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THREE-DIMENSIONAL SIMULATION OF POLLUTANT DISPERSION OF AN OPEN CHANNEL FLOW WITH A SIDE DISCHARGE

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An attempt has been made in this paper to study the pollutant dispersion behavior from Arges River as a tributary on the Danube River using three-dimensional numerical model. Numerical computations were carried out using Fluent 6.2.16, which is based on the finite volume approach. Both the volume of fluid (VOF) and user defined scalar (UDS) methods were used in this study. VOF method was used to allow the free-surface to deform freely with the underlying turbulence. Moreover, the pollutant (BOD) is assumed to be mixed throughout the system as a passive scalar. The study comprised the effect of flow rate on the dispersion behavior for different scenarios. The numerical simulation results show a good fit with observed data in the literature. The findings of this study may provide a proper basis for water quality management in rivers.

Keywords: computational fluid dynamics (CFD), Pollutant dispersion, Open channel flow, Danube River.

1. Introduction

Open channel flow such as rivers and streams are the major sources of water for many human activities such as farming, water supply and industry. Recently, the deterioration in water quality of rivers and stream have been increased due to the growth of population, urbanization, industrialization, and agriculture activities all over the world which forcing developing countries into remediation options of river water quality [1]. Although the river system is complex, different studies have been conducted to assess, evaluate and simulate the water quality in rivers [2-5].

Moreover, the fate and transport of pollutants in rivers is relatively important for reliable water quality management. Numerical model has been widely used as an effective tool to simulate and predict pollutant transport in rivers and stream. Numerous studies have been carried out to understand and simulate the transport phenomena and the change in the pollutants concentration in order to gain insight into the impact of these pollutants, and to provide a basis for water quality management [6-8].

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Various commercial and public domain models have been developed in literature to consider the changes in contaminated concentration based upon physical, chemical, and biological principles such as QUAL2Kw, QUASAR, MIKE11, SIMCAT and WASP [9]. In contrast, computational fluid dynamics (CFD) tools have also been used for certain researches to provide valuable information relating the description of the water flow hydrodynamics and the pollutant behavior along the river and stream [10-13].

The main aim of this study is to predict the pollutant dispersion behavior with different scenarios in a curved open channel flow with a side discharge by setting different values of flow rate and diffusivity coefficient using volume of fluid (VOF) method and scalar transport. This study may serve as a basis for understanding the effect of the flow rate on the concentration of pollutant from the polluted tributary on the river.

2. Materials and Methods

Assumptions

A CFD code (FLUENT), has been used in the present paper for analysis of 3D curved open channel flow with a side discharge. The geometry used in this study is shown in Fig. 1, along with mesh generation (Gambit was used for meshing). A real open channel flow (Danube River) was chosen for calibration in order to validate the simulation results. It was assumed that the main open channel flow is representing the Danube River at the lower course and the side discharge is represented as a tributary of the Danube (Arges River). Curved shape of open channel flow was considered to provide valuable information on the pollutant dispersion behavior. Different set of flow rate and diffusivity were adopted to explore the dispersion of pollutant behavior during different flow condition along the channel. Biochemical oxygen demand (BOD) was chosen as a pollutant and the aim is to produce different scenarios of the BOD dispersion along the channel on the basis of the discharges. Table 1 shows the adopted values of flow rate in the Danube and Arges Rivers along with BOD values in the rivers.

Both Multiphase free surface flow (volume of fluid) and user defined scalar (UDS) were used in this study. For volume of fluid (VOF), Euler-Euler multiphase models were used. Furthermore, this study assumed that the BOD is in a liquid form and mixed throughout the system as a passive scalar and there are no sources or sinks of the pollutant in the channel. The main aim of this assumption was to account only for the changes in the pollutant concentration due to the physical process of dispersion without considering the transformation process of the pollutant and compare the results with the observed values of BOD in the river. This may provide a quick estimate for BOD dispersion along the river, especially when the results are somewhat acceptable.

