Heavy Metal Pollution and numerical Modeling in the River and Dam (Case study: Zarineh river and Bookan dam in Iran)

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Abstract: Based on the deep studies of existing mathematical models, a mathematical model that expresses the dynamic of transport and transformation of heavy metals in the rivers has been presented. In this model, the basic principles of chemistry in the environment, hydraulic and fluid transfer dynamics have been used as well as recent studies of researchers. The effects of sediment on the transfer and evolution of heavy metals pollution can be investigated by the proposed models. For example, the evolution and transport of heavy metal pollutants in a steady state flow containing sediment are studied using the present model. The results of theoretical analysis and calculations show that transport and transformation of heavy metal pollution in sediment laden flows, not only have common characteristics of general pollutant but also have features of transport and transformation induced by the movement of sediments.

Keywords: Numerical Simulation; Heavy Metal; Pollution; Sediment; Finite Difference Method.

1-Introduction:

Prediction of flowing water quality and characteristics is having a remarkable place in the research work at global level due to the need to counteract the effects of the natural disasters or accidents that might take place. The concern for water environmental pollution by heavy metals has recently increased due to the negative effects it might have in human beings (Kavcar et al., 2009; Mahato et al., 2016). Some heavy metals as Cadmium (Cd), Chromium (Cr) and Lead (Pb) may transform into persistent metallic compounds with high toxicity (Cao et al., 2016). Due to their damaging effects on the ecological environment and in human health, it is necessary to study heavy metal contamination in aquatic ecosystems (Zhang et al., 2014). Properties of pollutants play a key role when numerical models are used to predict their fate, transport- transformation in surface water bodies. As there occurs sediment motion ubiquitously in natural rivers, lakes and other surface water bodies, pollutants can be generally categorized into two groups. They are sediment motion-related pollutants or (particulate-) sediment associated pollutants (SAPs) and sediment-motion-nonrelated ones (Hart, 1986; Huang, 1993; Ellison and Brett, 2006; Huang et al., 2007). This paper focused on the governing equations of heavy metals and their physical interpretations. It is considered in the paper that the formulated model equations can be extended to describe SAPs transport-transformation in fluvial rivers. By reviewing existing mathematical models of heavy metal pollutant transport-transformation, the authors think that it is useful and proper to establish a mathematical model of heavy metal pollutant transport transformation (dynamics) in its entity, rather than a model of separated-phases (water phase or dissolved phase, particulate phase on suspended particles and on bed sediment). The preceding principal is followed throughout this paper.

2-Equation of Adsorption Reaction Kinetics of Heavy Metal Pollutants in Rivers:

Many experiments have been done to study the adsorption and desorption mechanism of heavy metals in the presence and absence of sediment particles. Using the experimental data, the adsorption and desorption phenomena can be expressed by the dissolved heavy metal concentration equation that is:

$$\frac{dN}{dt} = k_1 c(b - N) - k_2 N \qquad (1)$$

where, k_1, k_2 and b are the coefficients of adsorption and desorption rate and content of saturation adsorption in unit weight of sediment particles, respectively. With the combination of Equation (1) and the mass conservation equation, equations N − t and c − t are formed. Heavy metal absorption by sediment particles is influenced by different factors such as the chemical-environmental conditions and sediment and hydraulic conditions. In general, in rivers, the chemical-environmental conditions do not change much over a given time range; this is while the sediment, hydraulic and hydrology conditions are associated with important changes. Therefore, the chemical-environmental conditions can be fixed for a certain period of time. In contrast, the sediment and flow conditions, the dissolved concentration of heavy metals, c, and the adsorption content of unit weight of sediment, N, (or the particulate concentration of heavy metals) varies with space and time. Therefore, in the case of uniform sediment, the following equation is used for the adsorption phenomena.

$$\frac{dN}{dt} = k_1 c(b - N) - k_2 N \qquad (2)$$

Here, the constants of the equation are extracted from the experimental laboratory experiments, which are under the same chemical-environmental conditions in the rivers.

