

A Two Dimensional Numerical Model For Simulation of The Dispersion of Pollutants in Shatt Al-Hilla

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Abstract

A two-dimensional numerical model was developed and applied to study the unsteady continuous discharge of pollutant from a single source into the river with considering the effect of the turbulent eddy viscosity resulted from density difference between the pollutant and river water. This model can be applied for soluble as well as for miscible pollutant with density equals or slightly greater than river water density. The governing equations in the present model are momentum and mass fraction conservation equations. The turbulent dynamic viscosity and diffusion coefficients were calculated by using $(k-\varepsilon)$ turbulence model. The partial differential equations were converted into finite difference form by using (ADI) finite difference technique with application the upwinding scheme. Then the set of the linear algebraic equations were solved by Gauss-Seidel Point-by-Point Method. The results of the system were verified by using a numerical model presented by (Petrus, 1990) for simulating pollutant dispersion in Tigris river. The verification showed a good agreement between the present and the previous work. A sensitivity analysis was carried out to study the effect of variations of different parameters on the concentration distribution resulting from the application of the model.

الخلاصة

تم إنشاء وتطوير نموذج رياضي ثنائي البعد لدراسة طرح الملوث إلى النهر من مصدر مفرد وبشكل مستمر وغير مستقر مع الأخذ بنظر الاعتبار تأثير اختلاف اللزوجة الاضطرابية الناتج عن اختلاف الكثافة بين الملوث وماء النهر. يمكن تطبيق هذا النموذج الرياضي على الملوث الذائب بالإضافة إلى الملوث القابل للامتزاج على أن تكون هذه الملوثات ذات كثافة مساوية أو أكبر بشكل قليل جداً إلى ماء النهر. تم استخدام معادلات حفظ الزخم ومعادلة حفظ الكتلة في إنشاء وتطوير النموذج وتم حساب اللزوجة الاضطرابية ومعامل الانتشار باستخدام النموذج الاضطرابي $(k-\varepsilon)$. تم تحويل المعادلات التفاضلية الجزئية إلى معادلات جبرية خطية باستخدام طريقة الاتجاه المتناوب الضمني-الصريح للفروقات المحدودة (ADI) مع تطبيق منظومة (Upwinding) ومن ثم تم حل المعادلات الجبرية الخطية باستخدام طريقة (Gauss-Seidel). تم التحقق من صحة النتائج باستخدام نموذج رياضي لانتشار الملوث في نهر دجلة للباحث (Petrus, G. B. (1990) وتبين من خلال المقارنة أن هناك توافق جيد بين النموذج الحالي والنموذج السابق. تم إجراء تحليل الحساسية لدراسة تأثير تغير عوامل مختلفة على توزيع التراكيز الناتج من تطبيق النموذج الرياضي.

1. Introduction

Water pollution is a subject of growing public concern. The environmental problems caused by the increase of pollutant loads discharged into natural water bodies due to the growth in municipal, industrial and agricultural activities. These activities contribute significantly to water pollution problems in natural water bodies and cause pollution problems in rivers which are the main source for the fresh water in Iraq and in Hilla City specially.

The development and application of computer-operated mathematical models to simulate the movement of pollutants in rivers and thus to anticipate environmental problems has been the subject of extensive research by government agencies, universities, and private companies for many years and become an important implement of solution of water management problems. The mathematical models of pollution

mixing in open channels can be effectively used for determination of transport, mixing and self purifying characteristics of channels, optimum location of outlet structures in stream, delineation of mixing zones, prediction of spreading of accidental contaminant waves, etc. The ability to solve these problems may have a big influence upon the improvement of water quality, and thus upon ecology (Velísková, 2002).

Many studies were conducted to treat water pollution problems and some of the related previous models are:

Razoky (1984) developed a numerical model for dispersion of pollutants in rivers near drainage or sewer outfalls. The results showed that the decreasing of the mean velocity cause lateral widening and longitudinal shortening in the mixing zone, while Increasing the lateral dispersion coefficient cause a slight lateral narrowing and a longitudinal extension in the mixing zone.

Petrus (1990) developed a two-dimensional numerical model for the simulation of the spreading and mixing of a pollutant in a river considering the effect of an initial pollutant density that differs from the river water density. The results showed that the model was sensitive to the variations in the river velocity and to variation of both longitudinal and vertical dispersion coefficients and it showed that the model was insensitive to the variations in the turbulent eddy viscosity.

Abdul-Hussain (1992) developed a three-dimensional numerical model for the simulation of the spreading and mixing of gaseous pollutants in air. The model showed that the pollutants with high injection velocities are disperse higher in the atmosphere than the pollutants with low injection velocities, while the low density pollutants are disperse higher in the atmosphere than the high density pollutants.

