Digital Simulation Programming Technology of Contaminated Surface Water boundaries

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Abstract

A 3D unsteady model in homogenous anisotropic media is developed to simulate the contaminate transport in surface runoff. The model technology is based on a numerical solution of the partial differential diffusion-advection equation. A finite difference numerical solution is preferred. A model technology firstly requires to discretize the model domain into finite number of meshes and the implementation of the base map. The case study indicates that concentration ratio C/Co is lowered to be (0.1) at 1600m downstream of the pollutant setting point. The model is so flexible in the input and output of the data.

Keywords : dispersivity**,** base map, time step, error

Introduction

Chapra (1997) derived one dimensional non-steady partial deferential equations that govern the changes in pollutant and dissolved oxygen concentration. The equations includes the additions of pollutants (q) and removal by oxygenation which is consumed by pollutants as follows:

$$\frac{\partial(AP)}{\partial t} = D_x \frac{\partial^2(AP)}{\partial x} - \frac{\partial(vAP)}{\partial x^2} + qH(x) \quad subjected\ to \quad (x < L < \infty),\ \ t > 0$$

Baffaut and Benson (2009) construct a SWAT model to simulate quick movement of water through vertical conduit connecting river bed with overlying aquifer. The model was calibrated for the James River basin of a watershed (3,600 km^2) in southwest Missouri. Losing. Results indicate that the changes improve the partition of stream flow between surfaces and return flow. Water quality results indicated that the SWAT model can be used to simulate the frequency of ccurrence of pollutant concentrations.

Pimpunchat et al (2010) developed 1D model based on the solution of Chapra (1997) to simulate the pollution of Chin River in Thailand to be used as a basis for future practices. The river is exposed to heavy impact of fertilizer and insecticides moreover it passing through an urban and industrial areas. The river endures a combined pollution namely as industrial, domestic and rural inflows before reaching the sea.

Zhi et al (2013) adopted 2D numerical model to investigate roughness, infiltration by using the diffusion wave equation. The model firstly is compared with analytical and experimental data. The simulated results show that roughness and micro-topography are the main factors affecting solute concentration.

The current 3D model is a contribution for simulation a pollutant transport in a surface water flow. It is based on a numerical transient solution of diffusion-advection partial differential equation in homogenous anisotropic media.

Mathematical Background

The general form of 3D advection-dispersion equation is (Erwin Kreyszig, (1972):-

$$\frac{\partial c}{\partial t} = \nabla(D\nabla c) - \nabla.(vc) + Q \qquad \dots\dots\dots \quad (1)$$

Where:

$\frac{\partial c}{\partial t}$ represent the temporal variation of chemical species concentration, the term $\nabla(D\nabla c)$ describes the variation diffusivity of the chemicals within the media, $\nabla.(vc)$ quantitates the advection of the chemical species, and finally Q is the sink source discharge of the chemicals within media or in other words the creation or destruction of the quantity and how the molecule can be created or destroyed by chemical reactions. Briefly, concentration c for each discretized location should be solved by simultaneous differential equations.

Stationary advection-dispersion equ. describes the steady state system behavior that $\frac{\partial c}{\partial t} = 0$. Accordingly Equ.(1) becomes:

$$0 = \nabla(D\nabla c) - \nabla.(vc) + Q \qquad \dots\dots\dots \quad (2)$$

The expansion form of transient Eq.(1) in Cartesian system is as:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D_x \frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y \frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_z \frac{\partial c}{\partial z}\right) - \frac{\partial v_x c}{\partial x} - \frac{\partial v_y c}{\partial y} - \frac{\partial v_z c}{\partial z} + Q$$

……….. (3)

Where:- c is the pollutant concentration,

D_x, D_y *and* $D_z (m^2/day$ *dispersion coefficient in* x, y *and* z *directions*,

Q is the pollutant discharge (m^3/day) and t is the differential time (day)

$D_x, D_y and D_z$ are considered to be constant in x, y and z directions respectively therefore Equ. (3) may be reduced to

$$\frac{\partial c}{\partial t} = D_x \frac{\partial 2c}{\partial x^2} + D_y \frac{\partial 2c}{\partial y^2} + D_z \frac{\partial 2c}{\partial z^2} - \frac{\partial v_x c}{\partial x} - \frac{\partial v_y c}{\partial y} - \frac{\partial v_z c}{\partial z} + Q \qquad \dots\dots\dots.. \quad (3)$$

