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INVESTIGATION OF BEHAVIOR AND TRANSPORT OF HEAVY METALS BY NUMERICAL MODELLING

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Abstract

In recent years, the importance of investigation of behavior and transportation of heavy metals in water systems that are dangerous for human health with toxic characteristics has been increasing and hence work on developing new methods and models are undertaken. The aim of this study is to implement a heavy metal model in a three - dimensional numerical model, ECOMSED in order to investigate the behavior and transportation of heavy metals. ECOMSED is capable of predicting flow circulation, salt and non-cohesive sediment transportation, deposition and re-suspension with hydrodynamic and sediment modules. In the heavy metal model adopted, the behavior of heavy metals was investigated by taking into consideration the effect of partition coefficient (k_d) on particulate and dissolved heavy metal concentrations. The model is set up for a simple open channel test case and the effect of flow structure, partition coefficient, concentration of suspended sediment and bed load on particulate and dissolved heavy metal concentrations are investigated. This study is an attempt in modeling transportation of heavy metals and the results found to be encouraging for this initial state.

Keywords: Heavy metals; behavior and transportation of heavy metals; numerical modeling; partition coefficient.

1. Introduction

As a result of continuing increase of economic activities in gulf, lake, river, estuary and coastal waters, environmental problems and especially pollution problem has been increasingly emerging. In recent years, a significant increase in the number of studies related to the development of water quality models used in prediction of the spatial and temporal distribution of the quantity and quality of a pollutant constituent has been observed. Particularly with the help of numerical model studies in this area, the aim is to predict the spatial and temporal distributions of the concentrations of heavy metals harmful to human health present in water bodies either in dissolved form or particulate form absorbed onto sediment.

Heavy metals are of particular concern in aquatic environment because of their toxicity, persistence, bioaccumulation and carcinogenicity [1]. In case of exceeding certain values of concentrations of heavy metals, toxic and carcinogenic properties can be seen not necessarily in the form of large doses but resulting from bioaccumulation [2]. The metabolism of human beings can be affected both physically and psychologically with the accumulation of heavy metals taken from nutrition chain and drinking water. The concentrations of various heavy metals must therefore be kept under control within certain definite limits. Many vital health problems would otherwise be inevitable over time when required attention to the concentrations and transportations of heavy metals in water systems that are harmful to human health is not given and important measures aren't taken.

Heavy metal pollution, measurements of evaluation as well as the use of new emerging numerical model convections enable better understanding of the behavior of heavy metals without harming the environment and efficient methods of struggle can thus be determined and applied over time. With the developments in computer technology and numerical modeling techniques, the goal of present studies is to develop numerical models enabling better understanding of heavy metal behavior and capable of predicting the transportation of heavy metal pollution validated with field data.

With regard to environmental pollution, metals can be classified according to three criteria as (1) non-critical, (2) toxic but very insoluble or very rare and (3) very toxic and relatively accessible. For instance sodium (Na), potassium (K), magnesium (Mg) and calcium (Ca) are non-critical since they are widely present and not considered as trace metals but as macro-elements while nickel (Ni), copper (Cu), zinc (Zn), cadmium (Cd), mercury (Hg) and lead (Pb) can be considered very toxic and relatively accessible metals [1],[3].

Essential trace metals become toxic when the nutritional supply becomes excessive. A metal in trace amounts is essential when an organism fails to grow in the absence of that metal. However, the same trace metal is toxic when concentration levels exceed required levels [3].

Heavy metals can be present in the water column in two phases, namely dissolved and particulate phase [4]. The dissolved metal phase changes to the particulate phase in the water column principally according to a number of possible pathways, for example sorption onto clay minerals, sorption and co-precipitation on hydrous Fe/Mn oxides and sorption and complexation on metals by humic substances [1].

The aim of this study is to investigate the behavior and transportation of heavy metals by implementing a heavy metal model in ECOMSED, which is a three - dimensional numerical model [5]. With hydrodynamic and sediment modules ECOMSED, is capable of predicting flow circulation, salt and non-cohesive sediment transportation, deposition and re-suspension. Thus, the behavior of heavy metals can be investigated by taking into consideration the effect of partition coefficient (k_d) on particulate and dissolved heavy metal concentrations by considering various conditions for hydrodynamic, salt and non-cohesive sediment. The model is set up for a simple open channel test case and the effect of flow structure, partition coefficient, concentration of suspended sediment and bed load on particulate and dissolved heavy metal concentrations are investigated.

2. Behavior and Partioning of Heavy Metals

The dissolved and particulate metal phases are transported differently. It is therefore important to understand the mechanisms effective on the behavior, phases and transport of heavy metals. All fine grained materials with a large surface area are capable of accumulating heavy metal ions at the solid-liquid interface as a result of intermolecular forces which is termed as adsorption [1]. Many researches were carried out about the dissolved and particulate heavy metals [3],[6],[7],[8],[9],[10].

Particulate material within water bodies such as estuaries is transported as both bed load and in suspension. The suspended material is affected by turbulent diffusion and vertical settling. The settling velocity of any particle will depend on its size, morphology and specific gravity [1].

When metals are introduced into water containing suspended particulate matter (SPM), a portion of the metal is dissolved in the water and the remainder is absorbed onto surface of the SPM. The distribution of the metal fractions between these two phases can be described by a partition coefficient, k_d, defined as:

$$k_d = \frac{P}{C} \tag{1}$$

where P is the concentration of heavy metal absorbed on suspended sediments (μg/L) and C is the concentration of heavy metal dissolved in the water column (μg/L). The coefficient k_d is function of spatially varied water chemistry and is notoriously difficult to quantify in marine waters. It is well documented and generally accepted that there is a strong functional relationship between k_d and salinity. In many studies only the influence of salinity are considered and other direct water chemistry effects are ignored [11]. In an estuary, where fresh and salt water mix, changes in the dissolved metal concentration are known to occur within the water column, with the dissolved metal concentrations increasing with increasing salinity [3].