Modenesi et al (2004) developed a three-dimensional numerical model for pollutant dispersion in rivers. The results showed that the model is capable of giving detailed information on the dispersion of inert soluble particles in a river. The experimental data used in this work were obtained from the Atibaia River in the state of São Paulo in Brazil, where effluent is discharged from several industries. The results show a good agreement with the experimental data.

Ayyoubzadehs, et al., (2006) developed a numerical model for pollutant transport in open channel. The validity of the model was shown by a comparison with the results of the analytical solution under certain initial and boundary assumed condition and also with the results of the previous model (DHI, 2003) under same condition.

2. Model description

The problem that is considered in the present work is the unsteady continuous discharge of pollutant from a single source into the river. To simplify the problem to a two-dimensional problem in a rectangular vertical plane, as shown in Fig.(1), the following assumptions are used:

1. The flow is uniform.
2. The fluid is incompressible.
3. The river reach is a rectangular vertical plane. The x-axis is along the water surface in the direction of flow, and the z-axis is along the upstream downward.
4. The slope of the river is vary small and the river surface is planar.
5. Hydrostatic pressure in the vertical direction.
6. The river reach plane is constant across the river width.

7. The pollutant is conservation, soluble or miscible substance having a density equal or slightly greater than river water density.
8. The pollutant concentration at the outfall is constant at any time and it is disposed continuously in the direction of the river flow with only horizontal velocity component equal to ambient river flow velocity.
9. Neglect the wind shear on the flow velocity.

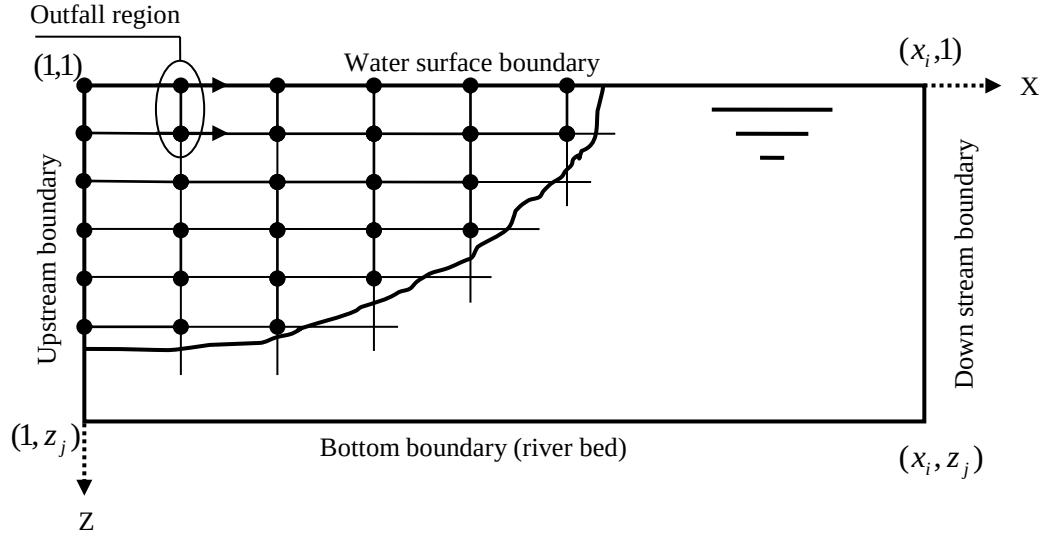


Fig.(1) : River reach domain

2.1 Governing and auxiliary equations:

The numerical model base on the equations which are compatible with the above assumptions. These equations are listed below:

1. Vertical momentum equation:

$$\frac{\partial \rho W}{\partial t} + \frac{\partial \rho U W}{\partial x} + \frac{\partial \rho W W}{\partial z} = \frac{\partial}{\partial x} \left(\mu_t \frac{\partial W}{\partial x} \right) + \frac{\partial}{\partial z} \left(\mu_t \frac{\partial W}{\partial z} \right) - \frac{\partial P}{\partial z} + \rho g \quad (1)$$

2. Horizontal momentum equation:

$$\frac{\partial \rho U}{\partial t} + \frac{\partial \rho U U}{\partial x} + \frac{\partial \rho W U}{\partial z} = \frac{\partial}{\partial x} \left(\mu_t \frac{\partial U}{\partial x} \right) + \frac{\partial}{\partial z} \left(\mu_t \frac{\partial U}{\partial z} \right) \quad (2)$$

3. Mass conservation equation:

$$\frac{\partial \rho m}{\partial t} + \frac{\partial \rho U m}{\partial x} + \frac{\partial \rho W m}{\partial z} = \frac{1}{\sigma_m} \frac{\partial}{\partial x} \left(\mu_t \frac{\partial m}{\partial x} \right) + \frac{1}{\sigma_m} \frac{\partial}{\partial z} \left(\mu_t \frac{\partial m}{\partial z} \right) \quad (3)$$

