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ORIGINAL RESEARCH ARTICLE

NUMERICAL MODELING OF HEAVY METALS IN RIVERINE SYSTEMS IN ELDORET, UASIN-GISHU COUNTY, KENYA.

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ABSTRACT
Heavy metals are gradually being added into water resources due to the rise in Municipal, industrial and agricultural activities. The fate of heavy metals being in water systems is mainly controlled by transport processes. Transportation of heavy metals by rivers can be both as metal in solution and adsorbed to suspended solids. A one-dimension environmental model has been developed in this work to simulate the transport of heavy metals discharged into a riverine system. The model has been developed by solving a mass transport equation. The governing equation describing the mathematical model is discretized implicitly by the integral finite difference method (IFDM). Heavy metal samples were collected along River Sosiani as it passes through Eldoret town. The concentration levels of copper, zinc and lead metals were analysed. The maximum values obtained for copper, zinc and lead were 0.35 mg/l, 0.48 mg/l and 0.23 mg/l respectively. The World Health Organisation (WHO) standards for drinking water are 0.2 mg/l, 0.05 mg/l and 0.5 mg/l for copper and lead and zinc respectively. The concentration values for copper and zinc were above WHO standards. The model developed in this study was validated for spatial variation of heavy metal concentration where field parameters like flow rate and dispersion coefficient were varied. The model also considered multiple sources of pollutants. There was close agreement between the measured and the simulated values. The results obtained in this study show that the model demonstrated good capabilities for describing spatial characteristics of heavy metals in riverine systems. It can be concluded that by using mass balance model it is possible to simulate heavy metal transport in surface waters for risk assessment purposes and is shown to be a useful management tool in monitoring water quality in River Sosiani.

Keywords: Environmental model; contaminants; Integral Finite Difference Method; Mass transport equation; Water quality.

1.0 Introduction

There is a great concern of the presence of heavy metals in the environment because of their nature in toxicity, increase in discharge, and negative impact on aquatic life and human beings. Heavy metals do not degrade, volatilize or decay and therefore transport processes control their fate in natural waters (Novotny and Salomons, 1995). Their concentration in the dissolved phase as well as of that adsorbed to the sediments are dependent mainly on the levels of metal concentration flowing in the water stream (Pintilie *et al*., 2007).

Heavy metals are gradually and progressively being added into the water sources. Their origin in rivers can be from either Point or diffuse sources which vary in both time and space (Hermond and Fechner, 1994). Point sources release pollutants at well-defined places along the watercourse while non-point sources are distributed along the watercourse. Point sources examples are effluents from factories and sewage treatment facilities while those of diffuse sources include agricultural run-off, mining waste and industrial activities. Sources can further be divided into continuous and instantaneous sources. Continuous sources release pollutants to the river for an extended period of time. Instantaneous sources on the other hand discharge pollutant mass to the river over very short periods. An example is an accidental spill where pollutants enter a river in a matter of minutes (Bencala and Runkel, 1995).

The analytical methods used by environmentalists to assess the quality of water are too general to predict the effect of contaminants released in rivers over a period of time. Direct measurements are expensive since they must be taken periodically and are affected by the prevailing conditions which cannot be generalized to represent an area constantly. In order to understand the river transport behaviour, a long-term programme requires establishment.

There is the extensive use of mathematical modelling in the management of water resources for hydrological purposes (Coulthard and Macklin, 2003). It is now a useful management tool for forecasting the effect of different management policies. A powerful and essential tool for the solution of problems associated with water resources is provided by numerical methods (Wood, 1983). Advection-dispersion equations which are in form of partial differential equations are used by numerical models which have specific initial and boundary conditions depending on the type of the source releasing the pollutants. This allows the numerical model to predict points and multiple kinds of release.

This research focuses on the development of a one-dimensional model which solves the mass transport equation which governs the concentration of heavy metals in riverine systems. The transport equation which incorporated the sources and sinks and the adsorption terms are solved so as to predict the concentration variation of heavy metals in rivers.