[12] describes the application of the k_d concept to the study of heavy metal desorption in the Humber Estuary. Heavy metal solid-solution partitioning, represented by k_d was studied along the salinity gradient of the Humber Estuary. In a study by [13], a depth averaged velocity and sediment transport model (DIVAST) of the Humber Estuary was used which also modelled salinity and sediment transportation. In [10] a review of partition coefficients derived from field measurements was conducted. Equilibrium k_d for Cd, Cr, Cs and Zn were determined for the Clyde, Tweed, Dee, Humber and Tamar estuaries from field measurements gathered from several studies. The dependence of the k_d on salinity was then explored. It was found that there is a general reduction in partitioning with increasing salinity. In a study by [14], the transport of suspended sediment over intertidal mudflats was investigated as part of the LOIS program at the upper shore of Spurn Bight in the Humber estuary.

Especially in the last two decades many numerical studies have been carried out for prediction of heavy metal concentrations and transportations among some of which are [13], [15], [16], [17], [18], [19], [20], [21] and [22].

3. Methodology

Three-dimensional numerical model ECOMSED is used to predict velocities and non-cohesive suspended sediment fluxes. The parameters needed for the prediction of pollutant fluxes are the flow depths and velocities which are required for pollutant transport in the dissolved phase, suspended sediment concentration which is required for pollutant fluxes in the particulate phase, bed elevation, required to determine water column-bed exchange of sediment and salinity with which to predict the partition coefficient variation.

3.1. Hydrodynamic Model

The ECOMSED is an integrated three-dimensional hydrodynamic, wave and sediment transport model designed to simulate time-dependent distributions of water levels, currents, temperature, salinity, tracers, cohesive and non-cohesive sediment and waves in marine and freshwater systems. ECOMSED uses an orthogonal curvilinear coordinate system, greatly increasing model efficiency in treating complex topography and irregularly shaped coastline. It consists of various modules such as the ECOM hydrodynamic module and the SED sediment transport module. The governing hydrodynamics equations which are the continuity and the Reynolds Averaged Navier-Stokes equations with hydrostatic pressure assumption and Boussinesq approximation are given in orthogonal curvilinear coordinate system with sigma co-ordinate in vertical direction as

$$h_1 h_2 \frac{\partial \eta}{\partial t} + \frac{\partial}{\partial \xi_1}(h_2 U_1 D) + \frac{\partial}{\partial \xi_2}(h_1 U_2 D) + h_1 h_2 \frac{\partial \omega}{\partial \sigma} = 0 \tag{2}$$

$$\begin{aligned}
&\frac{\partial (h_1 h_2 D U_1)}{\partial t} + \frac{\partial}{\partial \xi_1}(h_2 D U_1^2) + \frac{\partial}{\partial \xi_2}(h_1 D U_1 U_2) + h_1 h_2 \frac{\partial (\omega U_1)}{\partial \sigma} \\
&+ D U_2 \left(-U_2 \frac{\partial h_2}{\partial \xi_1} + U_1 \frac{\partial h_1}{\partial \xi_2} - h_1 h_2 f \right) \\
&= -g D h_2 \left(\frac{\partial \eta}{\partial \xi_1} + \frac{\partial H_0}{\partial \xi_1} \right) - \frac{g D^2 h_2}{\rho_0} \int_\sigma^0 \left[\frac{\partial \rho}{\partial \xi_1} - \frac{\sigma}{D} \frac{\partial D}{\partial \xi_1} \frac{\partial \rho}{\partial \sigma} \right] d\sigma \\
&- D \frac{h_2}{\rho_0} \frac{\partial P_a}{\partial \xi_1} + \frac{\partial}{\partial \xi_1}(2 A_M \frac{h_2}{h_1} D \frac{\partial U_1}{\partial \xi_1}) + \frac{\partial}{\partial \xi_2}(A_M \frac{h_1}{h_2} D \frac{\partial U_1}{\partial \xi_2}) \\
&+ \frac{\partial}{\partial \xi_2}(A_M D \frac{\partial U_2}{\partial \xi_1}) + \frac{h_1 h_2}{D} \frac{\partial}{\partial \sigma}(K_M \frac{\partial U_1}{\partial \sigma})
\end{aligned} \tag{3}$$

$$\begin{aligned}
&\frac{\partial (h_1 h_2 D U_2)}{\partial t} + \frac{\partial}{\partial \xi_1}(h_2 D U_1 U_2) + \frac{\partial}{\partial \xi_2}(h_1 D U_2^2) + h_1 h_2 \frac{\partial (\omega U_2)}{\partial \sigma} \\
&+ D U_1 \left(-U_1 \frac{\partial h_1}{\partial \xi_2} + U_2 \frac{\partial h_2}{\partial \xi_1} - h_1 h_2 f \right) \\
&= -g D h_1 \left(\frac{\partial \eta}{\partial \xi_2} + \frac{\partial H_0}{\partial \xi_2} \right) - \frac{g D^2 h_1}{\rho_0} \int_\sigma^0 \left[\frac{\partial \rho}{\partial \xi_2} - \frac{\sigma}{D} \frac{\partial D}{\partial \xi_2} \frac{\partial \rho}{\partial \sigma} \right] d\sigma \\
&- D \frac{h_1}{\rho_0} \frac{\partial P_a}{\partial \xi_2} + \frac{\partial}{\partial \xi_2}(2 A_M \frac{h_1}{h_2} D \frac{\partial U_2}{\partial \xi_2}) + \frac{\partial}{\partial \xi_1}(A_M \frac{h_2}{h_1} D \frac{\partial U_2}{\partial \xi_1}) \\
&+ \frac{\partial}{\partial \xi_1}(A_M D \frac{\partial U_1}{\partial \xi_2}) + \frac{h_1 h_2}{D} \frac{\partial}{\partial \sigma}(K_M \frac{\partial U_2}{\partial \sigma})
\end{aligned} \tag{4}$$

