A New Two Dimensional Model for Pollutant Transport in Ajichai River

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Abstract

Accurate prediction of pollution control and environmental protection need a good understanding of pollutant dynamics. Numerical model techniques are important apparatus in this research area. So a 2500 line FORTRAN 95 version code was conducted in which using approximate Riemann solver, couples the shallow water and pollution transport agents in two dimensions by the aid of unstructured meshes. A multidimensional linear reconstruction technique and multidimensional slope limiter were implemented to achieve a second-order spatial accuracy. The courant number ruled as a control parameter for stability conditions and a third order Runge-Kutta method was performed for equation discretizations. For Code verifications another author's case study was examined.

The numerical results show that the model could accurately predict the flow dynamics and pollutant transport in Ajichai River.

Keywords: FORTRAN Program, Courant Number, Pollution, Finite Volume, Ajichai River.

1. Introduction

The damage caused to the quality of water, can be regarded as an important source of pollution making it very important in Environmental Engineering Areas. The pollution concentration and distribution rate of each case helps then to control its water quality standard levels.

The numerical models have a good performance in modeling shallow water equations, besides advection- dispersion equations in pollution propagation cases. This is because of the unstructured nature and boundaries of most of Engineering problems, causing them have no direct analytical solution as a result. Among the available Numerical methods such as Finite difference, Finite element and finite volume method, the last method meets our case better, because it not only has a better accuracy in real cases, but also needs fewer memory and time for solution. Among many researchers who focused on water pollution control and flow equations are: Jawahar p and Kamath H. (2000), Zhou JG et al. (2001), Delis AI. (2003), Komatsu T. et al. (1997), Alcrudo , F. and Benkhaldoun, F.(2001), Benkhaldoun, F. and Quivy L.(2006), Benkhaldoun, F.(2002), Heniche M. (2000), James I.D. (2002), Komatsu T. et. al. (1997), Roe P.L. (1981), Vazquez M.E. (1999). For a comprehensive review of recent developments in finite volume methods for shallow water equations we refer to benkhaldoun's papers. By the aforementioned reasons, finite volume model was our choice as a research target for pollution analysis of a case study, namely Ajichai river in west of Iran (Tabriz city). To do this, in this paper we introduce a FORTRAN code whereby we can couple the flow and pollution equations to simulate finally the pollutant dispersion pattern in Ajichai river. The code was calibrated firstly by Fayssal benkhaldoun et al. model (2007) to see its robustness and finally it was used to the real Ajichai river case. According to complex and variant geometry of the river, an unstructured triangular mesh scheme was introduced to represent the river area. The Riemann solver was the discretization agent of the equations, our code may consider the advection and/or dispersion effects in pollution transmit ion besides the shallow water equations in which the continuity and momentum effects in x and y directions were considered.

2. Theory and governing equations

The procedure considered in the logic of code has been shown in the Figure 1, from which the necessary relations and governing equations are as bellows:

