Two-dimensional simulation of pollutant dispersion at the confluence of Diyala river with Tigris river using CFD technique

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Abstract

The main aim of this paper is to simulate the pollutant dispersion behavior from Diyala River as a tributary on the Tigris River using a two-dimensional numerical model. Numerical computations were achieved using computational fluid dynamic (CFD) code, which is based on the finite volume approach. Biochemical oxygen demand (BOD) was selected as a pollutant for the simulation process as it is a very important water quality parameter in rivers and streams. It is presumed that BOD is mixed throughout the system as a passive scalar. Furthermore, 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. The numerical simulation results show a good fit with observed data. The findings of this study may provide a proper basis for water quality management in rivers.

Keywords: Water dispersion, BOD, Tigris river, Diyala river, CFD

محاكاة ثنائية الأبعاد لتشتت الملوثات عند التقاء نهري ديالى مع نهر دجلة باستخدام تقنية CFD

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الخلاصة

ان الهدف الرئيسي في هذا البحث هو عمل محاكاة لسلوك تشتت الملوثات من نهر ديالى كرافد على نهر دجلة باستخدام نموذج رياضي ثنائي الأبعاد. تم إجراء الحسابات الرياضية باستخدام تقنية ديناميكيات الموائع الحسابية Computational Fluid Dynamics (CFD) ، والذي يعتمد على طريقة الحجم المحدود. تم اعتماد المطلب الحيوي للأوكسجين (BOD) في عملية المحاكاة كعامل تلوث مهم لجودة المياه في الانهار والجداول. وقد تم أفتراض ان BOD كملوث يختلط في جميع أنحاء النظام باعتباره عددًا سلبيًا. من جانب اخر ، تم استخدام حجم المائع Volume of Fluid (VOF) والطرق الرياضية المعرفة من قبل المستخدم user defined scalar(USD). في هذه الدراسة، تم استخدام طريقة VOF للسماح للسطح الحر بالتداخل بحرية مع الاضطراب الأساسي. أظهرت نتائج المحاكاة الرياضية توافقًا جيدًا مع البيانات المرصودة. وقد توفر نتائج هذه الدراسة أساسًا مناسبًا لإدارة جودة المياه في الأنهار.

الكلمات المفتاحية: تشتت الملوثات، المطلب الحيوي للأوكسجين، نهر دجلة، نهر ديالى، ديناميكيات الموائع الحسابية

Introduction

Open channel flow such as rivers and streams are the major sources for drinking and irrigation. The water quality of rivers and streams has deteriorated in recent years, especially in developing countries including Iraq (Ismail , et.al.,2014; Zowain and Ismail 2015). This deterioration is due to several reasons such as misuse of water, increasing demand for water, and discharge of wastewater into rivers without adequate treatment (Ismail, et.al.,2019; Ismail , et.al.,2020). Moreover, the shortage of water flows was another reason for the deterioration of water quality (Abbas , et.al.,2016; Ghalib 2017).
The present study attempts to study the pollutant dispersion at the confluence of Diyala river with Tigris river. Diyala river in its lower course is characterized by poor water quality due to many outfalls that are discharged into the river without sufficient treatment, such as the Alrustumiah wastewater treatment plant and the army canal (Ismail and Muntasir 2018; Ismail and Abed 2013; Al-Rubaie and Al-Musawi 2019).
Furthermore, the fate and transport of pollutants in rivers are most significant for best water quality management. Mathematical modeling has been extensively used as an effective tool to predict pollutant transport in rivers. Numerous studies have been conducted to understand the transport phenomena and the change in the concentration of the pollutant in order to explore the impact of these pollutants and to aid the decision-makers in preserving the surface water quality (Deng and Jung 2009; Duarte and Boaventura 2008; Abderrezzak , et.al.,2015; Popescu , et.al.,2015).
Numerous studies were carried out to assess and monitor the water quality in the Diyala river. However, few studies were conducted on the dispersal of pollutants in the confluence area between Tigris and Diyala rivers (Dawood and Rasheed 2005; Ismail and Muntasir 2018; Al-Rubaie and Al-Musawi 2019; Abed , et.al.,2021). Therefore, the present study aimed to simulate the pollutants dispersal using the CFD code (Ansys-Fluent). CFD technique has been extensively used for different engineering applications (Babaali , et.al.,2015). The study examined the effect of different scenarios of flow rate on the BOD dispersion at the confluence area between Diyala and Tigris rivers.

Materials and Methods

Assumptions

Ansys-Fluent (CFD code) was used in this study in order to predict the dispersal of polluting behavior of Diyala River, which is one of the sources points of pollution in Tigris River. Fig. 1 shows the geometry and the boundary condition of the study beside the meshing generation. Based on different flow conditions, BOD was chosen as a non-conservative pollutant for the simulation process in order to investigate the different BOD dispersal scenarios. If the BOD is a passive scalar, it is assumed to be a liquid form and mixed throughout the system, and there are no sources or sinks of pollutants in the study area (Ismail and Robescu 2017).