3- Mathematical Model of the Evolution and Transportation of Heavy Metal Pollutants in the Rivers:

By combining the equations obtained in the preceding two paragraphs with the equations of sediment motion and flow, the mathematical model is obtained for the transformation and transport of heavy metal contaminants for uniform sediment, which is

Flow continuity equation:

$$\frac{\partial}{\partial x}(Bhu) + B\frac{\partial y}{\partial t} = 0 \qquad (3)$$

Flow dynamic equation:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + g\frac{\partial y}{\partial x} + g\frac{u^2}{c_1^2 R} = 0 \qquad (4)$$

Sediment continuity equation:

$$B\frac{\partial}{\partial t}(hs) + \frac{\partial}{\partial x}(Bhus) = -\alpha B\varpi(s - s_*) \qquad (5)$$

River bed deformation equation:

$$\rho' B \frac{\partial y_0}{\partial t} = -\alpha B \varpi (s - s_*) \qquad (6)$$

Suspended sediment transfer capacity:

$$s_* = s_*(u, h, \varpi, \ldots) \qquad (7)$$

The equation for the transformation and transport of heavy metal contaminants:

$$\begin{aligned} &\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} - \frac{1}{A} \frac{\partial}{\partial x} (A E_l' \frac{\partial c}{\partial x}) \\ &= \frac{1}{A} \rho' N_1 \frac{\partial A_3}{\partial t} - \frac{1}{A} \frac{\partial}{\partial t} (N_3 L (1 - p')) \\ &-(s \frac{\partial N_1}{\partial t} + us \frac{\partial N_1}{\partial x} - E_l'^s \frac{\partial s}{\partial x} \frac{\partial N_1}{\partial x}) \end{aligned} \qquad (8)$$

The kinetic equation of the suspended sediments adsorption reaction:

$$\frac{\partial N_1}{\partial t} = k_1 c (b - N_1) - k_2 N_1 \qquad (9)$$

The kinetic equation of the bed sediments adsorption reaction:

$$\frac{\partial N_3}{\partial t} = k_1^b (b^b - N_3) - k_2^b N_3 \qquad (10)$$

In these equations, h mean depth, y water level, y_0 mean level of river bed, s_* suspended sediment transport capacity, s suspended sediment concentration, ϖ average deposition rate, c_1 Chezy coefficient, R hydraulic radius, B channel width on the surface, g gravity acceleration, α coefficient, k_1 adsorption rate coefficient, k_2 desorption rate coefficient, b saturation absorbance per unit weight of suspended sediment, k_1^b bed absorption rate coefficient, k_2^b desorption rate coefficient of bed and bb amount of saturated adsorption per unit area of bed. For ease of reference, the index w has been deleted. In the results of the last two equations, the fluctuations of suspended sediments adsorption is neglected. In addition, the cross section is considered rectangular and the effect of bed sediments on the bed deformation or the transformation and transport of heavy metals has been ignored. The previous equations form the mathematical model and the boundary conditions are determined according to real conditions.

4-Application of Mathematical Model:

The explained mathematical model is applied in two case studies. In both cases, the flow is steady and uniform and the bed changes are negligible. In the case of the first studies, the incoming water is contaminated, but the sediment is clean. In the second study, the intake water is clean and contains contaminated sediments. Some concepts related to the effect of sediment transport on the evolution and transport of heavy metal contaminants are derived from these two studies. By considering the uniform sediment and regardless of the adsorption by boundary sediments, Equation (3) through Equation (10) are simplified as follows. h = constant, u = constant, s = s∗

$$\frac{\partial y_0}{\partial t} = 0, \qquad s_* = k_s \left(\frac{u^3}{gR\varpi} \right)^m$$