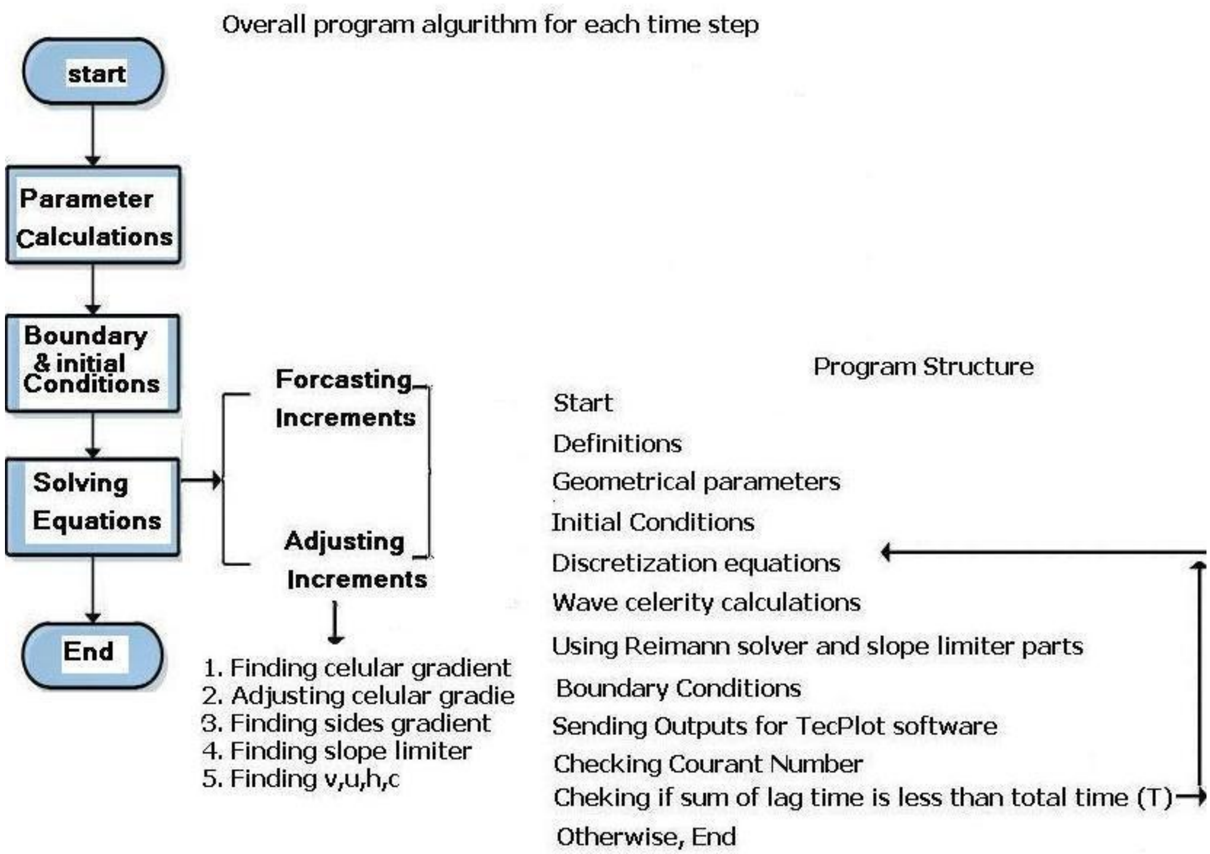

Fig. 1 Building block of Code structure for each step

General shallow depth Flow equations are:

$$\frac{\partial h}{\partial t}+\frac{\partial (hu)}{\partial x}+\frac{\partial (hv)}{\partial y}=0 \tag{1}$$

$$\frac{\partial (hu)}{\partial t}+\frac{\partial (hu^2+0.5gh^2)}{\partial x}+\frac{\partial (huv)}{\partial y}=-gh(S_{0x}-S_{fx}) \tag{2}$$

$$\frac{\partial (hv)}{\partial t}+\frac{\partial (huv)}{\partial x}+\frac{\partial (hv^2+0.5gh^2)}{\partial y}=-gh(S_{0y}-S_{fy}) \tag{3}$$

Advection –dispersion equation is presented as:

$$\frac{\partial(hc)}{\partial t}+\frac{\partial(huc)}{\partial x}+\frac{\partial(hvc)}{\partial y}=\nabla.(\nabla(\mathrm{hc}))+\mathrm{Sd} \qquad (4)$$