Rivers Modeling Consideration and Simplifications

Usually, the surface runoff in the rivers and stream is considered to be one-dimensional flow but in really there is a local traverse flow in a right hand angle. Currently to proceed the solution of Equ.(3) easily, many assumptions should be taken; they are:-

1- The media is considered non-homogenous isotropic. Accordingly the dispersivity is equal in x,y and y directions therefore $D_x = D_y = D_x = D \quad (\frac{m^2}{day})$.
2- Because of non-homogeneity The average runoff velocity in x direction along the Euphrates River $v_x = \quad m/day$ and $v_y = v_z = 0$ for one dimensional flow
Subsequently the transient form of the governing Equ.(3) becomes:-

$$\frac{\partial c}{\partial t} = D\left(\frac{\partial 2c}{\partial x^2} + \frac{\partial 2c}{\partial y^2} + \frac{\partial 2c}{\partial z^2}\right) - v_x\left(\frac{\partial c}{\partial x}\right) + Q \qquad \dots\dots\dots\dots\dots\dots\dots.(4)$$

General Numerical Solution

The discretization of 3D model domain requires a discretizing of a modeled domain in the three dimensions. The number of column is denoted by Nc, the number of Rows in y direction is denoted by N_R and the number of layers in Z direction is denoted by $N_{L.}$

The discretized model domain is shown in Fig.(1)

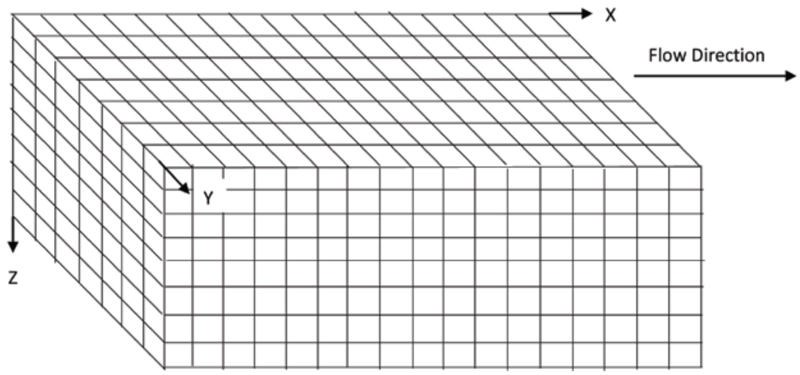

Fig.(1) Discretization of the Model Domain

According to the model in Fig.(2) $NC = 17$, $NR = 7$ and $NL = 8$

To solve Eq. (4) numerically by using the finite difference approximation of Taylor series expansion briefly, the first and second derivatives in x-axis according to Taylor are as follows: Erwin Kreyszig [13]

$$\frac{\partial C}{\partial x}_{i,j,k} = \frac{C_{i,j+1,k} - C_{i,j-1,k}}{2\Delta x}$$

$$\frac{\partial 2C}{\partial x^2}_{i,j,k} = \frac{C_{i+1,j},k - 2C_{i,j,k} + C_{i-1,j,k}}{\Delta x^2}$$

Similarly, the first and second derivatives in y and z coordinates are as follows:

$$\frac{\partial C}{\partial y}_{i,j,k} = \frac{C_{i+1,j,k} - C_{i-1,j,k}}{2\Delta y}$$

$$\frac{\partial 2C}{\partial y^2}_{i,j,k} = \frac{C_{i+1,j,k} - 2C_{i,j,k} + C_{i-1,j,k}}{\Delta y^2}$$

$$\frac{\partial C}{\partial z}_{i,j,k} = \frac{C_{i,j,k+1} - C_{i,j,k-1}}{2\Delta z}$$

$$\frac{\partial 2C}{\partial z^2}_{i,j,k} = \frac{C_{i,j,k+1} - 2C_{i,j,k} + C_{i,j,k+1}}{\Delta z^2}$$

$$\frac{\partial C}{\partial t}_{i,j,k} = \frac{C_{i,j,k} - Co_{i,j,k}}{\Delta t}$$

The numerical solution of Equ.(4) based on a finite difference approach which is required to discretize the domain into a number of nodes as shown in Fig.(2) to construct a number of simultaneous algebraic equations.