where ξ_1 and ξ_2 are the arbitrary horizontal curvilinear orthogonal coordinates, respectively, σ is the vertical sigma coordinate, U_1 and U_2 are the velocity components along ξ_1 and ξ_2 directions, respectively, h_1 and h_2 are the computational grid sizes in ξ_1 and ξ_2 directions, respectively, η is the free surface, D is the total water depth, ρ_0 is the reference density, ρ is the in situ density, g is the gravitational acceleration, f is the Coriolis parameter, A_M and K_M are the horizontal and vertical eddy diffusivity of turbulent momentum mixing and ω is the vertical velocity component in sigma coordinate system given as

$$\omega = W - \frac{1}{h_1 h_2} \left[h_2 U_1 \left(\sigma \frac{\partial D}{\partial \xi_1} + \frac{\partial \eta}{\partial \xi_1} \right) + h_1 U_2 \left(\sigma \frac{\partial D}{\partial \xi_2} + \frac{\partial \eta}{\partial \xi_2} \right) \right] - (\sigma \frac{\partial D}{\partial t} + \frac{\partial \eta}{\partial t}) \tag{5}$$

in which W is the vertical velocity component in Cartesian coordinate system and t is the time. A second-order turbulence closure scheme developed by [23] is adapted in the module where all details of the model can be found in [23]. Mode splitting technique is used to solve the governing equations. Further details of the transformation of governing equations, turbulence model, boundary conditions and the solution technique of the equations can be found in [24].

3.2. Sediment Transport Model

The SED module of ECOMSED is the three-dimensional sediment transport model which simulates cohesive and non-cohesive sediments. The three-dimensional advection-dispersion equation for transport of sediment in Cartesian coordinate system is given as

$$\frac{\partial C}{\partial t}+\frac{\partial UC}{\partial x}+\frac{\partial VC}{\partial y}+\frac{\partial (W-W_s)C}{\partial z} = \frac{\partial}{\partial x}\left(A_H\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(A_H\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_H\frac{\partial C}{\partial z}\right) \tag{6}$$

where C is the suspended sediment concentration, U,V and W are the velocity components in x, y and z-directions, respectively, A_H is the horizontal diffusivity, K_H is the vertical eddy diffusivity and W_s is the sediment settling velocity. Output from SED module includes the spatial and temporal distribution of total suspended solids, water column concentrations of cohesive and non-cohesive sediments, bed fractions of cohesive and non-cohesive sediments, the mass of sediment deposited/eroded and subsequent change in bed elevations. Re-suspension of sediments from a non-cohesive sediment bed is based on the suspended load theory of [25], [26].

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3.3. Description of the Heavy Metal Model

In modelling heavy metals consideration has to be taken into account of the partitioning of the heavy metal between the dissolved and the particulate phases. This partitioning could be described in the form of the partition coefficient k_d given by Eq. (7).

$$\ln k_d^n = b\left[\ln(S^n+1)\right]+\ln k_d^0 \tag{7}$$

where k_d^n is the partition coefficient in cell n and S^n is the salinity in cell n, k_d^0 is the partition coefficient of the heavy metal in freshwater, is metal specific and is typically in the range 2000-200,000 l/kg. The constant b is determined experimentally and is typically in the range b = -0.5 to -1.5.

The heavy metal model was implemented into the existing ECOMSED model to enable the prediction of particulate and dissolved phase heavy metal concentrations and the exchange of contaminated sediments between the water column and the bed. A similar work was also carried out in which this metal geochemistry model algorithm was implemented into to a 2-D model, DIVAST [1]. Fig.1 shows a 1-D schema of the model working.

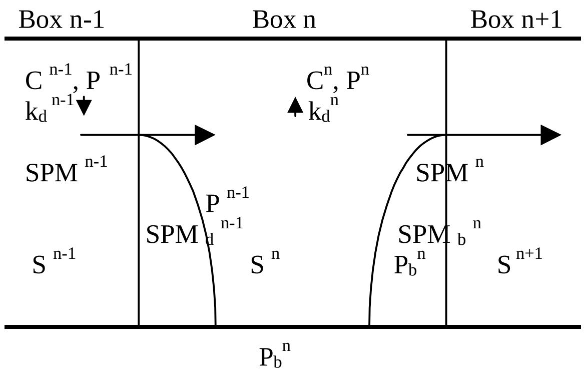

Figure 1: Box model of adjacent segments and governing parameters [1]