2.0 MATERIALS AND METHODS

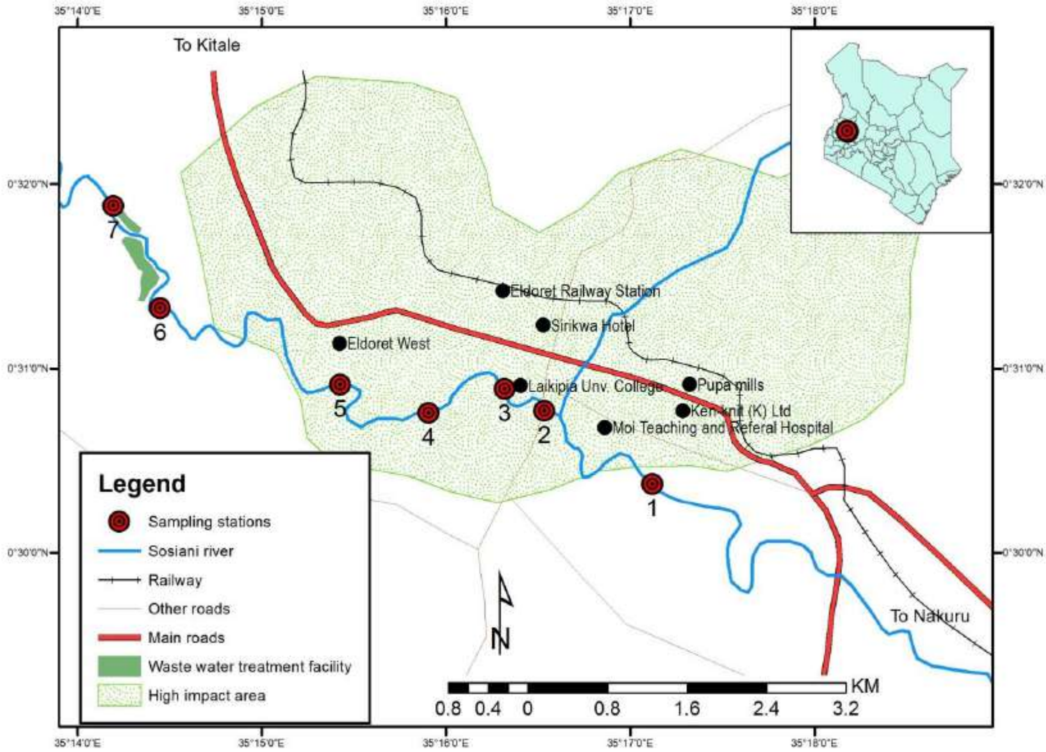
2.1 Study area

Sosiani River passes through Eldoret town which is the largest city in Uasin-Gishu County, Kenya. The river is facing alarming levels of pollutants originating from both point and non-point sources mainly caused by anthropogenic activities such as urbanization, industrialization, agriculture, municipal sewage disposal, population pressure and settlements within the Uasin-Gishu area. The study area is outlined in Fig.1

2.1.1 Sample collection and analysis

Water samples were collected from a section of Sosian River where it passes through Eldoret town. Samples were taken from each of the seven stations using 0.5 L plastic bottles which had been cleaned earlier. The plastic bottles were rinsed with the river water, before collecting the samples. Without infiltration, the collected water samples were digested with 5 ml of nitric acid to pH < 2. The acid was added to acidify and preserve the water samples.

To prepare the samples for analysis, a sample from each sampling bottle was mixed thoroughly by shaking. A 50 ml of water sample was pipetted into a digestion flask. The sample was brought to boiling slowly on a hot plate controlling the temperature at 70^0 C evaporating it to about 15 ml, followed by addition of 3 ml concentrated nitric acid and 5 ml concentrated sulphuric acid while continuing heating until the solution cleared and brown fumes were no longer evident. The digested samples were cooled and filtered then topped to the mark with de-ionized water. Using Atomic Absorption Spectrophotometer the digest was analyzed for total copper, zinc and lead metals.



(1. Fig 1: Study area and sampling sites location along Sosiani River.
(2. Moi Teaching and Referral Hospital (MTRH), 2.Langas bridge, 3. Pioneer, 4.Kipkaren, 5. West Indies, 6.Kipkenyo dumpsite 7. Waste Water Treatment Facility (WWTF))

2.1.2 Hydrodynamic model

In surface waters, the most commonly used models fall under the classification of the equations of shallow waters, in which the assumption is that the flow is shallow relative to the dimensions of the problem in consideration. The flow is considered as one-dimensional and the velocity is constant over a cross-section, the level of the water is horizontal across the section and the cosine of the angle made by the bed's and the horizontal is given as unity since the average slope of the beds channel is too small. The density is also constant in time and in space. The flow rate is constant such that only the velocity changes with change in the cross-section area of the section.