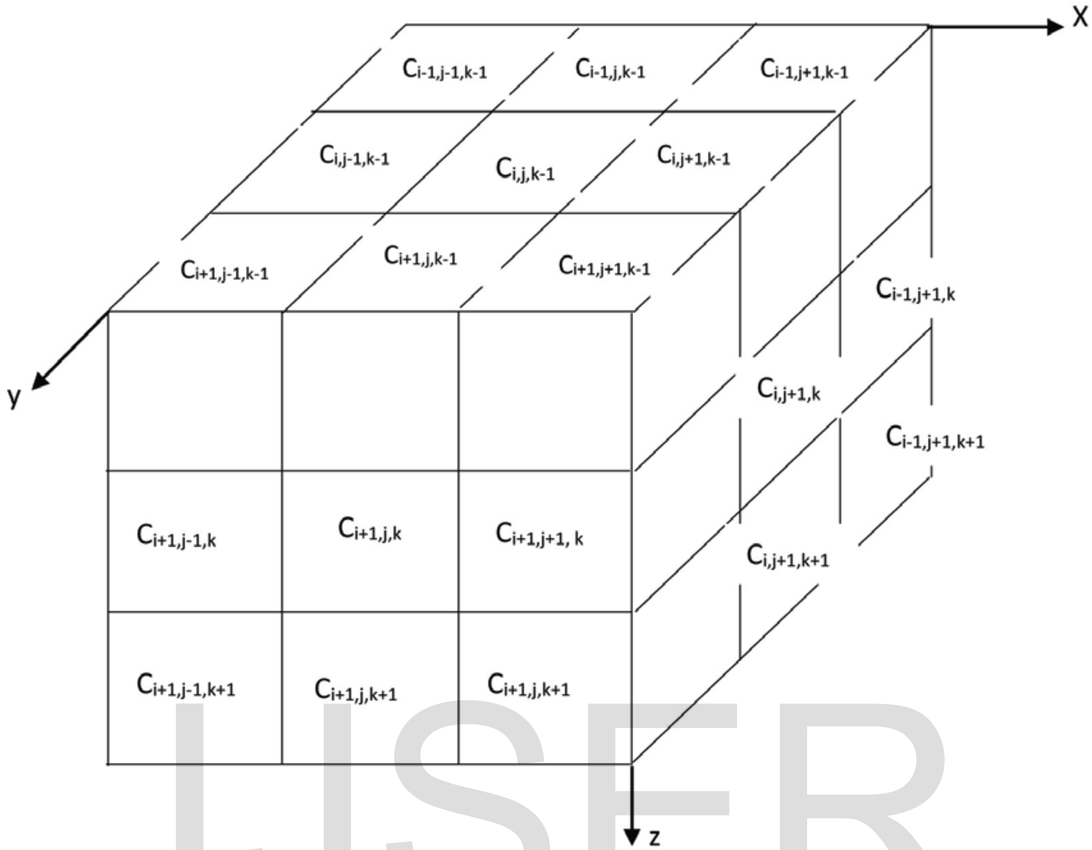

Fig.(2) 3D explicit method of nodal points

The governing Equ. (4) of the modal domain may be reformed as shown in Equ.(5) by using the central difference in x &y coordinates.

$$\frac{C_{i,j,k}-Co_{i,j,k}}{\Delta t} = D\left(\frac{C_{i,j-1,k}-2C_{i,j,k}+C_{i,j+1,k}}{\Delta x^2} + \frac{C_{i+1j,k}-2C_{i,j,}k+C_{i-1,j,k}}{\Delta y^2} + \frac{C_{ij,k-1}-2C_{i,j,}k+C_{i,j,k+1}}{\Delta z^2}\right) - v_{i,j,k}\left(\frac{C_{i,j+1,k}-C_{i,j-1,}k}{2\Delta x}\right) + Q_{i,j,k} \qquad \ldots\ldots\ldots\ldots..(5)$$