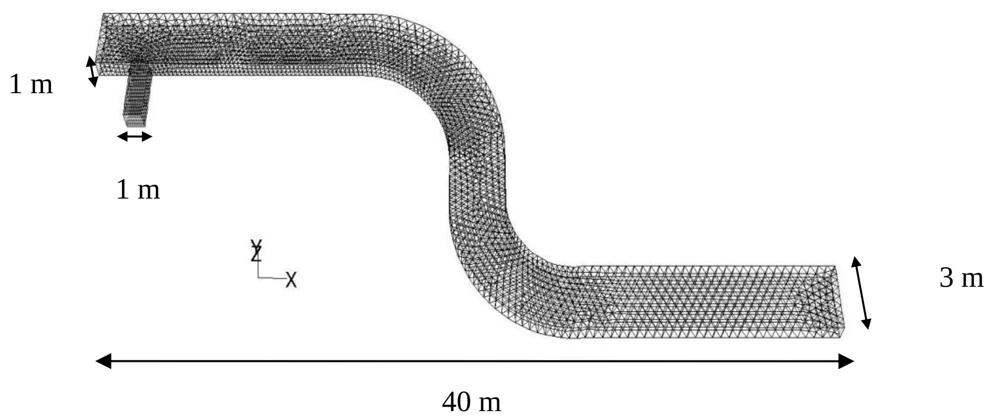

Fig. 1. Geometry and mesh of the study

Table 1

Water quality and quantity data used in this study.

Variables / **River name**	**BOD (mg/L)**	**Flow rate (m^3/sec)**
Danube River	5	4000 - 10000
Arges River	40	50 - 90

Governing equations

The VOF formulation relies on the fact that two or more fluids are not interpenetrating. This is the case with dispersion process in open channel flow (Rivers). The governing differential equations of mass and momentum balance for unsteady free surface flow can be expressed as:

$$\frac{\partial \rho}{\partial t} + \sum_{i=1}^{3}\left[\frac{\rho U_i}{\partial x_i}\right] = 0 \tag{1}$$

$$\frac{\partial(\rho U_i)}{\partial t} + U_j \frac{\partial(U_i)}{\partial x_i} = \frac{\partial \tau_{ij}}{\partial x_j} + \frac{\partial P}{\partial x_i} + \rho g_i + S_i, s \tag{2}$$

where U is the velocity vector in the three directions; p is the pressure; v is the molecular viscosity; g is the gravitational acceleration in the three directions, and ρ

is the density of flow. In the momentum Eq. (2) the interaction between the phases is modeled by the surface tension *Si,s* .

In the present study air is set as primary phase and water is set as the secondary phase. The tracking of the interface between the phases is done with the solution of the continuity Eq. (1) for the secondary phase (water). This interface is so calculated with the following equation [10]:

$$\frac{\partial(\alpha_2\rho_2)}{\partial t}+\frac{\partial(\alpha_2\rho_2 U_i)}{\partial x_i}=S_2 \tag{3}$$

where S_2 is the source of the phase 2 (S_2 is equal to zero in this work), ρ_2 is the density of the secondary phase and α_2 is the volume fraction of the secondary phase ($\alpha_2 = V2/V$). V is the total volume of fluids ($V = V1 + V2$); $V1$ is the volume of phase 1 and $V2$ is the volume of phase 2. The volume fraction of the primary phase ($\alpha_1 = V1/V$) is calculated as

$$\sum_{i=1}^{2}\alpha_{i=1} \tag{4}$$

The standard κ-ε model has been used in the present case. It is a semi-empirical model based on model transport equations for the turbulent-kinetic energy 'κ' and its dissipation rate 'ε', and is expressed by the following equations:

$$\frac{\partial k}{\partial t}+\frac{\partial(U_j k)}{\partial x_i}=\frac{\partial}{\partial x_i}\left[\left(v+\frac{v_t}{\sigma_k}\right)+\frac{\partial(k)}{\partial x_i}\right]+P_k-\varepsilon \tag{5}$$

$$\frac{\partial \varepsilon}{\partial t}+\frac{\partial(U_j \varepsilon)}{\partial x_i}=\frac{\partial}{\partial x_i}\left[\left(v+\frac{v_t}{\sigma_\varepsilon}\right)+\frac{\partial(\varepsilon)}{\partial x_i}\right]+C_{1\varepsilon}P_k\frac{\varepsilon}{k}-C_{2\varepsilon}\frac{\varepsilon^2}{k} \tag{6}$$

where v = viscosity of fluids and P_k = production for turbulence given by:

$$Pk=\overline{u'_i u'_j}\frac{\partial U_j}{\partial x_i}=\left[v_t\left(\frac{\partial U_i}{\partial x_j}+\frac{\partial U_j}{\partial x_i}\right)-\frac{2}{3}\delta_{ij}\right]\frac{\partial U_j}{\partial x_i} \tag{7}$$

The values of the model constants are as follows: $\sigma_k = 1.0$, $\sigma_\varepsilon = 1.3$, $C_{1\varepsilon} = 1.44$, $C_{2\varepsilon} = 1.92$, $C\mu = 0.09$ [11].