Where t = time, x and y = horizontal coordinates, h = flow depth, u and v = depth-averaged flow velocity in x- and y-directions, C = depth-averaged volumetric pollutant concentration, The equations may be transformed to the following form:

$$\frac{\partial(U)}{\partial t}+\frac{\partial(F)}{\partial x}+\frac{\partial(G)}{\partial y}=\mathrm{S(U)} \qquad (5)$$

$$\frac{\partial U}{\partial t}+\nabla.E=\mathrm{S(U)} \qquad (6)$$

Where **U** is the vector of the conservative variables, **F** and **G** are the flux vectors in x- and y-direction; **S** is the vector of source terms, **E** = $(\mathbf{F},\mathbf{G}^T)$

$$U=\begin{pmatrix} h \\ hu \\ hv \\ hc \end{pmatrix}, F(U)=\begin{pmatrix} hu \\ hu^2+0.5gh^2 \\ huv \\ huc \end{pmatrix}, G(U)=\begin{pmatrix} hu \\ huv \\ hu^2+0.5gh^2 \\ hvc \end{pmatrix}$$
$$S(U)=S_0+S_f+Sd=\begin{pmatrix} 0 \\ ghS_{0x} \\ ghS_{0y} \\ 0 \end{pmatrix}+\begin{pmatrix} 0 \\ -ghS_{fx} \\ -ghS_{fy} \\ 0 \end{pmatrix}+\begin{pmatrix} 0 \\ 0 \\ 0 \\ \nabla.(\nabla(\mathrm{hc}))+Sd \end{pmatrix} \qquad (7)$$

In which the dispersion matrix would be:

$$D=\begin{pmatrix} D_{xx} & D_{xy} \\ D_{yx} & D_{yy} \end{pmatrix} \qquad (8)$$

The bottom slope is:

$$S_{0x}=\frac{\partial z}{\partial x}, S_{oy}=\frac{\partial z}{\partial y} \qquad (9)$$

Manning equation for friction slope calculation is:

$$S_{fx}=\frac{n^2u\sqrt{(u^2+v^2)}}{h^{4/3}}, S_{fy}=\frac{n^2v\sqrt{(u^2+v^2)}}{h^{4/3}} \qquad (10)$$

Bed slope, friction slope and diffusion equation terms are:

$$\begin{aligned} S_0&=\begin{pmatrix}0 & -ghS_{0x} & -ghS_{0y} & 0\end{pmatrix}^T \\ S_f&=\begin{pmatrix}0 & -ghS_{fx} & -ghS_{fy} & 0\end{pmatrix}^T \\ Sd&=\begin{pmatrix}0 & 0 & 0 & \nabla.(D\nabla(hc))+Sc\end{pmatrix}^T \end{aligned} \qquad (11)$$

g = gravitational acceleration, S_{0x} *and* S_{0y}= bed slopes in x-and y-directions, S_{fx} and S_{fy} = friction slopes in x-and y-directions, D_{xx}, D_{xy}, D_{yx}, and D_{yy} = empirical dispersion coefficients accounting for turbulent diffusion and shear flow dispersion (L2/T), *S*d= the additional source/sink for the pollutant.

For decomposition of domain we have:

$$\int \frac{\partial U}{\partial t} dA + \int \nabla.E dA = \int S(U) dA \qquad (12)$$

Considering Gauss theorem makes this equation form to:

$$\int \frac{\partial U}{\partial t} dA + \oint E.n dL = \int S(U) dA \qquad (13)$$

In which a Delaunay-type triangle-shaped control volume is considered during a cell-centered finite volume method and can be converted to a new form by mid-point rule as:

$$\frac{\partial U_i}{\partial t} = -\frac{1}{A_i} \sum_{j=1}^{3} (E_{ij}.n_{ij}) L_j + S_i \qquad (14)$$

Here we used cell center as data saving place instead of joints.

U_i has a mean value over the control volume A_i , and E_{ij} is the numerical flux vector through the edge j, and is calculated by a HLL approximate Riemann solver as:

$$E.n_{ij} = \begin{cases} E_L.n_{ij} & if \quad S_L \ge 0 \\ \dfrac{S_R(E_L.n_{ij}) - S_L(E_R.n_{ij}) + S_L S_R (U_R - U_L)}{S_R - S_L} & if \quad S_L < 0 < S_R \\ E_R.n_{ij} & if \quad S_R \le 0 \end{cases} \qquad (15)$$

In which U_L and U_R are value on cell I and the adjacent cell to side j respectively, and S_R and S_L are the related wave celerity estimates.