Equ. (5) can be simplified to the form of Equ.(6) taking into account $\Delta x = \Delta y = \Delta z = \Delta$:-

$$\left(\frac{1}{\Delta t} + \frac{6D}{\Delta^2}\right)C_{i,j,k} = \left(\frac{D}{\Delta^2} + \frac{v_{i,j,k}}{2\Delta}\right)C_{i,j-1,k} + \frac{D}{\Delta^2}C_{i-1,j,k} + \frac{D}{\Delta^2}C_{i,j,k-1} + \left(\frac{D}{\Delta^2} - \frac{v_{i,j,k}}{2\Delta}\right)C_{i,j+1,k} + \frac{D}{\Delta^2}C_{i+1,j,k} + \frac{D}{\Delta^2}C_{i,j,k+1} + \left(\frac{Co_{i,j,k}}{\Delta t} + Q_{i,j,k}\right) \qquad \ldots\ldots\ldots\ldots\ldots(6)$$

Further rearrangement offers:-

$$C_{i,j,k} = \frac{\left(\frac{D}{\Delta^2}+\frac{v_{i,j,k}}{2\Delta}\right)}{\left(\frac{1}{\Delta t}+\frac{6D}{\Delta^2}\right)}C_{i,j-1,k} + \frac{\frac{D}{\Delta^2}}{\left(\frac{1}{\Delta t}+\frac{6D}{\Delta^2}\right)}C_{i-1,j,k} + \frac{\frac{D}{\Delta^2}}{\left(\frac{1}{\Delta t}+\frac{6D}{\Delta^2}\right)}C_{i,j,k-1} + \frac{\left(\frac{D}{\Delta^2}-\frac{v_{i,j,k}}{2\Delta}\right)}{\left(\frac{1}{\Delta t}+\frac{6D}{\Delta^2}\right)}C_{i,j+1,k} + \frac{\frac{D}{\Delta^2}}{\left(\frac{1}{\Delta t}+\frac{6D}{\Delta^2}\right)}C_{i+1,j,k} + \frac{\frac{D}{\Delta^2}}{\left(\frac{1}{\Delta t}+\frac{6D}{\Delta^2}\right)}C_{i,j,k+1} + \frac{\left(Q_{i,j,k}+\frac{Co_{i,j,k}}{\Delta t}\right)}{\left(\frac{1}{\Delta t}+\frac{6D}{\Delta^2}\right)} \qquad \ldots\ldots\ldots\ldots\ldots(7)$$

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If it is assumed that:-

$AA_{i,j,k} = \frac{\left(\frac{D}{\Delta^2}+\frac{v_{i,j,k}}{2\Delta}\right)}{(\frac{1}{\Delta t}+\frac{6D}{\Delta^2})}$, $BB_{i,j,k} = \frac{\frac{D}{\Delta^2}}{(\frac{1}{\Delta t}+\frac{6D}{\Delta^2})} = (\frac{\Delta^2}{D\Delta t}+6)^{-1}$, $CC_{i,j,k} = \frac{\left(\frac{D}{\Delta^2}-\frac{v_{i,j,k}}{2\Delta}\right)}{(\frac{1}{\Delta t}+\frac{6D}{\Delta^2})}$, and $DD_{j,j,k} = \frac{(Q_{i,j,k}+\frac{Co_{i,j,k}}{\Delta t})}{(\frac{1}{\Delta t}+\frac{6D}{\Delta^2})}$

By substitution of AA_{ijk}, BB_{ijk}, CC_{ijk} $and\ DD_{ijk}$in Eq.(7) we may obtain:-

$$C_{i,j,k} = AA_{i,j,k}C_{i,j-1,k} + BB_{i,j,k}C_{i-1,j,k} + BB_{i,j,k}C_{i,j,k-1} + CC_{i,j,k}C_{i,j+1,k} + BB_{i,j,k}C_{i+1,j,k} + BBC_{i,j,k+1} + DD_{i,j,k}$$
……………(8)

may be rearranged to gives the compacted form of the algebraic governing equation of transient non-homogenous isotropic diffusion surface runoff of the river.

$$C_{i,j,k} = AA_{i,j,k}C_{i-1,j,k} + BB_{i,j,k}(C_{i-1,j,k} + C_{i,j,k-1} + C_{i+1,j,k} + C_{i,j,k+1}) + CC_{i,j,k}C_{i,j+1,k} + DD_{i,j,k}$$
…………(9)

Where $AA_{i,jk}$, $BB_{i,j,k}$, $CC_{i,j,k}$ and $DD_{i,j,k}$ are coefficients depend upon the physical properties of each cell within the model domain.