Where:

$$m = \frac{r_p \rho_p}{\rho} \quad (4)$$

4. k -equation:

$$\frac{\partial \rho k}{\partial t} + \frac{\partial \rho U k}{\partial x} + \frac{\partial \rho W k}{\partial z} = \frac{1}{\sigma_k} \frac{\partial}{\partial x} \left(\mu_t \frac{\partial k}{\partial x} \right) + \frac{1}{\sigma_k} \frac{\partial}{\partial z} \left(\mu_t \frac{\partial k}{\partial z} \right) + G - \rho \varepsilon \quad (5)$$

Where:

$$G = \mu_t \left(2 \left[\frac{\partial U}{\partial x} \right]^2 + 2 \left[\frac{\partial W}{\partial z} \right]^2 + \left[\frac{\partial U}{\partial z} + \frac{\partial W}{\partial x} \right]^2 \right) \quad (6)$$

5. ε -equation:

$$\frac{\partial \rho \varepsilon}{\partial t} + \frac{\partial \rho U \varepsilon}{\partial x} + \frac{\partial \rho W \varepsilon}{\partial z} = \frac{1}{\sigma_\varepsilon} \frac{\partial}{\partial x} \left(\mu_t \frac{\partial \varepsilon}{\partial x} \right) + \frac{1}{\sigma_\varepsilon} \frac{\partial}{\partial z} \left(\mu_t \frac{\partial \varepsilon}{\partial z} \right) + C_1 \frac{\varepsilon}{k} G - C_2 \rho \frac{\varepsilon^2}{k} \quad (7)$$

6. Mixture density equation:

$$\rho = \rho_p r_p + \rho_w r_w \quad (8)$$

9. Turbulent eddy viscosity:

$$\mu_t = C_\mu \rho \frac{k^2}{\varepsilon} \quad (9)$$

7. Mass fraction equations:

$$r_p = \frac{m}{m + \frac{\rho_p}{\rho_w} (1 - m)} \quad (10)$$

$$r_p + r_w = 1 \quad (11)$$

8. Hydrostatic pressure equation:

$$\frac{\partial P}{\partial z} = \rho g \quad (12)$$

Where t is the time; u , w are the velocity components in the x and z directions, respectively, in the Cartesian coordinate system; ρ is the mixture density (water and pollutant) at any point in the river; ρ_p is the pollutant density; ρ_w is the water density; P is the hydrostatic pressure; g is the gravitational acceleration; m is the mass fraction of the pollutant at any point in the river; k is the kinetic energy of turbulence; ε is the rate of dissipation of turbulent kinetic energy; μ_t is the turbulent eddy viscosity; r_p is the ratio of the pollutant concentration at any point in the river to the pollutant concentration at the discharge region (c/c_a); r_w is the ratio of the difference in concentration between the pollutant at the discharge region and the pollutant at any point in the river to the pollutant concentration at the discharge region ($1 - c/c_a$); and the values of empirical constants are chosen as recommended by Launder and Spalding (1974) as follows: $C_1 = 1.44$, $C_2 = 1.92$, $\sigma_m = 0.7$, $\sigma_k = 1.0$, $\sigma_\varepsilon = 1.3$, $C_\mu = 0.09$.

2.2 Initial Conditions:

The initial conditions of the problem are as follows:

- The horizontal velocity component is constant at every point in the vertical plane and the vertical velocity component equals to zero.

- The pollutant concentration equals to zero at every point in the vertical plane except at the discharge region where the pollutant concentration is constant. This leads to the mass fraction (m) of the pollutant equals to zero at every point in the vertical plane except at the discharge region where the mass fraction (m) of the pollutant is equal to one.
- (μ_t), (ε) and (k) are obtained at every point in the vertical plane from the following equations (Rastogi and Rodi; 1978, Babarutsi and Chu; 1998):

$$\mu_t = .0765 \rho V_f h \quad (13)$$

$$\varepsilon = sgU \quad (14)$$

$$k = \sqrt{\frac{\mu_t \varepsilon}{C_\mu \rho}} \quad (15)$$

where V_f = friction velocity = $\sqrt{sgR}$

h = water depth.

ρ = water density.

s = water surface slope.

U = longitudinal velocity component.

R = hydraulic radius.