The hydrodynamic model based on one-dimensional partial differential equation in steady-state describing the concentration of a constituent in a one horizontal dimension system as a function of space with adsorption effect is given as (Singh 2013);

$$D\frac{\partial^2 C}{\partial x^2} - AU\frac{\partial C}{\partial x} \pm P - kC = 0 \qquad (1)$$

Where C= concentration, mg/l, x= streamwise distance, U= mean longitudinal velocity of river flow, m/s, D = dispersion coefficient, m^2/s, A= cross-sectional area of the river, P= external sources/sinks, mg/s and K = adsorption value. A= cross-sectional area of the river, In each side of the model grid, a gradient of zero heavy metal concentration was stated as boundary conditions except at the source zone. Velocity was taken constantly over a cross-section.

2.1.3 Numerical discretization and solution.

Discretization of the governing equations is in space and time dimensions allow the reduction of partial differential equation to simultaneous solution of a set of algebraic equations (Konikow, 1996). The partial differential equation governing pollutant transports in surface water flow is discretised using finite difference method (FDM). On discretizing the advection and the dispersion terms equation (1) becomes;

$$D\left(\frac{C_{j+1}-2C_j+C_{j-1}}{\Delta x^2}\right)-AU\left(\frac{C_{j+1}-C_{j-1}}{\Delta x}\right)-KC_j=0 \qquad (2)$$

Where C_j is the concentration in block j, C_{j+1} is the concentration in the next block, C_{j-1} is the concentration in the previous block, A is the cross-section area of the river, U is the longitudinal velocity of the river, D is the longitudinal dispersion coefficient, K is the adsorption value.

Implementation of the algorithms obtained from discretised solutions of the governing equations in equation 2 was done using a computer program. The modules were written using FORTRAN 77 language. The program was to determine the concentration of the heavy metals in the next space step. The problem under study comprised of the input information, the mathematical algorithm and the output data. The input data consisted of information like the size and properties of the river, initial and boundary conditions on the concentration of heavy metals. The grid designed for use in this study was Cartesian and node centred. The number of blocks in the entire grid was arbitrary. The boundary conditions were specified as zero concentration gradient for metal concentration at each side of the model grid except for the source zone.

The mathematical model involved the procedure for solving the resulting algorithm of the governing equations. Whereas the output data was the results obtained after the execution of the computer program.

3.0 RESULTS

The heavy metal concentration levels of samples collected along River Sosiani for zinc, lead and copper and the simulated values from the model are shown in Table 1;

Table 1. Total concentrations of heavy metal in water samples and the simulated values.

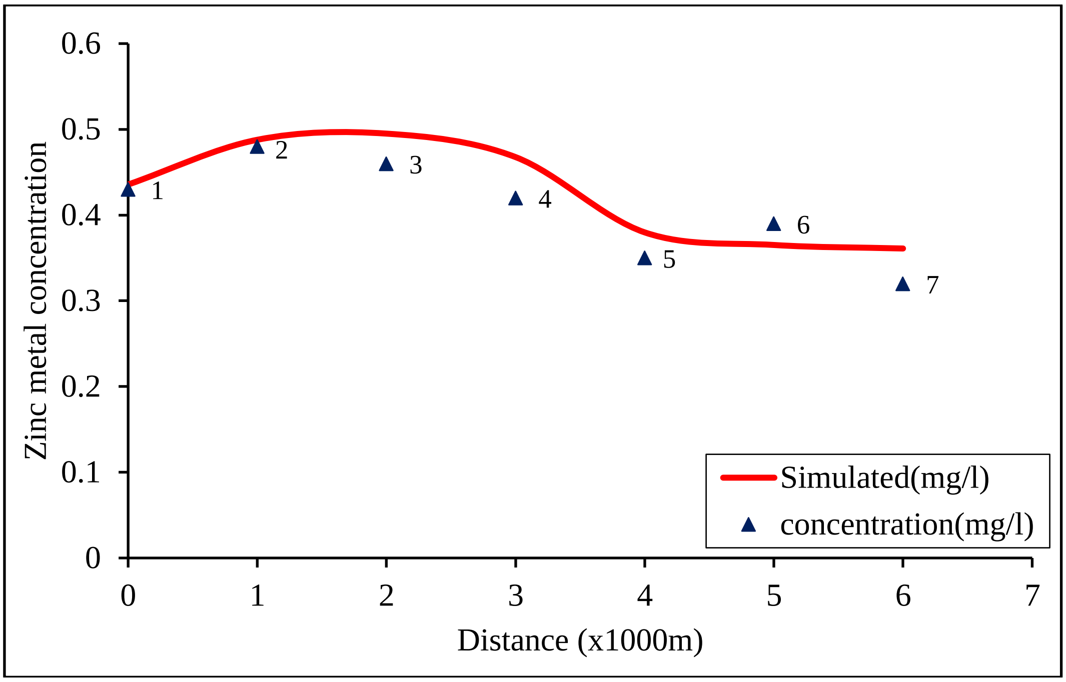
Distance (x1000m)	Zinc		Lead		Copper	
	Simulated mg\l	Measured mg\l	Simulated mg\l	Measured mg\l	Simulated mg\l	Measured mg\l
0	0.4356	0.43	0.1366	0.10	0.3520	0.32
1	0.4878	0.48	0.2091	0.23	0.2686	0.28
2	0.4950	0.46	0.1434	0.08	0.3766	0.35
3	0.4676	0.42	0.0881	0.06	0.3430	0.30
4	0.3798	0.35	0.0709	0.07	0.2384	0.27
6	0.3651	0.39	0.0910	0.09	0.3092	0.30
7	0.3710	0.32	0.1140	0.12	0.2745	0.22