The modified Gauss Seidel technique may be suitable for concentration algorithm at each node sequentially

The determination of $C_{i,j,k}$ in each node requires estimating the values of the coefficients $AA_{i,jk}$, $BB_{i,j,k}$, $CC_{i,j,k}$ and $DD_{i,j,k}$ in the nodal point $(i,j,k)$and concentration values in the surrounding nodes namely as; $C_{i-1,j,k}$, $C_{i,j-1,k}$, $C_{i,j,k-1}$, $C_{i+1,j,k}$, $C_{i,j+1,k}$, $C_{i,j,k+1}$.

Basic Simulation Programming

The simulation program is coded in Fortran Language for solving a set of simultaneous equations to operate with any consistent of units. Fig.(3) presents the flowchart of simulation program.

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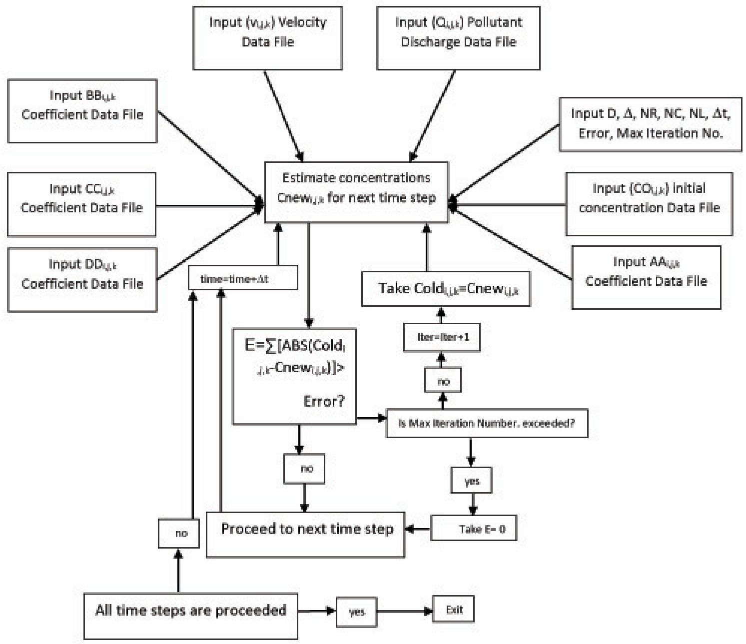

Fig.(3) Flowchart of Contaminant Transport Simulation Program

Simulation Setup & Modular Job

The first step in simulation job is the discretization of the model domain into a finite number of meshes. The number of meshes is depended upon the accuracy of the required output results. The more meshes the more accurate values. This is can be reached by superimposing a square papers on the scaled plain and vertical section maps of the domain. The number of meshes in x and y directions and the max number in Z direction are coded as NC, NR and NL respectively.

Base Map Implementation

It is defined as a number of the meshes which are bounded the modal domain. All these cells showed be traced in x and y direction (The diagonal tracing is not allowed) until the boundary of the domain is closed. The benefit of the base map technique is to omit the outside results of the simulated model domain and fixing the boundary conditions of the model domain. Fig.(4) presents the base map and the mesh design of typical model domain. The figure shows the enumeration the cells surrounding the boundary which should enclosed the XY boundary of the modeled domain. Table (1) presents the worksheet of the base map.

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Table (1) Base Map

Mesh No.	x	y
	148	0
1	8	2
2	7	2
3	6	2
4	6	3
5	6	4
6	5	4
⋮	⋮	⋮
⋮	⋮	⋮
⋮	⋮	⋮
⋮	⋮	⋮
146	10	1
147	9	1
148	8	1