At the discharge region, (k), (ε), and (μ_t) are obtained from the following equations (Rastogi and Rodi; 1978, Babarutsi and Chu; 1998):

$$\left(\frac{k_d}{k_r} \right) = \left(\frac{U_d}{U_r} \right)^2 \quad (16)$$

$$\left(\frac{\varepsilon_d}{\varepsilon_r} \right) = \left(\frac{U_d}{U_r} \right)^2 \quad (17)$$

$$\mu_t = C_\mu \rho \frac{k_d^2}{\varepsilon_d} \quad (18)$$

2.3 Boundary Conditions:

The boundary conditions of the problem are as follows:

- At discharge region:
 W, U, m, k , and ε equal to their initial condition (assumption No.8).
- At the upstream boundary:
 W, U, m, k , and ε equal to their initial condition (no reverse flow).
- At the down stream boundary:
 $\frac{\partial W}{\partial x} = 0, \frac{\partial U}{\partial x} = 0, \frac{\partial m}{\partial x} = 0, \frac{\partial k}{\partial x} = 0$, and $\frac{\partial \varepsilon}{\partial x} = 0$
- At the surface boundary:
 $P = 0, W = 0, \frac{\partial U}{\partial z} = 0, \frac{\partial m}{\partial z} = 0, \frac{\partial k}{\partial z} = 0$, and $\frac{\partial \varepsilon}{\partial z} = 0$

- At the bottom boundary:

$$W = 0, \frac{\partial U}{\partial z} = 0, \frac{\partial m}{\partial z} = 0, \frac{\partial k}{\partial z} = 0, \text{ and } \frac{\partial \varepsilon}{\partial z} = 0$$

2.4 Numerical scheme

The governing differential equations are converted to the finite-difference form by using (ADI) finite-difference technique in two steps:

1. Implicit in the z-direction and explicit in the x-direction for the time step $(t \rightarrow t + \Delta t / 2)$ to determine the unknown at time $(t + \Delta t / 2)$.
2. Implicit in the x-direction and explicit in the z-direction for the time step $(t + \Delta t / 2 \rightarrow t + \Delta t)$ to determine the unknown at time $(t + \Delta t)$.

Through the finite-difference transformations, to transform the governing differential from non-linear to linear equations, the variables $\rho, U, W, k, \varepsilon, \mu_t$, and P other than dependent variables were made constant from $(t \rightarrow t + \Delta t)$. All empirical constants $\sigma_c, \sigma_k, \sigma_\varepsilon, C_1$, and C_2 are always constant and not change during the time. The (ADI) finite-difference technique gives a set of linear algebraic equations for each step (equation 19, 20) and then the linear equations solved by Gauss-Seidel method.

$$\phi_{i,j}^{t+\Delta t/2} = \frac{d_{i,j} + a_{i,j}\phi_{i,j-1}^{t+\Delta t/2} + f_{i,j}\phi_{i,j+1}^{t+\Delta t/2}}{b_{i,j}} \quad (19)$$

$$\phi_{i,j}^{t+\Delta t} = \frac{d_{i,j} + a_{i,j}\phi_{i-1,j}^{t+\Delta t} + f_{i,j}\phi_{i+1,j}^{t+\Delta t}}{b_{i,j}} \quad (20)$$

where $\phi_{i,j}$ is a variable denoted to the unknown values of W, U, m, k , and ε .

3. Model verification

It is necessary to test the numerical model before examining its results in order to determine its validity. The success of any numerical model largely depends on the availability of the accurate field data specially when there is no analytical solution for the equations which are relate to relevant problem. These data should be adequate for model calibration and verification in terms of quantity and quality. In the present work, the field data are not available; therefore, the verification was conducted by comparing results of the present work with the results of the previous work for Petrus, G. B. (1990). The main characteristics of the Petrus model can be simply summarized as follows:

1. Three governing equations were used to study the unsteady continuous discharge of pollutant into river, these governing equations are momentum conservation and convective-dispersion equations.
2. The turbulent eddy viscosity of each point in the river was assumed to be constant in the momentum conservation equations. the horizontal eddy viscosity was taken equal to 10 N.s/m^2 and the vertical eddy viscosity was taken equal to 0.1 N.s/m^2 .
3. The convective-dispersion equation was used to study the pollutant concentration transport. This equation contains two different dispersion coefficients for each point in the river reach at each time, longitudinal and vertical dispersion

coefficients. These two coefficients were calculated using two different relations. These relations were developed by Mahender and Bansal (1971) and as follows:

$$D_L = \frac{V}{KV_s} UH * 10^{(6.45 - 0.762 \log(\frac{\rho UH}{\mu}))} \quad (21)$$

$$D_V = \nu * 10^{(-8.1 + 1.558 \log(\frac{\rho UH}{\mu}))} \quad (22)$$

Where D_L : longitudinal dispersion coefficient.

U : stream velocity (m/sec).

V : average velocity of flow in reach (m/sec)

V_s : effective mean velocity of flow at sampling station.

K : regional dispersion factor.

H : depth of flow (m).

D_V : vertical dispersion coefficient.

ν : kinematic viscosity (m²/s).