$$S_L = \begin{cases} \min(q_L.n - \sqrt{gh_L}, u_* - \sqrt{gh_*}) & if \quad h_L > 0, h_R > 0 \\ q_L.n - \sqrt{gh_L} & if \quad h_L > 0, h_R = 0 \\ q_R.n - 2\sqrt{gh_R} & if \quad h_L = 0, h_R > 0 \end{cases}$$

$$S_R = \begin{cases} \max(q_R.n + \sqrt{gh_R}, u_* + \sqrt{gh_*}) & if \quad h_L > 0, h_R > 0 \\ q_L.n + 2\sqrt{gh_L} & if \quad h_L > 0, h_R = 0 \\ q_R.n + \sqrt{gh_R} & if \quad h_L = 0, h_R > 0 \end{cases} \qquad (16)$$

$q=(u\ v)^T$ and $\sqrt{gh_*}$ and u_* have a form as (Toro, 2001):

$$u_* = 0.5(q_L + q_R) + \sqrt{gh_L} - \sqrt{gh_R} \qquad (17)$$

$$\sqrt{gh_*} = 0.25(q_L - q_R).n + 0.5(\sqrt{gh_L} + \sqrt{gh_R}) \qquad (18)$$

In which h_L , h_R are the related depths and the q_L , q_R are the corresponding water velocities. To avoid the oscillations around the discontinuities, a linear reconstruction was made by slope limiter provided by Jawahar and kamath (2000).

The modified Gausian diffusion term is :

$$\int \nabla.(Dh\nabla c)dA = \oint_i (Dh\nabla c).ndL \quad (19)$$

Or it can be rewritten in the form of:

$$\oint_i (Dh\nabla c).ndL = \sum_{j=1}^{3} (Dh\nabla c)ij.n_{ij} L_j \quad (20)$$

For time integration, the equation 15 is decomposed to these two equations to be solved in a semi implicitly manner.

$$\frac{\partial U_i}{\partial t} = -\frac{1}{A_i}\sum_{j=1}^{3}(E_{ij}.n_{ij})L_j + S_{0i} \quad (21)$$

In which The right hand side term consists of advection and bed slope source term while the right hand side term of the second equation (Equation 22) includes friction slope and pollutant diffusion source terms.

$$\frac{\partial U_i}{\partial t} = S_{fi} + S_{di} \quad (22)$$

These equations must be solved in conjunction with the equation 23 by a third order Runge - Kutta method:

$$\begin{aligned} u_1 &= u^n + \Delta t f(u^n) \\ u_2 &= \frac{3}{4}u^n + \frac{1}{4}u_1 + \frac{1}{4}\Delta t f(u_1) \\ u^{n+1} &= \frac{1}{4}u^n + \frac{1}{3}u_2 + \frac{2}{3}\Delta t f(u_2) \end{aligned} \quad (23)$$

In the first step, Equation 23 is solved by an explicit method, then using the values obtained from the first step as the initial conditions, Equation 22 is solved using an implicit method and the same run continues for the next steps.

The boundary conditions are described in the result part.

3. Results

A test example is selected to check the performance of the proposed scheme (Fig. 2). The example solves a pollutant transport in a squared cavity with smooth bottom. All the results presented in this section are computed with variable time step sizes Δt adjusted at each step according to courant Number constraint for stability conditions:

$$\Delta t \le \frac{\min(d_i)}{2\max\left(\left(\sqrt{u^2+v^2}+c\right)_i\right)} \quad (24)$$

where d_i is the distance between the centroid of two adjacent triangle meshes and Δt is less than 1 as a constraint.

