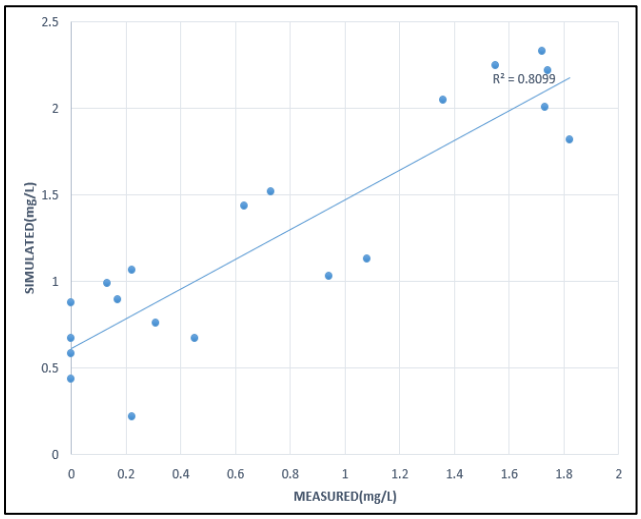


Fig 7 Comparison of Measured and Model Results of Iron in Water During the Wet Season

Figure 7 indicates that there was a strong positive relationship between the measured and simulated concentrations of iron metal in water and Zinc in sediments respectively. The correlation coefficient was 0.899 iron metal in water confirming that the models can be considered reliable for prediction of heavy metal concentration in river water and sediments.

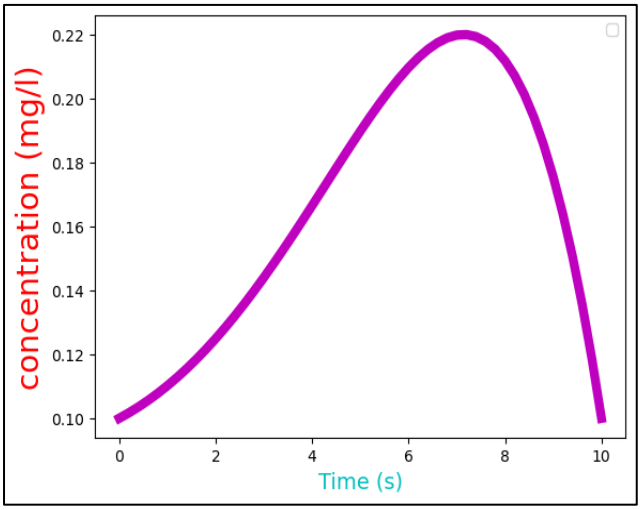


Fig 8 Temporal Variation of Concentration

Graph 8 indicated that heavy metal concentration increased with time This could indicate an ongoing pollution source that continuously added heavy metals into the river. Advection and diffusion effects (Heavy metals may have moved more downstream causing higher concentration at certain location over time)

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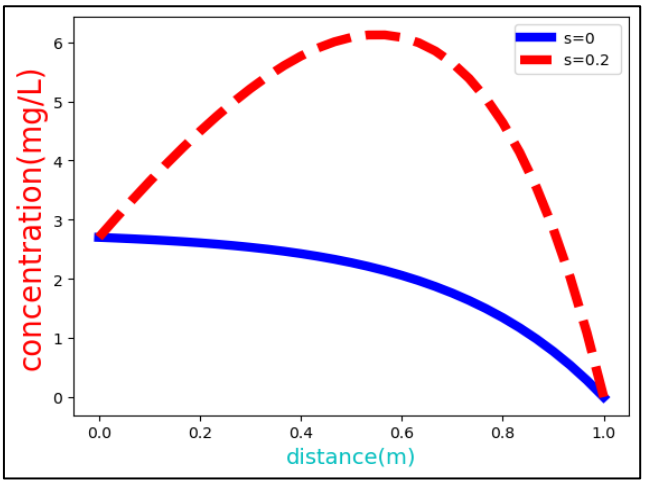


Fig 9 Spatial Variation of Iron Concentration

Figure 9 shows that the concentration of iron in river water decreases as it moves further away. The iron diffuse from a primary source point, when a source is added, the iron is introduced at a specific distance before the concentration reduces.

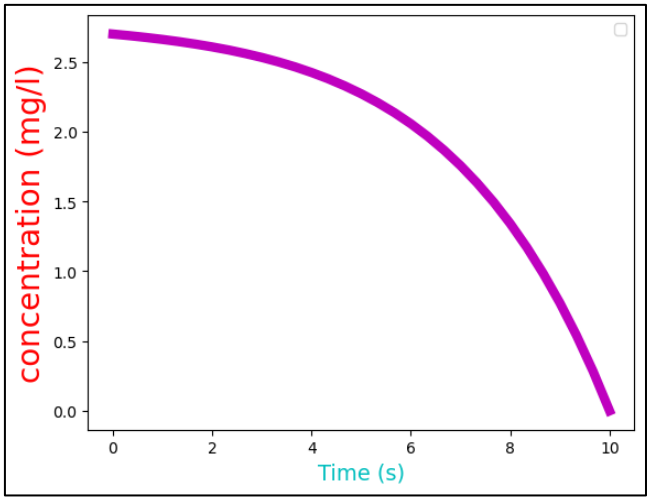


Fig 10 Temporal Variation of Iron Concentration

The model was applied to show the spatial and temporal variation of concentration of iron using the data that had been collected from the field in Rupingazi river Embu county Kenya. The variation of iron concentration was as indicated in figure 9 and figure 10.

V. CONCLUSIONS

Advection, diffusion, resuspension rate and settling were being quantified. The information can guide the prediction of how far and quickly a pollutant can move. Understanding the flow dynamics was crucial to predicting heavy metal concentration at various locations and times The model can identify areas of the river where heavy metal concentrations are likely to be highest allowing for targeted monitoring and remediation efforts. Model can provide insights into which parameters most strongly influence the results.

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