The input data which were used in this model were selected in which the input data are compatible with the previous work and based on some of the hydraulic conditions of the Tigris river in Baghdad City:

- The total length of the river reach 2000 m and the length increment 100 m.
- The total depth of the river reach 3 m and the depth increment 0.25 m.
- The time increment 1 sec and the program was run for various times.
- The slope of the river 6 cm/km (Euphrates center for studying and design of irrigation projects, 1992).
- The hydraulic radius of the river was taken equal to the river reach depth (i.e., 3 m).
- The initial horizontal velocity component of the river 0.8 m/sec (Euphrates center for studying and design of irrigation projects, 1992).
- The initial river water density 1000 kg/m³.
- The discharged pollutant density was taken equal to the initial river water density (i.e. , 1000 kg/m³).
- The discharged pollutant concentration at the discharge region was taken equal to 1.

The correlation coefficients were found for various times and as shown in Figs.(2, and 3).

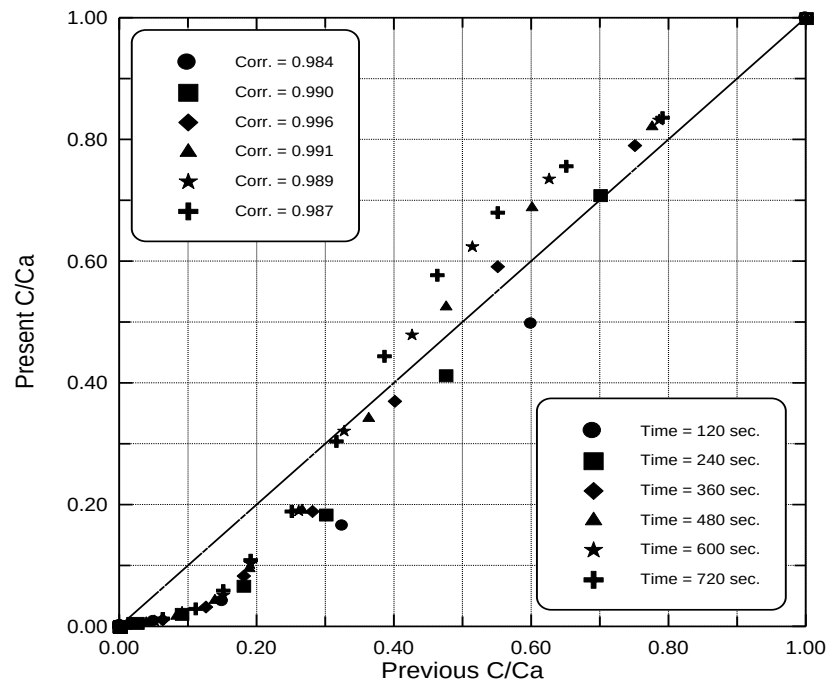


Fig.(2) : Verification by Comparison in C/Ca between the present and the previous work for the points located at the water surface.

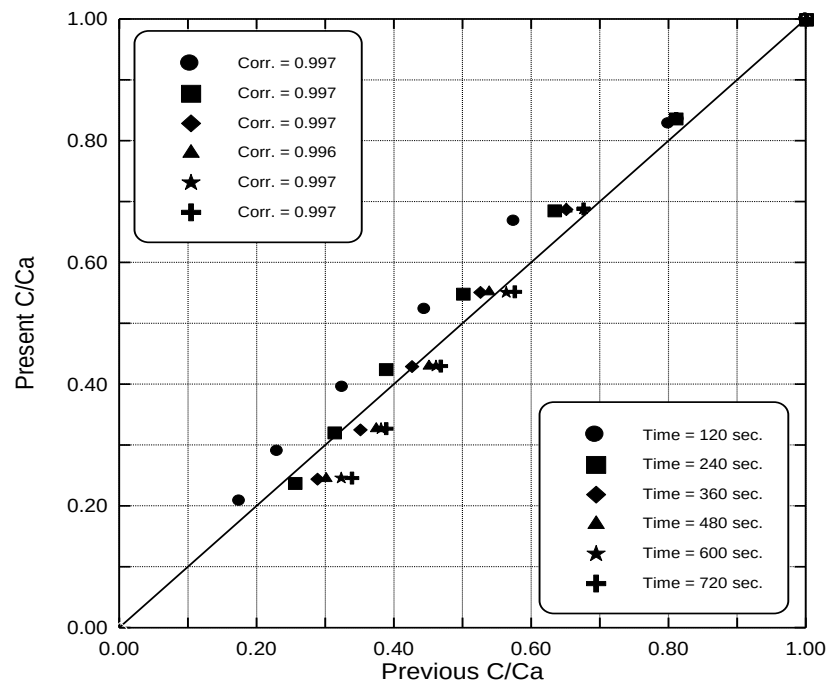


Fig.(3) : Verification by Comparison in C/Ca between the present and the previous work for the points located below the outfall region.