As for code verification example, we have a pure advection ($D \equiv 0$) of a pollutant transport in a squared cavity with smooth topography. The flow domain is a 9000 m × 9000 m squared channel with bottom slopes $S_{0x} = S_{0y} = -0.001$. The Manning resistance coefficient is set to n = 0.025 s/m$^{1/3}$. Uniform flow velocities u = v = 0.5 m/s and the uniform flow water depth are considered as initial condition. The initial condition for the pollutant concentration is given by the superposition of two Gaussian pulses centered in (x_1 = 1400 m, y_1 = 1400 m) and (x_2 = 2400 m, y_2 = 2400 m), respectively, where the pollution initial condition is:

$$c(0,x,y) = 10*\exp\left(-\frac{(x-1400)^2+(y-1400)^2}{264^2}\right) + 6.5*\exp\left(-\frac{(x-2400)^2+(y-2400)^2}{264^2}\right) \quad (25)$$

As boundary conditions, we use transparent flow conditions at all cavity boundaries. It is easy to check that the pollutant concentration is a wave that moves along the diagonal cross-section x = y preserving its shape with the constant speed u=v=0.5 m/s.

Figure 2 shows the results of this code for the example used by the mentioned specification.

The results for advection in three discrete times, namely t= 1628 s, t= 5235 s and t= 9600 s are also shown.

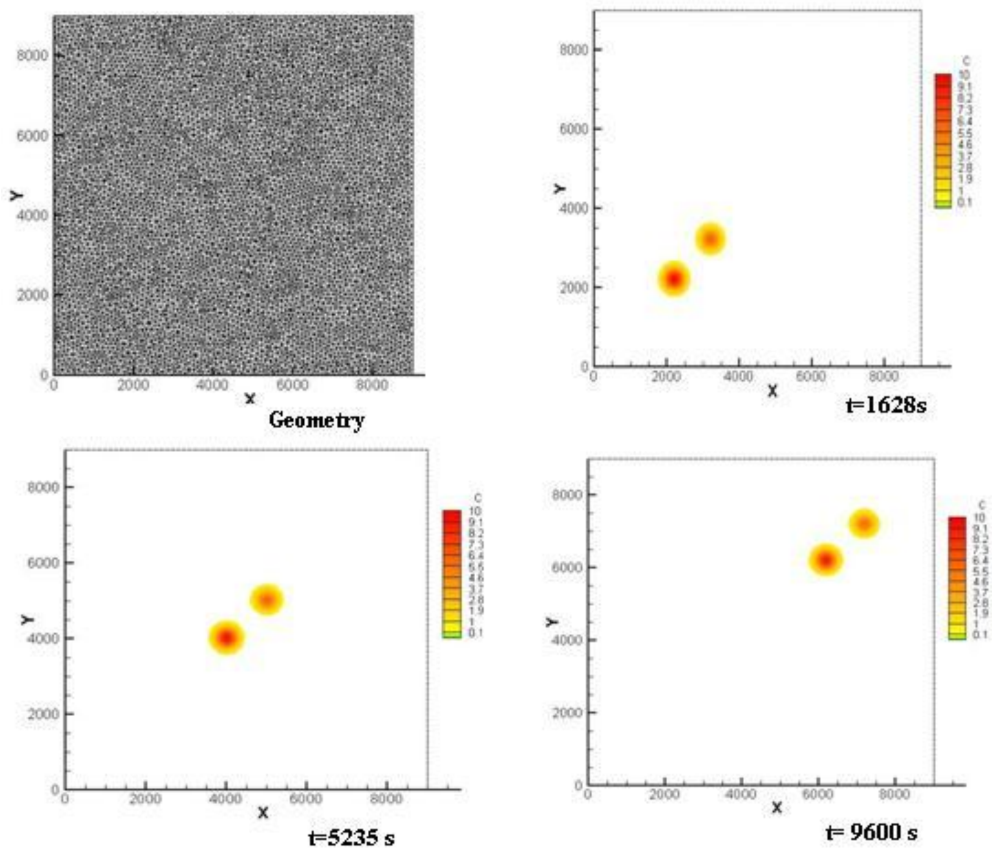

Fig. 2 adopted cavity meshes and the advection results throughout 3 different times. Which are comparable to the results given in Benkhaldoun's paper (2007) as in figure 3