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} - E_l' \frac{\partial^2 c}{\partial x^2} = -s\frac{\partial N}{\partial t} - us\frac{\partial N}{\partial x}$$

$$\frac{\partial N}{\partial t} = k_1 c(b - N) - k_2 N$$

Hydraulic and sediment flow conditions are: water surface gradient, $J = 1/10000$; Manning's roughness coefficient, $n = 0.015$; Comprehensive dispersion coefficients for the dissolved heavy metal concentration, $E_l' = \alpha h u_*$; where, $\alpha = 6.3$; $h = 0.1\text{m}$; shear velocity, $u_* = g^{1/2} h^{1/2} J^{1/2}$ gravity acceleration, $\varpi =$ $0.00010 m/s$; uniform characteristic length of sediments, 0.0124mm;

average deposition rate, $\varpi = 0.00010 m/s$;suspended sediments transport capacity, $s_* = 0.03u^{2.76}/(h\varpi)^{0.92} = 5.536\text{kg/m}^3$; k_s and m are constant coefficients; channel length, 10m.

4.1 First Case Study, Contaminated Water with Clean Sediments:

Based on laboratory experiments with cadmium ions, the parameters of Equation (9) are: $b = 0.534\text{mg/g}$, $k_1 = 0.0076(\text{l/mgs})$, $k_2 = 0.00084(\text{l/s})$. The initial conditions for heavy metal contaminants are: $c|_{t=0} = 0, N|_{t=0} = 0$ The boundary conditions are

$$c|_{x=0} = c_0\delta(t), \delta(t) = \begin{cases} 1 & t = 0 \\ 0 & t \neq 0 \end{cases}$$

where c_0 = 1*ppm* and $\frac{\partial c}{\partial x}|_{x=l} = 0$, $N|_{x=0} = 0$. The equation for the transfer of pollutants in clean water with the same hydraulic conditions and without the effect of bed sediments is:

$$\begin{aligned} &\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} - E_l'\frac{\partial^2 c}{\partial x^2} = 0; \qquad c|_{t=0} = 0 \\ &c|_{x=0} = c_0\delta(t); \qquad \frac{\partial c}{\partial x} = 0 \end{aligned}$$

It should be noted that the maximum amount of *N* and *c* decreases with time and space. This is due to the fact that the solution of cadmium (ions of cadmium) is adsorbed on suspended sediments. The effect of the sediments movement on the transport and transformation of cadmium ions can be clearly demonstrated. Due to adsorption of sediments, the concentration of dissolved cadmium, *c*, in a sediment laden water flow is lower than the clean water flow. Due to the adsorption of sediment, the difference between the concentration of dissolved cadmium with and without sediment motion is increased.

4.2 Second Case Study, Clean Water with Contaminated Sediments:

Based on laboratory experiments with cadmium ions, the parameters of the adsorption reaction kinetic equation, namely, the Equation (9), for suspended sediments are $b = 0.534(\text{mg/g})$, $k_1 = 0.0000071(\text{l/mgs})$ and $k_2 = 0.00000132(\text{l/s})$ which are used in simulation. The initial conditions for heavy metal contaminants are $c|_{t=0} = 0,\ N|_{t=0} = 0$. The boundary conditions are $N|_{x=0} = N_0 = 0.3\text{mg/kg}$. Under conditions where the water is clean and sediments are contaminated, the water will be contaminated due to the desorption of cadmium ions. As the time passes, the downstream water becomes more contaminated as the contaminated sediments move further downstream. Despite the fact that these issues are very simple and related to the high concentrations of fine-grained sediments, presents ideas about the effects of sediment transport on the transport and evolution of heavy pollutants in the rivers.