4. Results and analysis:

According to mass fraction conservation equation, mass of pollutant transports by two mechanisms; i.e., convection and diffusion. Convection is the direct process in which the tracer moves from place to place through a fluid system; thus, mass transport by convection means mass transport due to a local velocity. Diffusion is the transport caused by the molecular and turbulent action and is associated with time-average velocity-fluctuation (Al-Hashimy; 1979, Razoky; 1984).

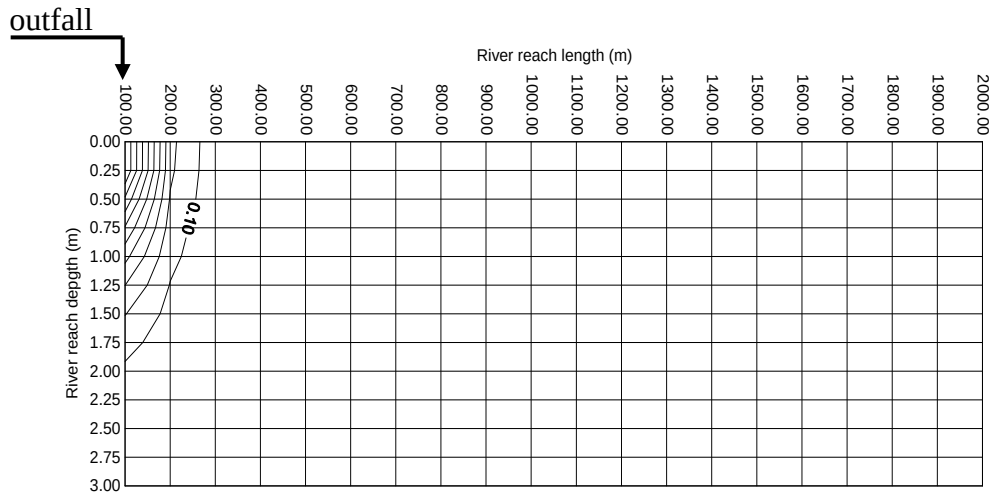
Pollutant density was increased slightly and the comparison between the case of the pollutant having a density equals to river water density and the case of the pollutant having a density greater than river water density has been done as follows:

For the case of the pollutant having a density equals to river water density, Figs.(4,5, and 6) show the C/Ca contours at different times. The horizontal mass transport occurs due to the effect of convection and diffusion mechanism with no change in horizontal velocity components with time but the vertical mass transport occurs due to the effect of diffusion mechanism only due to no change in vertical velocity component and stay zero with time. The vertical concentration gradient in this case will reduce with horizontal distance until the uniform vertical distribution is took place far from the outfall region where the pollutant concentration is increase with time.

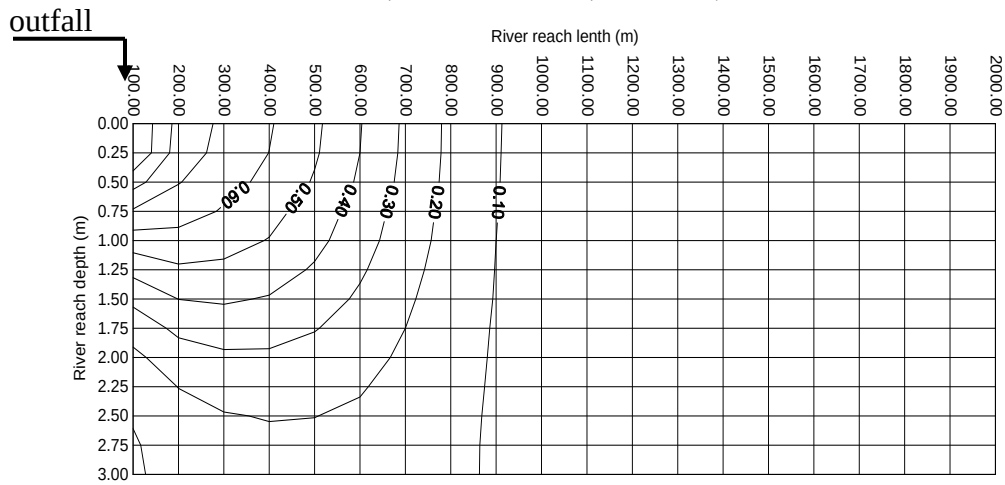
For the case of the pollutant having a density greater than river water density, Figs.(7,8, and 9) show the C/Ca contours at different times for a pollutant having a density equal to $1001\text{kg}/\text{m}^3$. These figures show that the vertical mass transport in this case is less than the vertical mass transport in the case of the pollutant having a density equals to river water density. For example, at time equal to 750 sec, the contour $C/Ca = 0.5$ is about 0.94 m away vertically from the outfall at the water surface in case of the pollutant having a density equals to $1001\text{kg}/\text{m}^3$, while it is about 1.19 m at the same time in case of the pollutant having a density equal to river water density. This can be attributed to the generating upward convection in an opposite direction to the vertical diffusion due to the presence of negative vertical velocity components in case of the pollutant having a density equals to $1001\text{kg}/\text{m}^3$. The uniform vertical distribution will not take place in case the pollutant having a density greater than river water density due to the presence of the vertical velocity components that cause vertical mass transport by convection and this leads to change in the vertical concentration gradient reduction with horizontal distance, then the two-dimensional phenomena of the pollutant transport in rivers can be considered as one-dimension in the longitudinal direction at distance far from the outfall region in case of the pollutant having a density equals to river water density.