The main heavy metal processes occurring within the water column can be summarized as follows:
If there is a bed-water column transfer of sediment as a result of erosion/deposition, then as a result, the bed level adjustment (positive for erosion) could be shown to be

$$M_s^n = A^n \rho (h_{t,0} - h_{t,1}) \tag{8}$$

where M_s^n is the mass of re-suspended/deposited sediment in cell n, A^n is the plan area of cell n, ρ is the density of bed sediment and $(h_{t,0} - h_{t,1})$ is the bed level adjustment (positive for erosion/re-suspension).
If re-suspension occurs in cell n then M_s^n is positive and V^n the volume of the overlying water column in cell n is used to calculate the re-suspended sediment concentration. This concentration is given as:

$$SPM_b^n = M_s^n / V^n \tag{9}$$

where SPM_b^n is the suspended sediment concentration gained to water column by re-suspension from bed in cell n arising from the bed and M_s^n is the mass of re-suspended/deposited sediment.
If deposition occurs in cell n then M_s^n is negative and the deposited sediment concentration is given by:

$$SPM_d^{n-1} = M_s^n / V^n \tag{10}$$

where SPM_d^{n-1} is the suspended sediment concentration lost to bed of cell n by deposition.
The bed concentration is adjusted for the added metal by:

$$P_b^n = \frac{(M_b^n.P_b^{n0} - M_s^n.P^{n-1})}{(M_b^n + M_s^n)} \tag{11}$$

where P_b^n is the particulate concentration of bed sediment and particles re-suspended from bed in cell n, M_s^n is the mass of re-suspended/deposited sediment, M_b^n is the mass of bed sediment in cell n ($M_b^n=A^n\rho h^n$ where h^n is the thickness of the bed involved in erosion/deposition), P_b^{n0} is the original particulate concentration of bed sediment and P^{n-1} is the particulate concentration of metal in cell n-1 carried into cell n. The net input of total metal to the cell n can be shown to be of the following form:

$$C^{n-1} + SPM^{n-1}.P^{n-1} + SPM_b^n.P_b^n + SPM_d^{n-1}.P^{n-1} \tag{12}$$

where C^{n-1} is the dissolved concentration of metal in cell n-1 carried into cell n, P^{n-1} is the articulate concentration of metal in cell n-1 carried to cell n, SPM^{n-1} is the suspended sediment concentration in cell n-1 carried into cell n. $SPM_b^n.P_b^n$ is therefore the erosional/re-suspension term and $SPM_d^{n-1}.P^{n-1}$ is the depositional term. $SPM^{n-1}.P^{n-1}$ is the particulate metal input from the previous cell. For mass balance, this must equal the output to cell n+1.

$$C^{n-1} + SPM^{n-1}.P^{n-1} + SPM_b^n.P_b^n + SPM_d^{n-1}.P^{n-1} = C^n + P^n.SPM^n \tag{13}$$

where C^n is dissolved metal concentration in cell n carried into cell n+1, P^n is the resultant particulate concentration in cell n carried into cell n+1, SPM^n is the resultant suspended sediment concentration in cell n carried into cell n+1 where $SPM^n = SPM^{n-1} + SPM_b^n + SPM_d^{n-1}$.

The fraction of metals on re-suspending particles relative to the particles entering the cell from the adjacent cell due to particle advection is given as:

$$\alpha = \frac{P_b^n}{P^{n-1}} \tag{14}$$

and the fractional loss of suspended sediment concentration entering the cell by advection SPM^{n-1} but then being deposited on the bed is:

$$\beta = \frac{SPM_d^{n-1}}{SPM^{n-1}} \text{ (-ve)} \tag{15}$$

The dissolved metal concentration in cell n is therefore given by:

$$C^{n-1} + SPM^{n-1}.P^{n-1} + SPM_b^n.P_b^n + SPM_d^{n-1}.P^{n-1} = C^n + P^n.SPM^n \tag{16}$$

and the particulate metal concentration in cell n is:

$$P^n = k_d^n . C^n \tag{17}$$

The advective and dispersive transport of metals in the dissolved and particulate phases is modeled using standard conservative advection-diffusion equation with no decay terms.

4. Modeling analysis of behavior and transport of heavy metals

Once the heavy metal model was implemented into the three-dimensional numerical model ECOMSED, the modified model was firstly set up to simulate simplified and idealized one dimensional open channel flow. The channel was assumed to be infinitely wide, with a flat bottom. The influence of a range of flow field, salinity and suspended sediment concentrations and changes in their values on the behavior and transportation of heavy metals together with the influence of partitioning coefficient on particulate and dissolved heavy metal concentrations have been investigated. The change of metal concentration with k_d varying with distance, increasing the value of k_d, variation of k_d with salinity, suspended sediment concentration and metal input from bed sediment was investigated. Fig. 2 shows the open channel with rectangular cross-section and Fig. 3 shows the grid cells in horizontal plane.