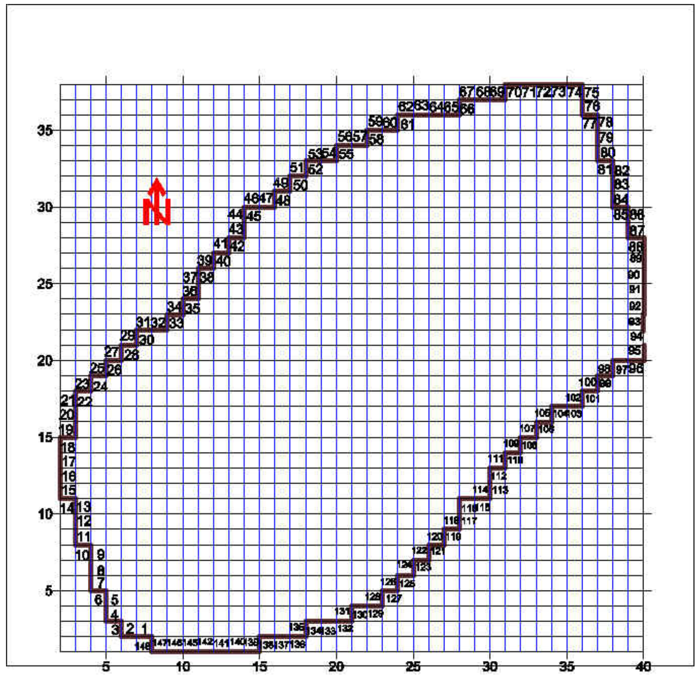

Fig.(4) Mesh Design & Base Map Implementation (1mesh=50m)

Case Study

A river reach of total discharge $Q=1500m^3/sec$ with an average velocity of 100km/day is chosen in this study. A contaminant $864m^3/day$ and concentration Co = 4 mg/liter is set at upstream of the river as shown in Fig.(5) with a diffusion factor of $3450000m^2/day$.

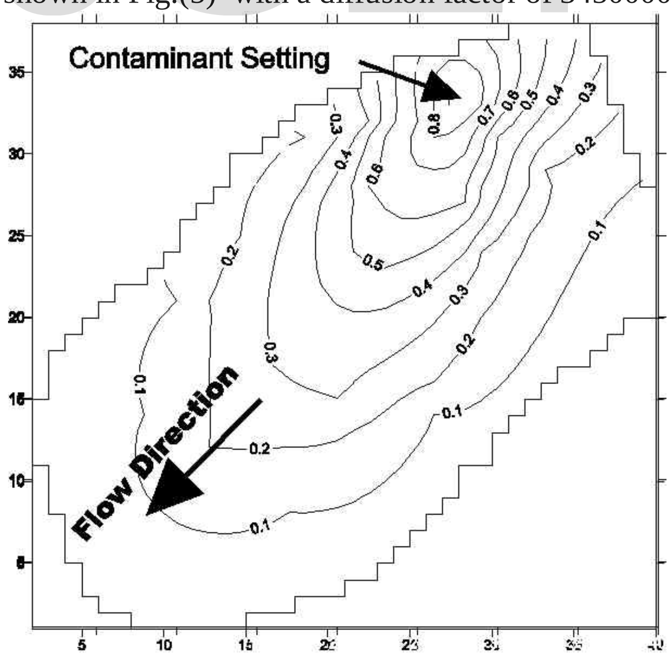

Fig.(5) Contaminant Concentration Ratios (C/Co) Distribution

The simulation program is run for a long period (30000days) until a steady state is obtained. The concentration ratios (C/Co) are presented in the contour map of Fig.(5).

Errors & Time Steps Treatments

The summation of allowable errors within the nodes in the model domain is the difference between two consecutive iterations. The errors summation of single iteration is added to the next and so on. If the summation exceeds the maximum of the allowable error (it is randomly assumed 0.1), it is set to zero and then the process is proceeded as shown in Fig.(3). This is not occurred as shown in the model simulation program results as presented in Fig.(6)