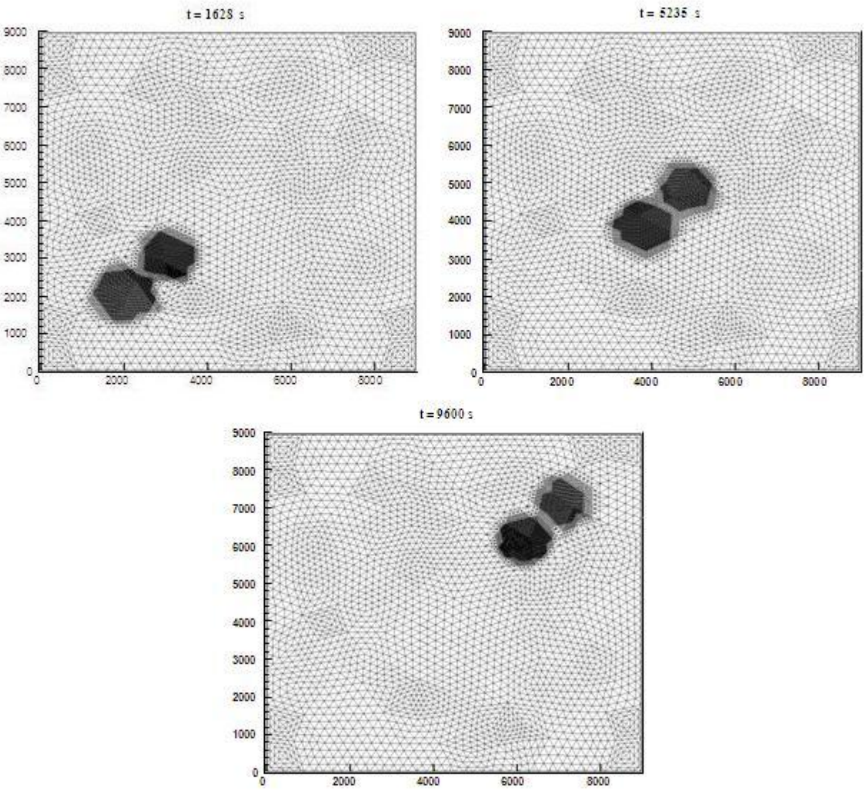

Fig. 3 contours of pollutant concentration at 3 simulation times: t = 1628 s, 5235 s and 9600 s

The real case study specifications:

The Ajichai river (figure 4) is a 147 km river in west of Iran (Tabriz), from which a 25 km; in-between two existent hydrometric stations; was chosen as our target to simulate its pollution concentration distribution.

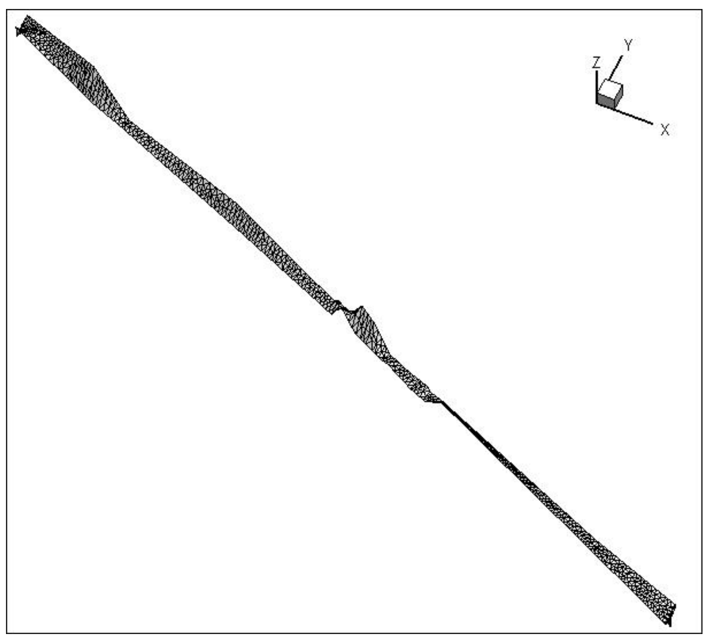

Fig. 4 Ajichai river layout in Iran (Tabriz) in specified river reach part

The related initial conditions are:

$$c(0,x,y) = 4.65*10\text{^}-5*(x\text{^}2+y\text{^}2)\text{^}0.5-32.2743 \quad (26)$$