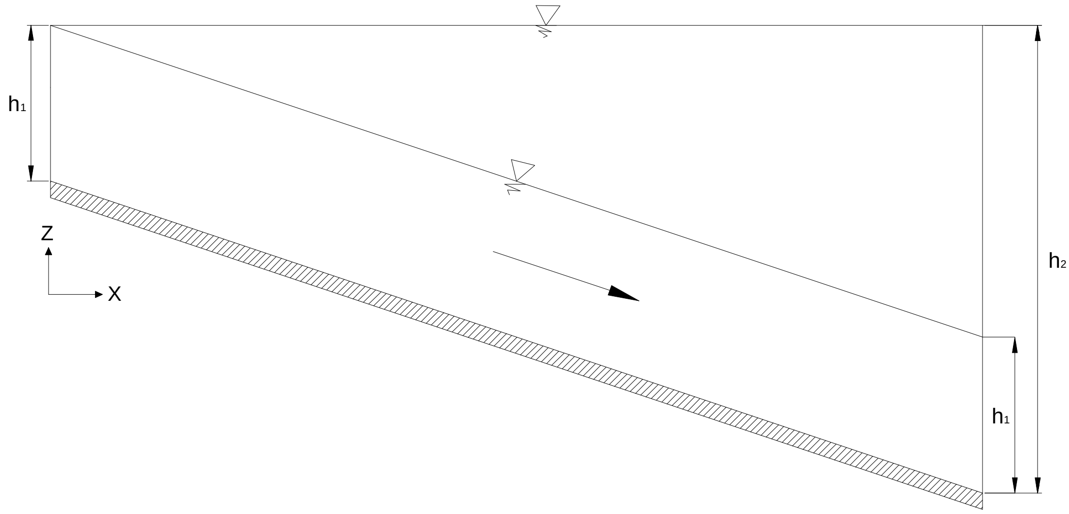

Figure 2: Longitudinal profile of the open channel used in the simulations

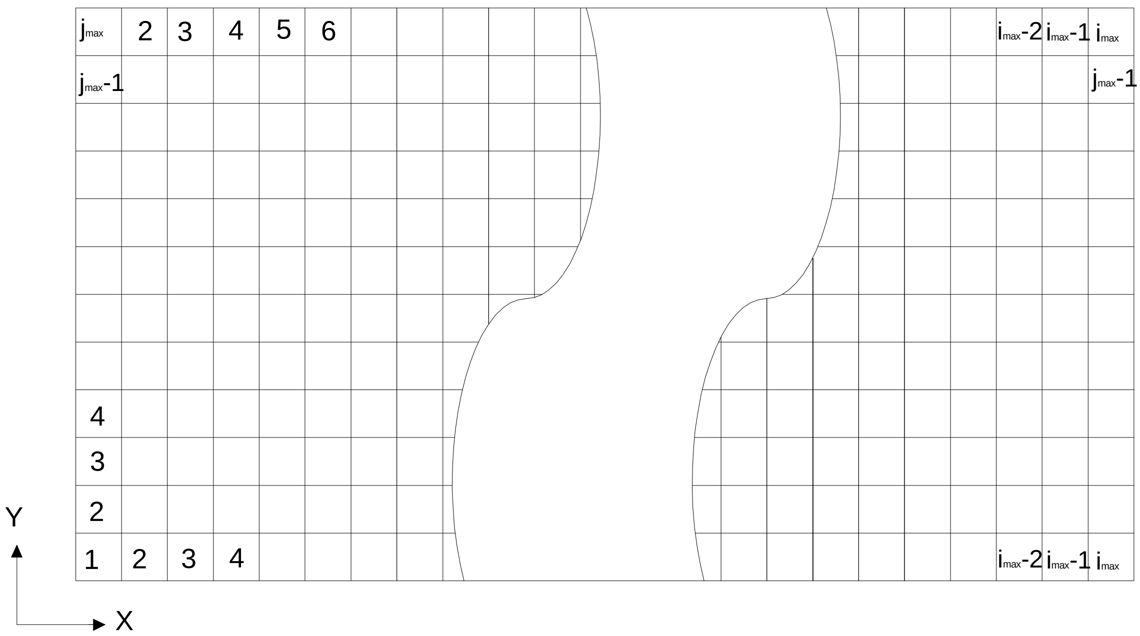

Figure 3: Computational domain in horizontal plane

In order to have a range of flow fields, three different channel slopes as 1:25000, 1:22500, 1:27500 were used and the depths and water elevations were chosen such that normal depth was obtained along the channel. For channel slopes of 1:25,000, 1:22 500 and 1:27 200, the depth below datum was 1.5m at distance 0.0m and the depth was 2.8m at distances 32 500m, 29250m and 35750m, respectively, for those sloped channels.

The simulation time was set to 62.5 hours where the time step for internal module was taken as 5sc, yielding 45000 computational time steps during simulations. In horizontal plane, the grid spacing along ξ_1 and ξ_2 directions was set to 500m. Thus for channel of slope 1:25000, 1:22500 and 1:27500, the number of grids along ξ_1 were 67, 61 and 74, respectively, while the number of grids along ξ_2 were 12 for all three channels. Free surface flow boundary condition was adapted at the entrance and exit of the channel. In the vertical direction, five layers were used for all three channels. At the beginning of simulation, all parameters were set to zero as initial condition.

When the influence of channel slope on the flow structure is investigated with three sloped channels given above, it is found that steady uniform flow is achieved such that the water surface is parallel to the channel bottom. The free surface is shown in Fig. 4 and the flow field in the surface, middle and bottom layer is given in Fig.5. Distribution of U velocity component along the centerline of the channel is illustrated in Fig.6. As can be seen from the figure, distribution of longitudinal U velocity is uniform along the channel centerline and logarithmic distribution of U is present along depth. It can thus be concluded that the numerical model is very much capable of simulating open channel flow.