5-Discretization of Equations for the First Study:

In the case of the first studies, the equations are:

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} - E_l'\frac{\partial^2 c}{\partial x^2} = 0, \qquad (11)$$

$$\frac{\partial N}{\partial t} = k_1 c(b - N) - k_2 N \qquad (12)$$

that are coupled and solved together. The dissolved and particulate contaminants concentration variables are calculated by time integration in the Euler method. Therefore Equation (11) and Equation (12) must have the right-side sentences representing the derivative of the considered variable in time. Equation (11) can also be written as follows:

$$\frac{\partial c}{\partial t} = E_l' \frac{\partial^2 c}{\partial x^2} - u \frac{\partial c}{\partial x} \qquad (13)$$

It should be noted that the discretization of the right terms of Equation (12) and Equation (13) are based on a finite difference method with a second order central difference scheme. The left hand term representing the time derivative of first order forward difference scheme. Therefore,

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} = E_l' \frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{\Delta x^2} - u \frac{c_{i+1}^n - c_{i-1}^n}{2\Delta x} = RHSC^n, \qquad (14)$$

$$\frac{N_i^{n+1} - N_i^n}{\Delta t} = k_1 c_i^n (b - N_i^n) - k_2 N_i^n = RHSN^n \qquad (15)$$

Using the first order time integration, one can obtain the dissolved and particulate concentration in next steps as follow,

$$c_i^{n+1} = c_i^n + \Delta t RHSC^n, \qquad (16)$$

$$N_i^{n+1} = N_i^n + \Delta t RHSN^n \qquad (17)$$

It should be noted that in the first study, the concentration of particulate pollutants is obtained from the exact solution of Equation (12) according to the initial conditions, which is:

$$N_i^{n+1} = \left(\frac{k_1 c_i^n b}{k_1 c_i^n + k_2}\right)\left(1.0 + e^{-(k_1 c_i^n + k_2) t^{n+1}}\right) \qquad (18)$$

Here t is the time and the indices n and i are temporal and spatial step counters, respectively.

6 -Discretization of Equations for the Second Study:

In this case, the equation for the variation of the dissolved concentration of pollutants is as follows

$$\frac{\partial c}{\partial t}+u\frac{\partial c}{\partial x}-E_l'\frac{\partial^2 c}{\partial x^2}=-s\frac{\partial N}{\partial t}-us\frac{\partial N}{\partial x} \tag{19}$$

The reason for the deformation of Equation (13) to Equation (19) is the entry of polluting sediments into the stream, so the particulate contaminants concentration affects the dissolved ones. The discretization of this equation, based on the description of the first case, is as follows:

$$\frac{c_i^{n+1}-c_i^n}{\Delta t}=E_l'\frac{c_{i+1}^n-2c_i^n+c_{i-1}^n}{\Delta x^2}-u\frac{c_{i+1}^n-c_{i-1}^n}{2\Delta x}-s\frac{N_i^{n+1}-N_i^n}{\Delta t}-us\frac{N_{i+1}^n-N_{i-1}^n}{2\Delta x} \tag{20}$$

Here it should be noted that the third sentence on the right hand side of the equation can be replaced by Equation (15). So,

$$\frac{c_i^{n+1}-c_i^n}{\Delta t}=E_l'\frac{c_{i+1}^n-2c_i^n+c_{i-1}^n}{\Delta x^2}-u\frac{c_{i+1}^n-c_{i-1}^n}{2\Delta x}-sRHSN^n-us\frac{N_{i+1}^n-N_{i-1}^n}{2\Delta x} \tag{21}$$

To calculate the variations in the particulate pollutants concentration, we use the numerical solution of Equation (12), that is Equation (15) and Equation (17).

7-Numerical Results:

In this section, the numerical results obtained from solving the equations for Problem 1 and Problem 2 are presented. As mentioned earlier, problem 1 is devoted to the state that input flow contain dissolved pollutants and clean sediments entering the stream. In this case, the adsorption and desorption reaction of sediments with dissolved contaminants results in variations in the dissolved and particulate concentration that its simulation result for Cadmium metal is presented in Figure 1.

In the second case, a situation is evaluated in which the input flow is clean, but the input sediments are contaminated. Therefore, as a result of sediments particulate pollutants, during adsorption and desorption reactions, contaminants are transferred to the fluid flow, which leads to the spread of contaminants downstream. The numerical results of this problem are shown in Figure 2.