In each cases, the change in concentration is high at early stage of disposal and reduces with time so that the pollutant concentration decreases with increases the pollutant density at the same time of disposal.

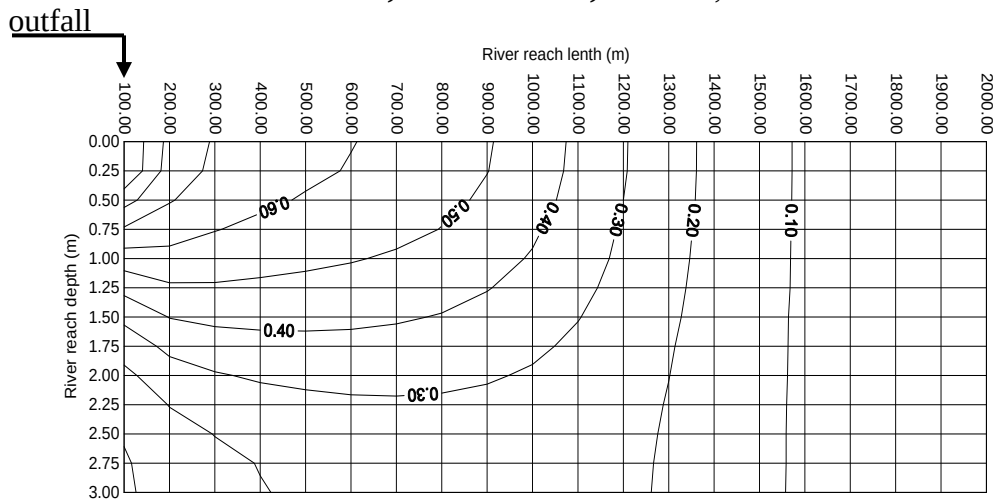
The above analysis indicates that the model is very sensitive to slightly changes in the initial pollutant density, initial river velocity, water surface slope, and turbulent eddy viscosity.



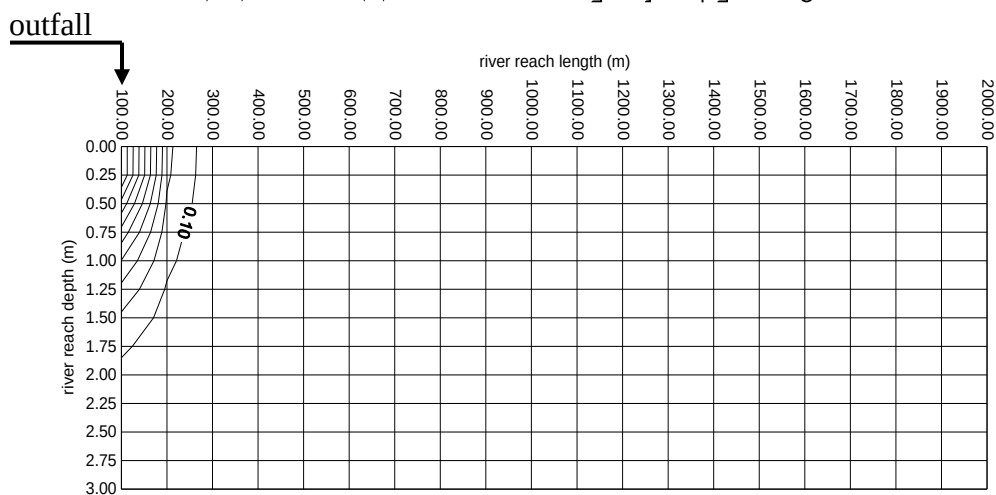
**Fig.(4) : C/C_a contours. pollutant density = 1000 kg/m^3 ,
 $U = 0.8 \text{ m/sec}$, $S = 6 \text{ cm/km}$, $R = 3 \text{ m}$, time = 50 sec.**