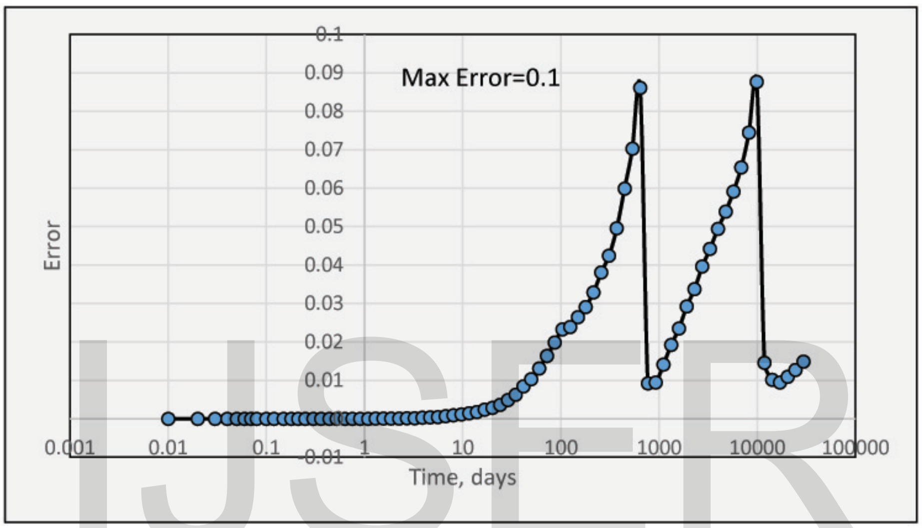

Fig.(6) Error Accumulation versus Operation Time

Fig.(7) presents the numbers of time steps versus operation time. It is reveals that the maximum number of time steps is (110).

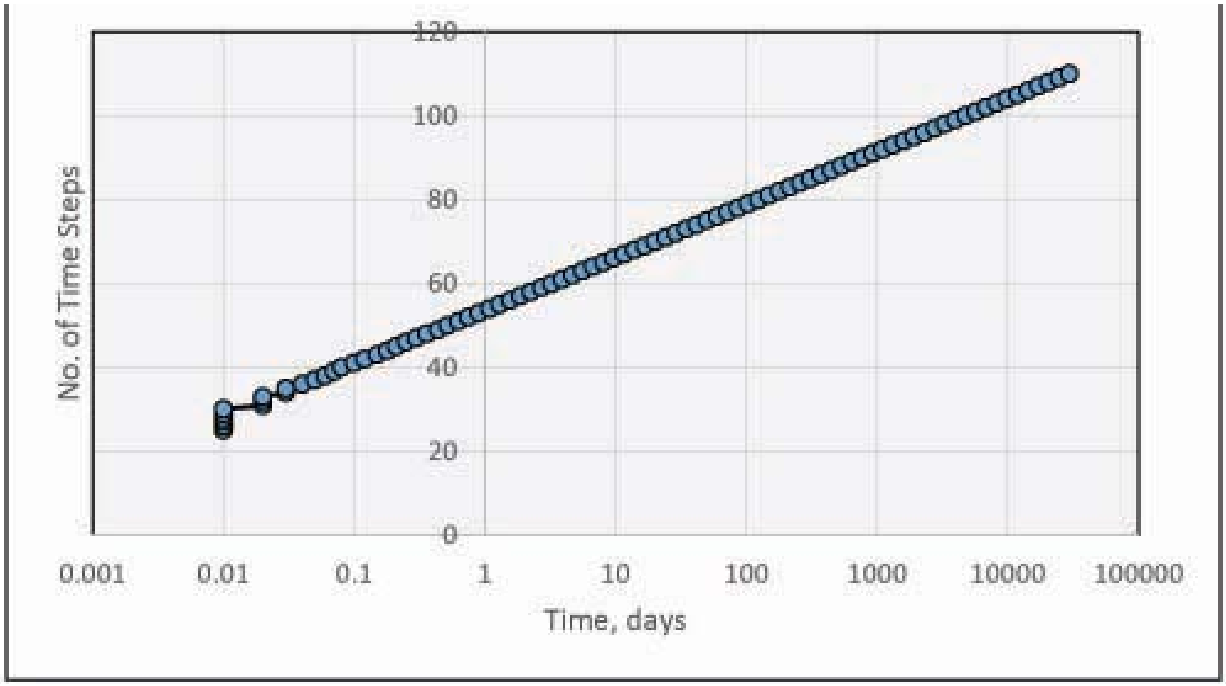

Fig.(7) Number of Time Steps Versus Operation Time

Conclusions:

It is concluded that:-

1- Concentration ratio C/Co is lowered to be (0.1) at 1600m downstream (D/S) of the pollutant setting point.
2- To avoid the model complications it is preferred to simplify the model into 2D model.
3- The model is characterized with high flexibility in input and output data.

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