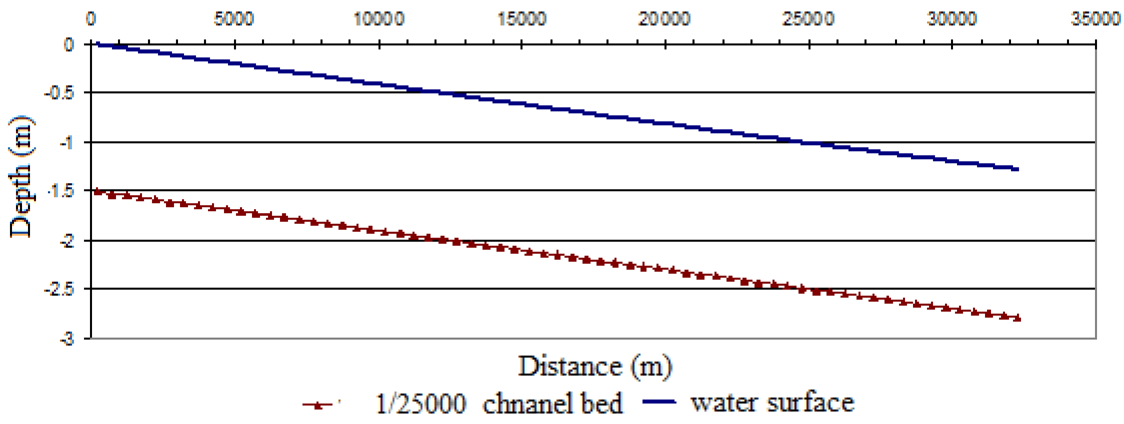

Figure 4: Channel bed and water surface in the channel of slope 1:25 000

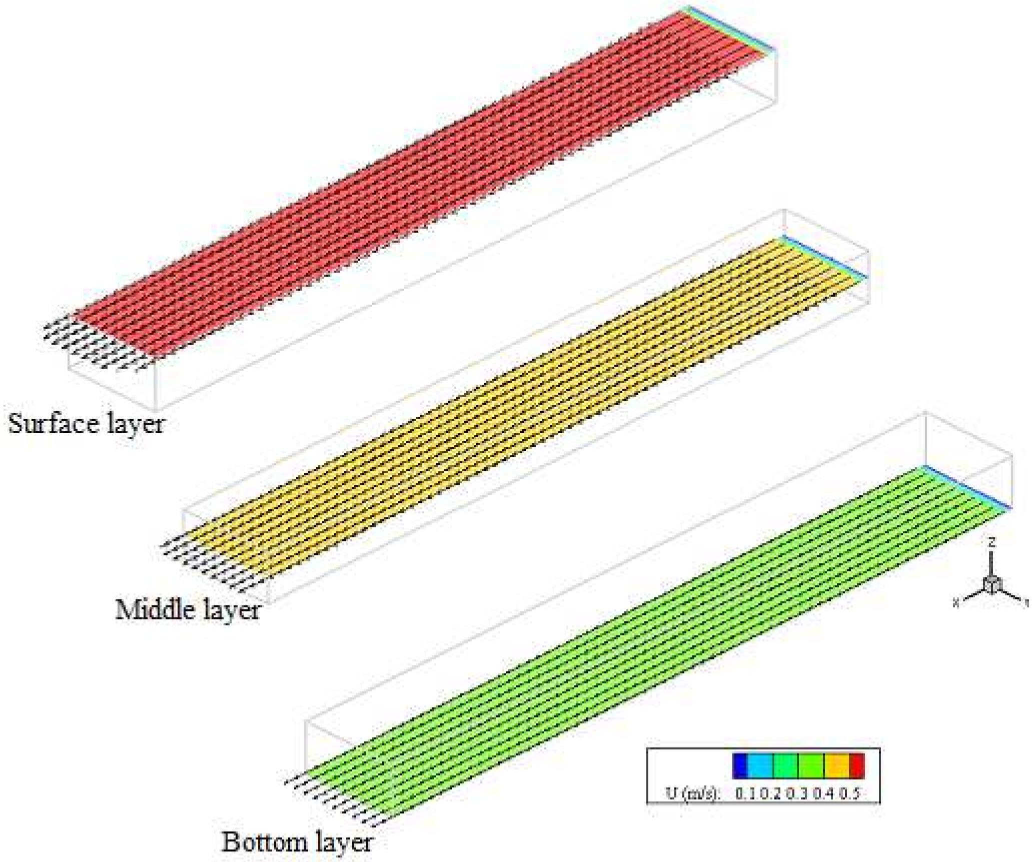

Figure 5:Distribution of longitudinal velocity component U in the surface, middle and bottom layers of channel of slope 1:25 000

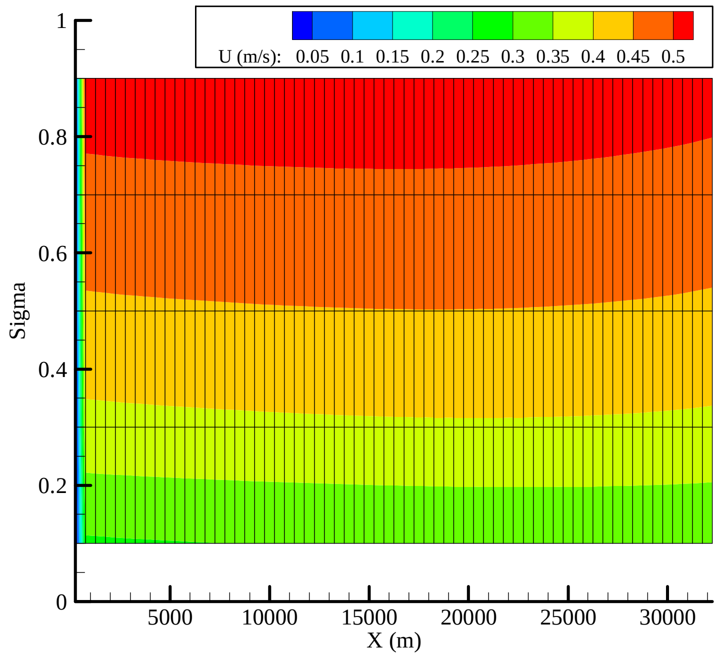

Figure 6:Distribution of longitudinal velocity component U along the centreline of the channel

Next, the model was set up to observe the ability of the model of simulating the variation of non-cohesive suspended sediment concentration (g/l). Thus, necessary boundary and initial conditions for sediment were introduced. The initial non-cohesive sediment thickness on the channel bottom was set to 2.0m and the non-cohesive suspended sediment concentration was set to zero at the outlet boundary condition. As can be seen in the Fig.7 and Fig.8, the distribution of non-cohesive suspended sediment shows variations along depth, as expected. It can be seen that non-cohesive suspended sediment transportation near surface was in the range of 0.001 – 0.01 g/l while it was in the range of 0.005 – 0.075 g/l near bottom.