The transport equation for an arbitrary, user-defined scalar (UDS) is solved similarly to the transport equation for a scalar such as species mass fraction. For multiphase flow, the generic transport equation for the scalar is given by

$$\frac{\partial \rho_m \varphi}{\partial t} + \nabla \cdot \left(\rho_m \overline{\upsilon} \varphi_m - \Gamma_m \nabla \varphi \right) = S \tag{8}$$

where φ is the local mean age of the fluid, ρ_m is the mixture density, $\overline{\upsilon}$ mixture velocity, Γ_m is the mixture diffusion coefficient for the scalar, S is the source term of the scalar and ρ_m, $\overline{\upsilon}$ and Γ_m are calculated according to

$$\rho_m = \sum_l \alpha_l \rho_l \tag{9}$$

$$\rho_m \overline{\upsilon}_m = \sum_l \alpha_l \rho_l \overline{\upsilon}_l \tag{10}$$

$$\Gamma_m = \sum_l \alpha_l \Gamma_l \tag{11}$$

where α is the volume fraction

Boundary condition

Different boundary condition was set until appropriate condition at domain boundaries have been specified. In the present study, mass flow inlet boundary condition for the inlet 1 and inlet 2 of the channel and pressure outlet boundary condition for the outlet of the channel is specified (see Fig. 2). The no-slip boundary condition is specified to set the velocity to be zero at the solid boundaries and walls and bed assumed to be rough. The solution is considered to be converged when the difference between successive iterations is less than 10^{-6} for all variables in all 3 different scenarios.

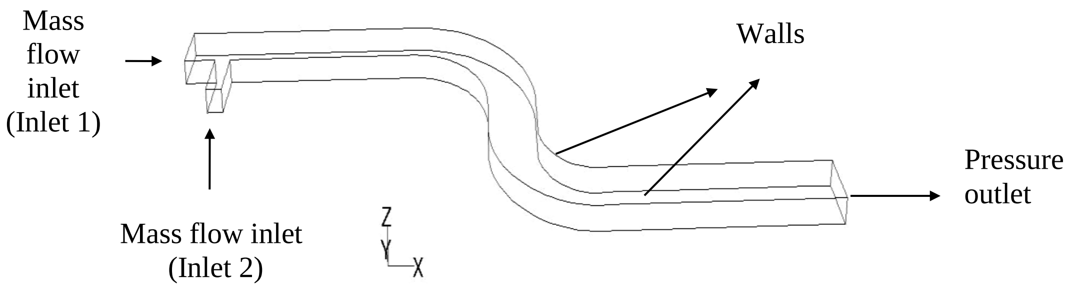

Fig. 2. Boundary condition adopted in the study

Numerical methods

Numerical computations were carried out using Fluent 6.2.16 which is based on the finite volume approach. It provides flexibility in choosing discretization schemes for each governing equation. The discretized equations, along with the initial and boundary conditions, were solved using the segregated solution method in which the governing equations were solved sequentially (segregated from one another) [10]. In order to discretize the solution, the first order upwind scheme was used which is one of the simplest and most stable discretization scheme. The PISO (Pressure implicit with splitting of operator) method was considered to calculate the pressure–velocity coupling. This method can maintain a stable pressure-velocity calculation for the Navier-Stokes equations for computation of unsteady free surface flow.

3. Results and discussion

In order to explore the effect of side discharges and velocities on the dispersion behavior of the pollutant from Arges River as a tributary on the Danube River, three different scenarios were considered and each scenario has three different values of diffusivity coefficients. As shown in Table 1 that the Danube River has discharges values ranging (4000 – 10000) m^3/sec and Arges River between (50 – 90) m^3/sec [14]. Consequently, three cases were presented in which it was assumed three different values of flow rate in the Danube River and a fixed value in Arges River in each case. Moreover, each case has three different values of diffusivity coefficient (see Table 2).

Table 2

The three adopted scenarios of this study.