8-Grid Independency Assessment:

In this section, grid independency for two methods of time integration that is Euler and fourth order

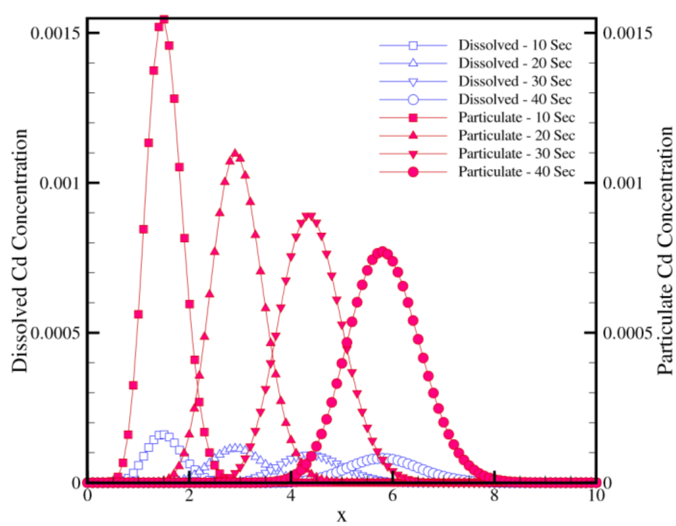

Figure1: Concentration variations of dissolved and particulate contaminants versus distance in various times in problem 1.

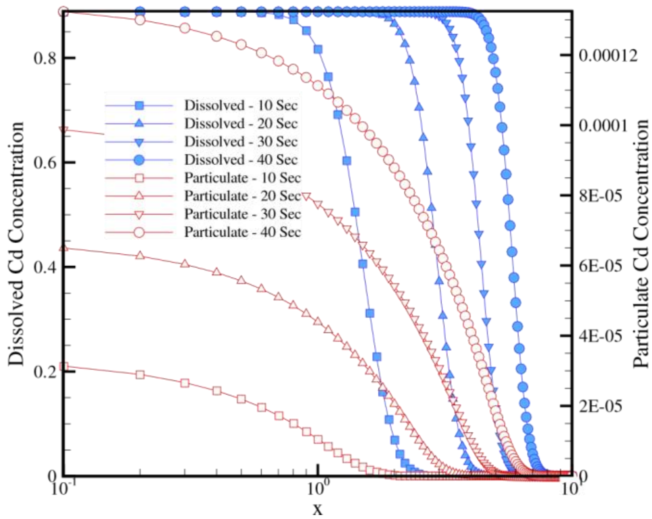

Figure 2: Concentration variations of dissolved and particulate contaminants versus distance in various times in problem 2.

Runge-Kutta are studied. Here, the convergence of the method for the first case study discussed in the previous sections is examined. The Euler time integration for Equation (16) and Equation (17) was explained earlier. Here we describe the algorithm of the fourth order Runge-Kutta integral method. Consider the following differential equation with the initial condition

$$y'_0 = f\,(t, y), y\,(t_0) = (y_0) \qquad (22)$$

To march in time for one step one can use the following relation

Where

$$y_{n+1} = y_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4) \quad (23)$$