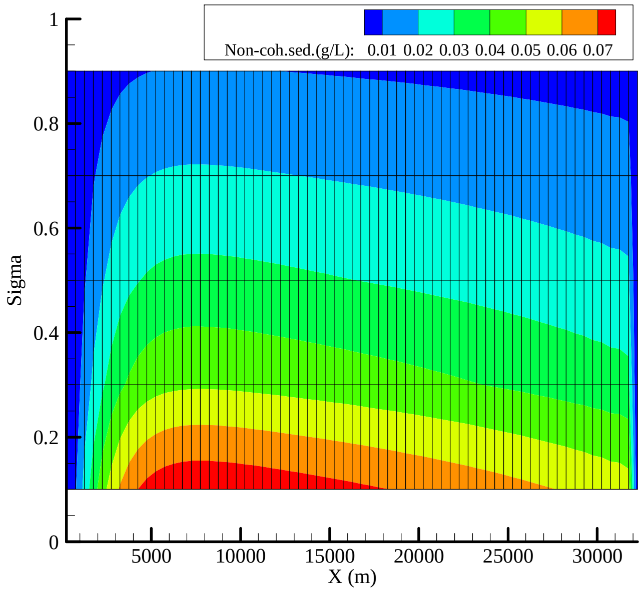

Figure 7: Distribution of non-cohesive suspended sediment concentration along longitudinal channel centerline in the vertical direction

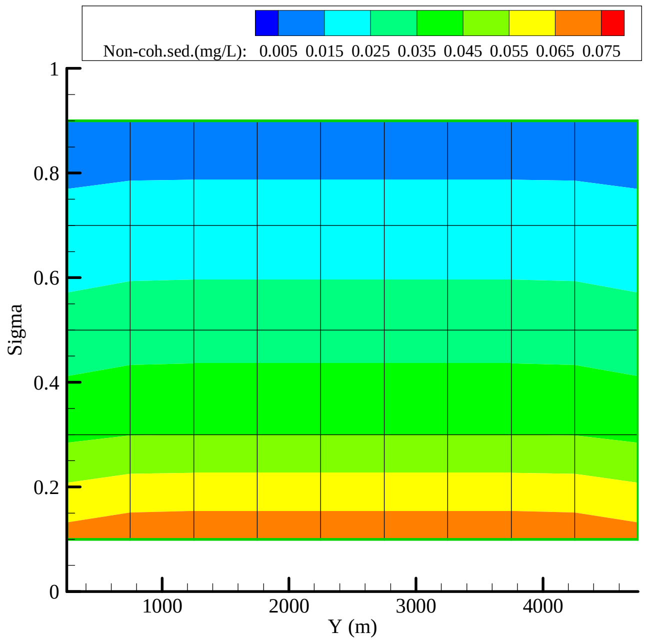

Figure 8: Distribution of non-cohesive suspended sediment concentration in the lateral channel section along depth

Next the model was set up to simulate the distribution of dissolved heavy metal concentration. As seen in Fig.9 and Fig.10, distributions of the dissolved heavy metal concentration varied along the depth of water where the concentration increased from surface to bottom. For instance, the dissolved heavy metal concentration at the surface was 0.475µg/l, while it was found to be 0.525 µg/l at the bottom.

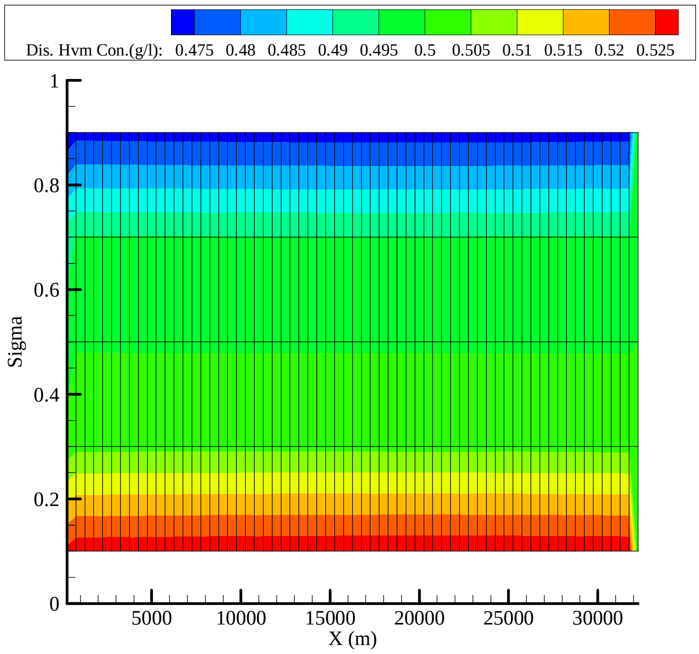

Figure 9: Distribution of heavy metal concentration in the vertical section along the longitudinal centerline of the channel section