Adopted Scenarios		Danube River Discharges (m^3/sec)	Arges River Discharges (m^3/sec)	Diffusivity coefficient (m^2/sec)
Case 1	**a**	4000	90	5
	b	4000	90	10
	c	4000	90	15
Case 2	**a**	7000	90	5
	b	7000	90	10
	c	7000	90	15
Case 3	**a**	9000	90	5
	b	9000	90	10
	c	9000	90	15

The value adopted in this study is demonstrating the present values in the Danube river and its tributary (Arges river). The BOD concentrations were set as fixed values in all cases and it was assumed 5 mg/L in the inlet 1 (main channel) and 40 mg/L in the inlet 2 (tributary) as these values stated in the previous technical reports and studies [15, 16]. The results of dispersion of BOD along the channel for all cases are shown in Fig 3. BOD concentration along Danube River in a plot direction (1, 0, 0) has been shown in Fig 4.

In case 1a, diffusivity = 5 m^2/sec, it can be seen that the BOD dispersed from the side discharge (Arges River) downstream which causing decreases in its concentration due to dilution process. Moreover, BOD concentration returns to its origin concentration of 5 mg/L at about 30 km downstream distance (Fig. 3a). It was observed that the increase in value of diffusivity (case 1b and 1c), the transverse dispersion of BOD increases (Fig. 3b and 3c). The self-purification process is one of the most important indicators for the river health. It can be seen that this process is highly affect the BOD concentration in this case.

In case 2a, the concentration of BOD was dispersed at long distance in this case in which Less BOD concentration was observed at almost 35 km longitudinal distance which is more than 5 mg/L (see Fig. 3d). Therefore, self-purification process is become slower than the self-purification process of case 1. It is clear that the increase in value of diffusivity (case 2b and 2c in Table 2), the transverse dispersion of BOD increases (Fig. 3e and 3f).