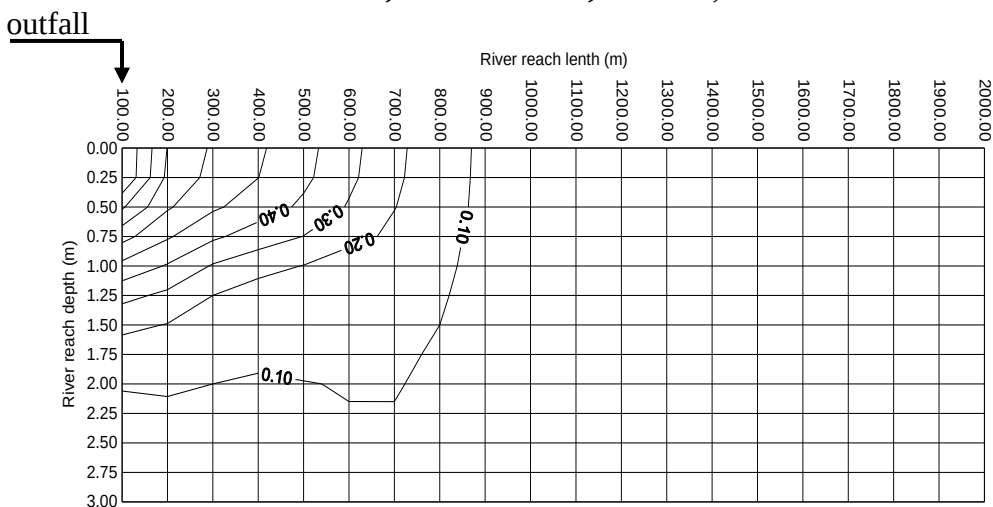
**Fig.(5) : C/C_a contours. pollutant density = 1000 kg/m^3 ,
 $U = 0.8 \text{ m/sec}$, $S = 6 \text{ cm/km}$, $R = 3 \text{ m}$, time = 750 sec.**



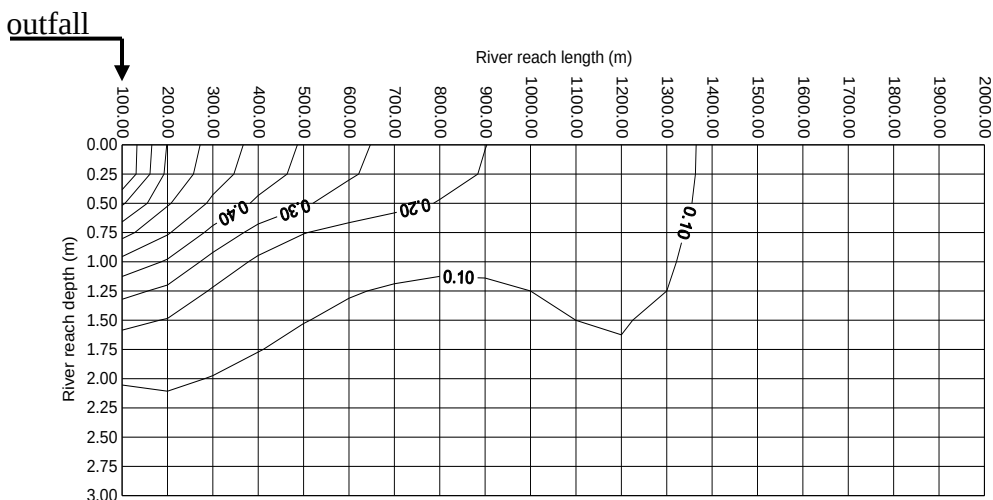
**Fig.(6) : C/C_a contours. pollutant density = 1000 kg/m^3 ,
 $U = 0.8 \text{ m/sec}$, $S = 6 \text{ cm/km}$, $R = 3 \text{ m}$, time = 1500 sec.**



**Fig.(7) : C/C_a contours. pollutant density = 1001 kg/m^3 ,
 $U = 0.8 \text{ m / sec}$, $S = 6 \text{ cm / km}$, $R = 3 \text{ m}$, time = 50 sec.**



**Fig.(8) : C/C_a contours. pollutant density = 1001 kg/m^3 ,
 $U = 0.8 \text{ m / sec}$, $S = 6 \text{ cm / km}$, $R = 3 \text{ m}$, time = 750 sec.**



**Fig.(9) : C/C_a contours. pollutant density = 1001 kg/m^3 ,
 $U = 0.8 \text{ m / sec}$, $S = 6 \text{ cm / km}$, $R = 3 \text{ m}$, time = 1500 sec.**

5. Conclusions

The results showed that a slight increase in the density of pollutant than river water density, reduces the pollutant mass transport longitudinally and vertically. The horizontal convection and diffusion are of a great influence in the pollutant mass transport longitudinally and vertically in case of the pollutant having the density greater than river water density. The results also showed that in case of the pollutant having the density equals to river water density, the horizontal convection and diffusion are dominate the pollutant mass transport in the horizontal direction while the vertical diffusion affects the pollutant mass transport in the vertical direction. A sensitivity analysis was carried out to study the effect of variations of different parameters on the concentration distribution resulting from the application of the model. The model was found to be very sensitive to the change in initial pollutant density, initial river velocity, water surface slope, and turbulent eddy viscosity.

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