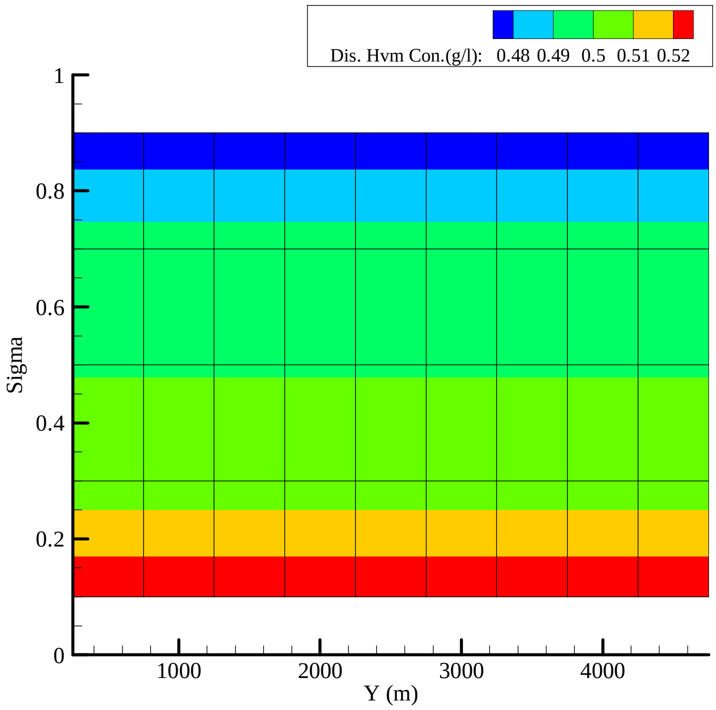

Figure 10: Distribution of heavy metal concentration in the vertical section along lateral cross section of the channel

The refined model was then set up to simulate the particulate concentration of heavy metals. In addition to the boundary and initial conditions given above, the values for partition coeffifient and the constant b were set to 6,600 l/kg and -1.50, respectively. Distribution of the particulate heavy metal concentration showed variations along depth as would be expected. However, the model should be set up for more complex test cases and then to a practical water body for validation.

5. Conclusions

In this study, a box model for heavy metal modeling is implemented into the ECOMSED, a three - dimensional numerical model to investigate the behavior and transportation of heavy metals. With hydrodynamic and sediment modules, ECOMSED, is already capable of predicting flow circulation, salt and non-cohesive sediment transportation, deposition and re-suspension. In the heavy metal module implemented, the behavior of heavy metals was investigated by taking into consideration the effect of partition coefficient (k_d) on particulate and dissolved heavy metal concentrations for various conditions for hydrodynamic, salt and non-cohesive sediment. The model is set up for a very simple open channel test case and the effect of flow structure, partition coefficient, concentration of suspended sediment and bed load on particulate and dissolved heavy metal concentrations were investigated. This study is an attempt in modeling heavy metal transportation and the results found to be encouraging for this initial state.

Acknowledgments

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Notations

A_n	plan area of cell n,
A_H and K_H	horizontal diffusivity, and vertical eddy diffusivity,
A_M and K_M	horizontal and vertical eddy diffusivity of turbulent momentum mixing and
b	constant,
P	the concentration of heavy metal absorbed on suspended sediments (μg/L),
C	suspended sediment concentration or the concentration of heavy metal, dissolved in the water column (μg/L),
C^n	dissolved metal concentration in cell n carried into cell n+1,
C^{n-1}	dissolved concentration of metal in cell n-1 carried into cell n,
D	the total water depth,
f	the Coriolis parameter,
g	the gravitational acceleration,
h_1 and h_2	the computational grid sizes in the ξ_1 and ξ_2 directions, respectively,
$(h_{t,0} - h_{t,1})$	bed level adjustment (positive for erosion/re-suspension),
i,j	Location of the grid cell in the x and y directions,
k_d	a coefficient which is function of spatially varied water chemistry and is notoriously difficult to quantify in marine waters,
k_d^n	the partition coefficient in cell n,

k_d^0	the partition coefficient of the heavy metal in freshwater,
m	time step,
M_s^n	mass of re-suspended/deposited sediment,
M_b^n	mass of bed sediment in cell n ($M_b^n = A_n \rho h^n$ where h^n is the thickness of the bed involved in erosion/deposition),
P_b^n	particulate concentration of bed sediment and particles re-suspended from bed in cell n,
P_b^{n0}	the original particulate concentration of bed sediment,
P^{n-1}	particulate concentration of metal in cell n-1 carried into cell n,
P^n	resultant particulate concentration in cell n carried into cell n+1,
S^n	salinity in cell n,
SPM^n	resultant suspended sediment concentration in cell n carried into cell n+1,
SPM_b^n	suspended sediment concentration gained to water column by re-suspension from bed in cell n arising from the bed,
SPM_d^{n-1}	suspended sediment concentration lost to bed of cell n by deposition,
SPM^{n-1}	suspended sediment concentration in cell n-1 carried into cell n,
$SPM_b^n.P_b^n$	the erosion/re-suspension term,
$SPM_d^{n-1}.P^{n-1}$	the depositional term,
$SPM^{n-1}.P^{n-1}$	the particulate metal input from the previous cell,
t	the time,
U,V and W	velocity components in x, y and z-directions, respectively,
$U_1$and U_2	the velocity components along the ξ_1 and ξ_2 directions, respectively,
V_n	the volume of the overlying water column in cell n,
W	the vertical velocity component in Cartesian coordinate system,
W_s	sediment settling velocity,
x and y	horizontal Cartesian co-ordinates ,
η	the free surface,
ρ_0	the reference density,
ρ	the in situ density or density of bed sediment,
σ	the vertical sigma coordinate,
ω	the vertical velocity component in sigma coordinate system,
ξ_1 and ξ_2	the arbitrary horizontal curvilinear orthogonal coordinates, respectively.

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