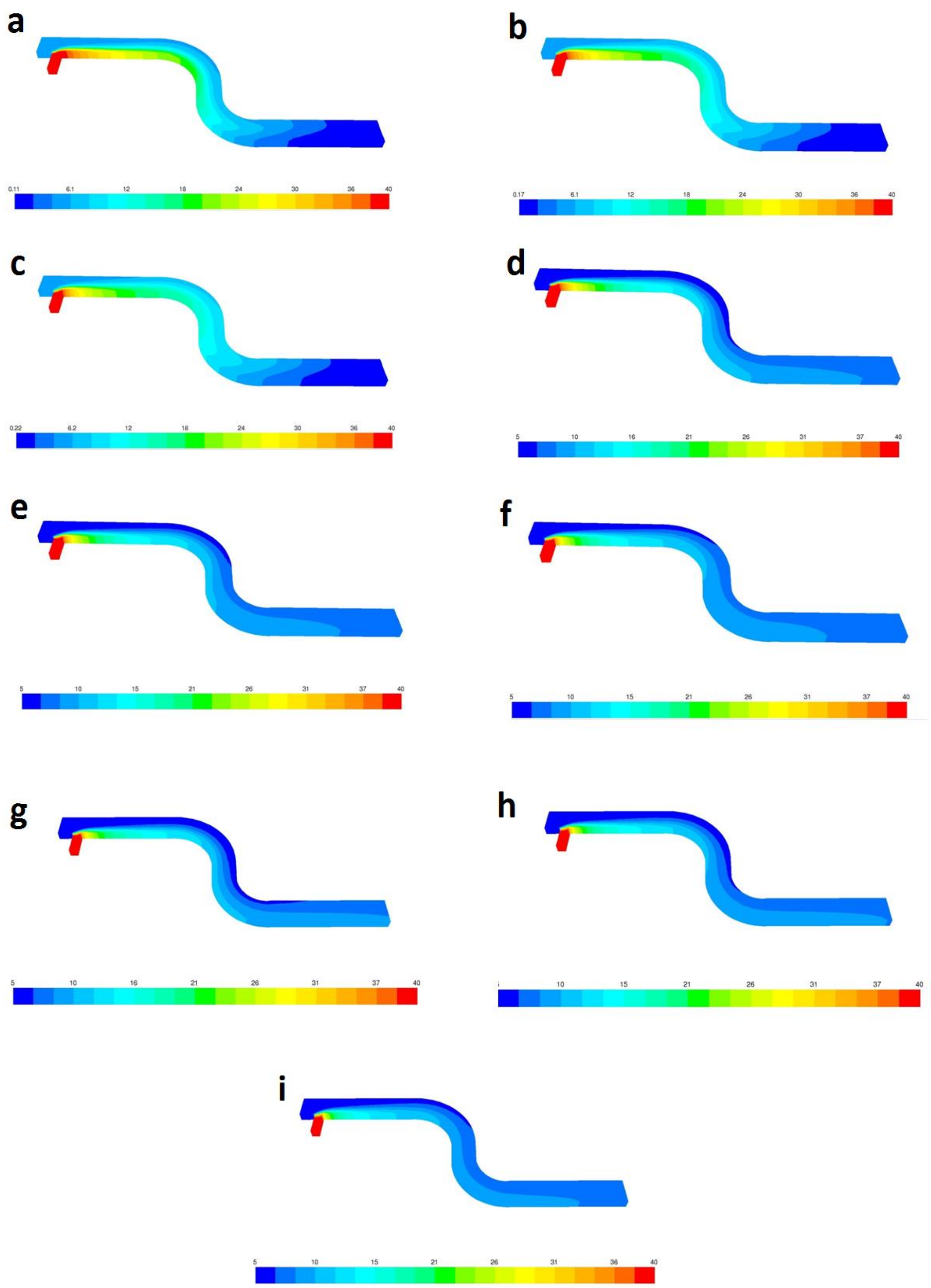

Fig. 3. The dispersion of BOD along the channel: a = case 1a, b = case 1b, c = case 1c, d = case 2a, e = case 2b, f = case 2c, g = case 3a, h = case 3b, i = case 3c in Table 2

In case 3, the concentration of BOD has been dispersed at longest distance than the two previous cases (1 and 2). BOD concentration does not return to its origin concentration of 5 mg/L. Less downstream BOD concentration was observed to be between (7 - 10) mg/L. Thus, self-purification process is become slower than the self-purification process of the previous cases (1 and 2).

Moreover, transverse dispersion of BOD in this case is very slow due to the high discharge in the Danube River (9000 m^3/sec) even with high variation of diffusivity coefficients (case 3a, 3b and 3c in Table 2).

Generally, according to high flow rate in the main channel, the dilution process of BOD concentration is quite clear in which the concentration of BOD is reduced downstream the channel (see Fig. 4). BOD concentration is dispersed more closely along the bank of the channel when the flow rate in the main channel is high (Case 3).

Comparison and agreement between the numerical simulation results and experimental data of BOD along the river which have been observed in the literature show some error between the results in cases 1, 2 and 3. The slight error in the simulation is evident and it is due to the obvious reason, in which the reaction kinetics process of BOD was not taken into consideration in the present study. However, the agreement between the prediction and the field observation is acceptable and the present model is reliable for the predictions the impact of Arges River as tributary on the Danube River. This may provide a quick estimate for BOD dispersion along the river.

The pollutant dispersion behavior in z-direction from the side discharge (Arges River) on the Danube River is tending to be different and dependent to the diffusivity coefficient. BOD concentration in z-direction decreases if the flow rate in the river is relatively high and thus, self-purification process is being slower. BOD reduction in the river is because of high dilution rates.

Furthermore, side discharge effluent into rivers is accompanied by the development of an area downstream due to reattachment of the effluent on the river bank. This phenomenon is linked to the presence of large scale turbulence is observed in rivers and natural flows where the lateral flow continues almost undisturbed along the river bank distances and even after long distance downstream of the river.