$$k_1 = f(t_n, y_n) \quad (24)$$

$$k_2 = f(t_n + \frac{h}{2}, y_n + \frac{h}{2}k_1) \quad (25)$$

$$k_3 = f(t_n + \frac{h}{2}, y_n + \frac{h}{2}k_2) \quad (26)$$

$$k_4 = f(t_n + h, y_n + hk_3) \quad (27)$$

and *h* is the time step. Selecting the temporal unit value is based on the required accuracy. The accuracy of the Runge-Kutta method increases with decreasing time steps. Of course, by reducing the time step, the volume of the calculations increases, and on the other hand, the rounding error also increases. Fourth order RungeKutta belongs to the explicit Runge-Kutta family. Here, the grid independency test is shown for variations of the Cadmium dissolved and particulate contaminants concentration in terms of distance at the 40th second in Problem 1. In Figure 3, the independency of the grid of problem 1 has been investigated for Euler's method. In this issue, five different meshes with the number of grid points 21, 41, 61, 81 and 101 are considered. It should be noted that by increasing the number of grid points and shrinking the spatial steps, the problem goes to a specific distribution. In Figure 4, the grid independency is also shown for problem 1 in the case of the fourth order Runge-Kutta method. Here, as the number of grid points increases, from 21 to 101, answers goes to a single distribution.

9-Conclusion:

Combining the equation of heavy metal pollutant transport-transformation, the equation of adsorption reaction kinetics and hydraulic equations, results in a mathematical model of heavy metal pollutant transport transformation in rivers. This model clearly explains the effect of sediment motion on heavy metal pollutant transport-transformation. Parameters b, k_1, k_2, can be verified without difficulty through preliminary laboratory experiments. Thus, the model is suitable for practical application. The concepts of the effect of sediment motion on heavy metal pollutant transport transformation is clarified via two case studies of the application of this model to a simple flow in a flume. The practical application of the model to natural rivers can obviously improve it.

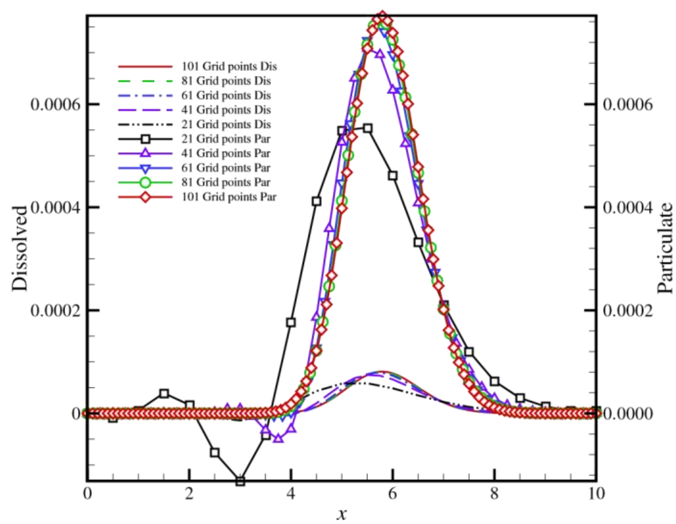

Figure 3: Grid independency of numerical solution for Euler time integration in problem 1 for variations of Cadmium particulate and dissolved contaminants concentration in the 40th second.

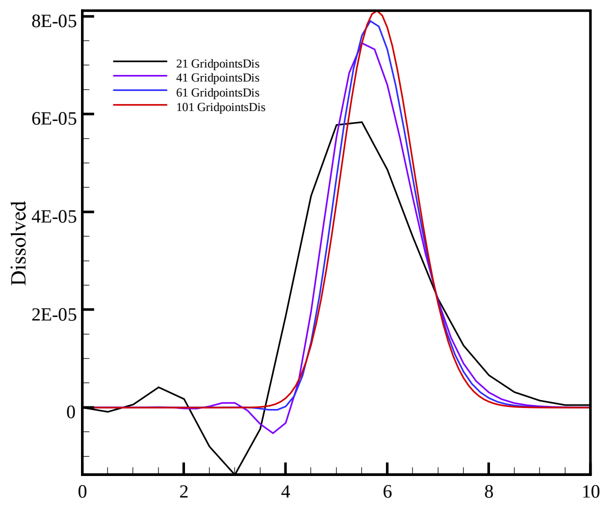

Figure 4: Grid independency of numerical solution for Runge-Kutta time integration in problem 1 for variations of Cadmium dissolved contaminants concentration in the 40th second.

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