*The sampling site Moi Teaching and Referral Hospital (MTRH) corresponds to the 0 Km in the research area.

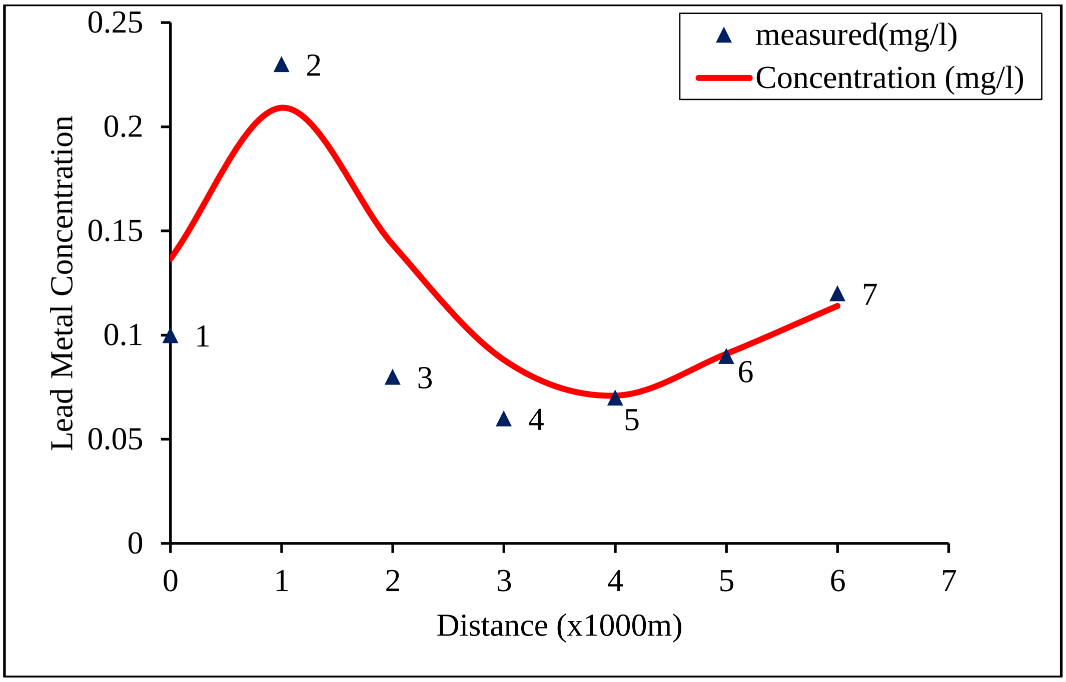
3.1 Model Validation

The model was compared with field-measured concentrations of copper, zinc and lead in River Sosiani. The simulator was validated for spatial variation of heavy metal concentration considering multiple sources of heavy metal pollutants. The initial heavy metal level of 2 mg/l was set in the entire model domain. The initial value of 2 mg/l was chosen to improve agreement with experimental outcomes. Field parameters like the dispersion coefficient, flow rate value and adsorptions values were varied by trial and error using graphical considerations in each case of the heavy metal concerned to obtain a match for simulated and measured values for specific metal. The measured data was approximated to correspond to the grid cells in the grid system of the simulated data for each case. Reducing the space steps, Δx improved the simulated data results giving more accurate curves, though it increased the computation time.