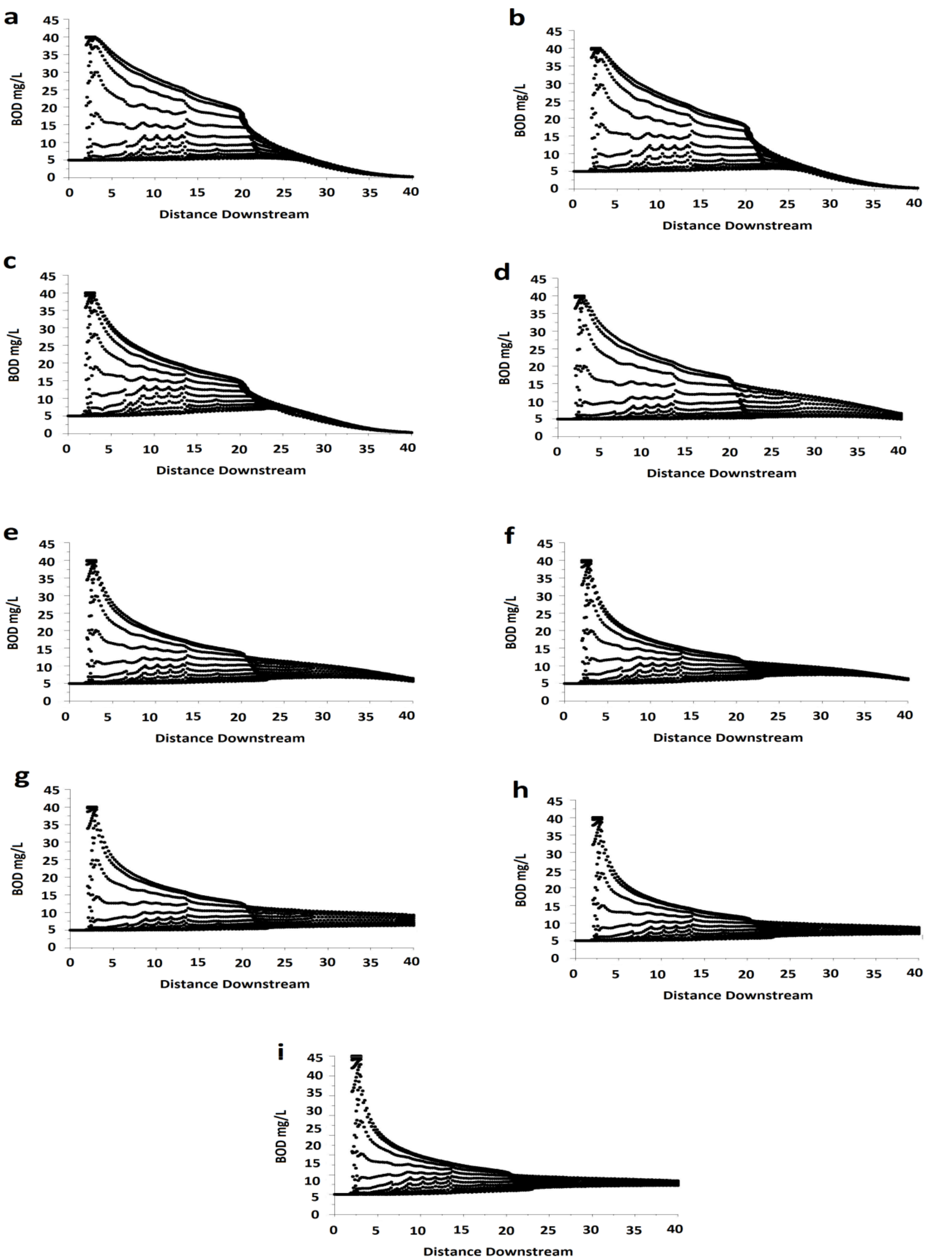

Fig. 4. BOD concentration along Danube River in a plot direction (1, 0, 0), a = case 1a, b = case 1b, c = case 1c, d = case 2a, e = case 2b, f = case 2c, g = case 3a, h = case 3b, I = case 3c in Table 2

4. Conclusions

Pollutant dispersion of curved-shaped open channel flow with a side discharge has been investigated using 3D numerical model. Numerical computations were carried out using Fluent 6.2.16, which is based on the finite volume approach.

The results revealed that according to high flow rate in the main channel (Danube river), the dilution process of BOD concentration is quite clear in which the concentration of BOD is reduced downstream the channel. BOD concentration is dispersed more closely along the bank of the channel when the flow rate in the main channel is high. The pollutant dispersion behavior from the side discharge (Arges River) on the Danube River is tending to be different and dependent to the diffusivity coefficient. It was observed that the increase in value of diffusivity, the transverse dispersion of BOD increases.

BOD concentration returns to its origin concentration of 5 mg/L at about 30 km distance for case 1. whereas in case 2, the concentration of BOD was dispersed at long distance in which less BOD concentration was observed at almost 35 km longitudinal distance which is more than 5 mg/L. In case 3, the concentration of BOD has been dispersed at longest distance than the two previous cases (1 and 2). BOD concentration does not return to its origin concentration of 5 mg/L. Flow rate can highly affect the self-purification process which it becomes slower at high flow rate

Furthermore, side discharge effluent into rivers is accompanied by the development of an area downstream due to reattachment of the effluent on the river bank. This phenomenon is linked to the presence of large scale turbulence which has been observed in the Danube River.

Moreover, this study may be extended to consider the transformation process of the conservative pollutant (BOD) in order to obtain the results in more representative form.

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