This is taken from logged data spreadsheet.
The entrance flow boundary condition is:
U=2.6 m/s, V=0
And for concentrations we have:

$$c(t,x,y) = ((j-1)/(nstep-1))*0.496+1.0185 \quad (27)$$

According to the data, the entrance B. C. depth variation is also as the following:

$$h(t,x,y) = 1646.24 - levelv(i) \quad (28)$$

The exit flow boundary condition is:
U=2.36 m/s, V=0
And for concentrations we have:
C=0
According the data, the exit B. C. depth variation is also as the following:

$$h(t,x,y) = 1604.87 - levelv(i) \quad (29)$$

The level is the height of points from the datum. The figure 5 reveals the 6 hr simulated pollutant concentration distribution along the river reach, while D=1.

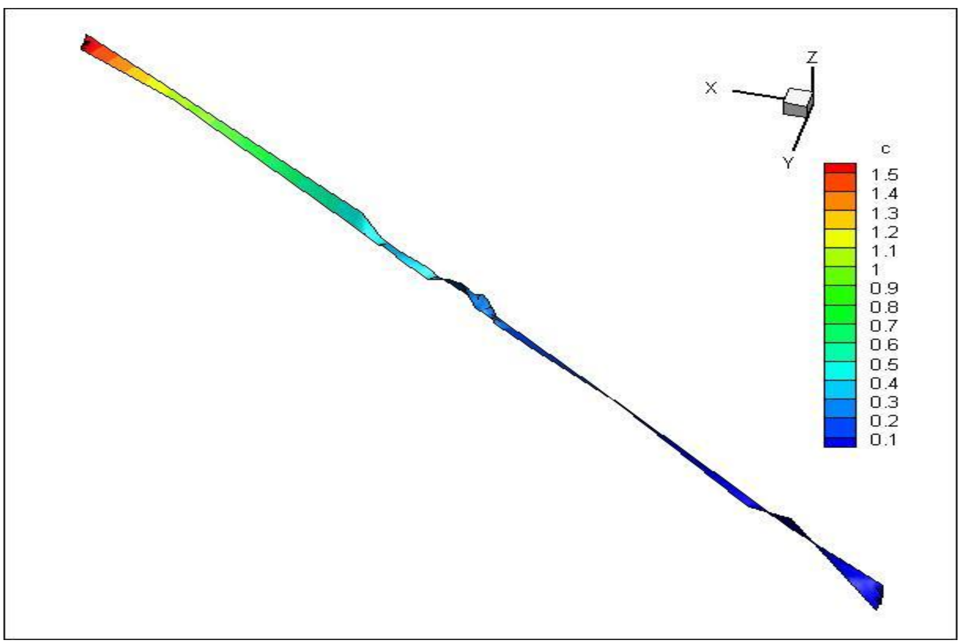

Fig. 5 simulated pollutant concentration in the Ajichai river reach

4. Conclusion

1. Numerical results of FORTRAN 95 code demonstrate the accuracy and robustness of the scheme to simulate the concentrations along the cavity, compared to reference example and its applicability in predicting pollutant transport under shallow water flow conditions.
2. The developed Fortran 95 code could handle the simulation of concentrations along the Ajichai river reach.
3. It is possible to monitor the concentrations according to standard levels in any point of the reach.
4. It could be extendable to other rivers to find their pollution map in case of mapping necessities.
5. The implementation on unstructured meshes allowing for local mesh refinement during the simulation process helps us predict in more real cases.
6. The courant stability condition was satisfied as a constraint throughout all the simulation process.

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