Figures 2 to 4 shows the match of the simulated data and the measured values of the three metals accessed i.e. zinc, lead and copper respectively;



(3. Fig.2. . Match of field data and the simulated breakthrough curve for zinc Concentration.
(4. (1. Moi Teaching and Referral Hospital (MTRH), 2. Langas bridge, 3. Pioneer, 4. Kipkaren, 5.West Indies, 6.Kipkenyo dumpsite, 7. Waste Water Treatment Facility (WWTF)).



(5. Fig.3. Match of field data and the simulated breakthrough curve for lead Concentration.
(6. (1. Moi Teaching and Referral Hospital (MTRH), 2. Langas bridge, 3. Pioneer, 4. Kipkaren, 5.West Indies, 6.Kipkenyo dumpsite, 7. Waste Water Treatment Facility (WWTF)).

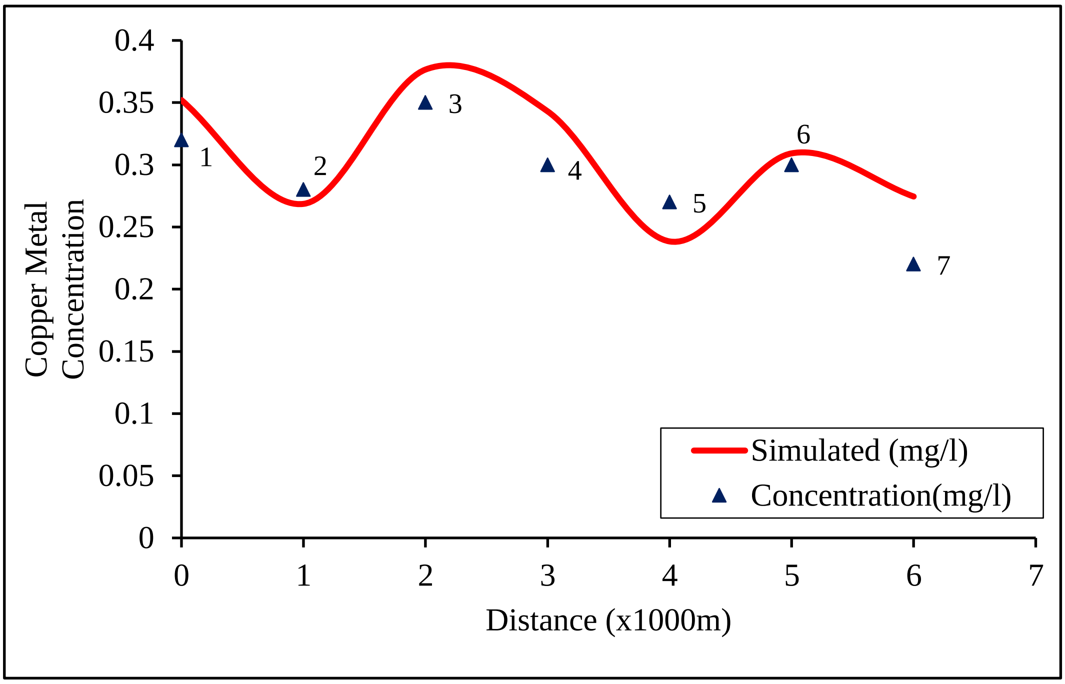


Fig.4. Match of field data and the simulated breakthrough curve for copper concentration.
(7. (1. Moi Teaching and Referral Hospital (MTRH), 2. Langas bridge, 3. Pioneer, 4. Kipkaren, 5.West Indies, 6.Kipkenyo dumpsite, 7.WWTF)

Correlation of simulated and measured values was plotted and correlation coefficients of 0.88789, 0.864395 and 0.79068 for zinc, lead and copper respectively were obtained.

4.0 DISCUSSION AND CONCLUSION

The maximum values obtained for copper, zinc and lead were 0.35 mg/l, 0.48 mg/l and 0.23 mg/l respectively. The WHO standards for drinking water are 0.2 mg/l, 0.5 mg/l and 0.05 mg/l for copper and zinc and lead respectively (WHO, 2008). The concentration values for copper and zinc were above WHO standards recommended for drinking water. Hence the water from River Sosiani is not safe for use domestically. There is a significant spatial variation of the lead concentration which can be attributed to the high degree of adsorption exhibited by lead on clay soils (Fernando *et al.,* 2019)

Generally, observation results agree with simulation results for the dissolved heavy metal transport. This proves the usefulness of the model as a possible management tool in monitoring water quality in the River Sosiani. The model can be regarded as a basic tool for assessing heavy metal dispersion in the riverine systems. The results obtained in this study show that the model can be a useful tool for describing spatial characteristics of heavy metal transport in riverine systems.

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