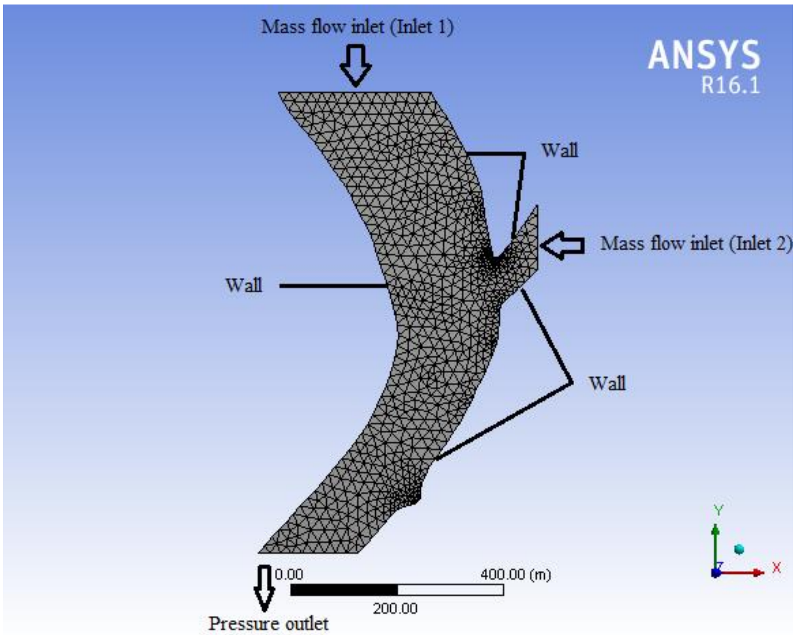

Figure (1) : Geometry, boundary condition and mesh of the study area.

To perform the numerical modeling, VOF and UDS techniques were used. For VOF, Euler-Euler multiphase models were chosen as this model is widely used for simulating the pollutant dispersion in an open channel flow (Ismail and Robescu 2017; Ismail and Robescu 2016; Khaldi , et.al.,2014; Khaldi , et.al.,2015).

Data required for modelling

The simulation process data in this study included two approaches: water quality data and river's hydraulic characteristics. In the first approach, grab water samples were collected from eighteen points (30 cm depth) in two different months April 2021 and August 2021. Fig. 2 shows the sampling locations in the study area. Table 1 shows the coordinates of water sampling in the study area. Water samples for BOD were collected in non-reactive borosilicate glass BOD bottles (300 mL capacity) and measured using Standard Winkler method at the Labs of the National Center for Water Resources Management. In the second approach, represented by the river hydraulic characteristics, the river discharge was obtained using an Acoustic Doppler Current Profiler (ADCP). This device is used to measure the total water transport in river. The process needs a rowboat with an ADCP mounted over the side to cross from one bank to another while measuring continuously (see Fig. 2). Table 2 shows the adopted values of flow rate in the Tigris and Diyala rivers, beside their BOD values for both rivers.

Figure (2) : Sampling locations in the study area and the ADCP device.

Table (1): Coordinates of water sampling

Sampling code	X	Y
TA	453217	3676596
TB1	453954	3675899
TB2	453934	3675897
TB3	453929	3675874
TB4	453913	3675848
TB5	453888	3675815
TB6	453856	3675781
TB7	453800	3675744
TB8	453769	3675736
TC1	453976	3675838
TC2	453969	3675831
TC3	453930	3675763
TC4	453895	3675724
TC5	453861	3675663
TC6	453794	3675568
TC7	453743	3675513
TC8	453666	3675480
TD1	453105	3674448
TD2	453022	3674492
TD3	452901	3674574
TE	452230	3673185
D1	457024	3683681
D2	456984	3683388
DA	457060	3681974
DB	456866	3681429
DC	456061	3681764
DD	455209	3681140
DE	456112	3679706
DF	455887	3678163
DG1	454597	3676734
DG2	454582	3676753
DG3	454557	3676779
DH1	454031	3675858
DH2	454019	3675853

DH3	454009	3675883
DH4	453995	3675893
DH5	453984	3675908

Model calibration

In this study, the model was calibrated using data from April 2021, besides applying a diffusion coefficient at a rate of 10 m2/s, as reported by Ismail and Muntasir , 2018. In order to obtain a high-quality data matrix, a lot of simulations were performed by adjusting these coefficients to obtain high-reliability outputs with the observed data. The model is validated using data from August 2021 without changing the calibrated coefficients to examine the ability of the calibrated model.

Table (2): Adopted scenarios of the present study

Adopted Scenarios	Tigris River		Diyala River		Date/status
	Discharges (m^3/sec)	BOD mg/L	Discharges (m^3/sec)	BOD mg/L	
Calibrated	455	5	30	12	26/4/2021
Verified	569	4	7.6	15	30/8/2021
Scenario 1	870*	3	850*	5	High flow
Scenario 2	355*	4	5*	25	Low flow
Scenario 3	520*	4	62*	16	Average flow

Governing equations

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

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

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

where U = velocity vector in the three directions; p = pressure; v = molecular viscosity; g = gravitational acceleration in the three directions, and ρ = density of flow. In the momentum Eq. (2) the interaction between the phases is modeled by the surface tension *Si,s*.

It is worth emphasizing, in this study, that the air is the initial phase, and water is the secondary phase. The interface between phases is traced with continuity solution Eq. (1) for the secondary phase (water). This interface is calculated using the following equation (Ismail and Robescu 2017):

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

where S_2 = source of the phase 2 (S_2 is equal to zero in this work), ρ_2 = density of the secondary phase and α_2 = volume fraction of the secondary phase (α_2 = $V2/V$). V = 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:

$$\sum_{i=1}^{2}\alpha_{i=1} \qquad (4)$$

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:

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

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

(6)

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

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

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, Cμ = 0.09 (Ismail and Robescu 2017).

Similar to the transport equation for a scalar, such as the mass fraction of species, the transport equation for an arbitrary user-defined scalar (UDS) is solved. For a multiphase flow, the generic transport equation for the scalar is presented as follows:

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

where φ = local mean age of the fluid, ρ_m = mixture density, $\overline{\upsilon}$ mixture velocity, Γ_m = mixture diffusion coefficient for the scalar, S = 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 = volume fraction

Boundary condition

When one determines a proper condition in the field boundaries, different boundary conditions can be determined. In this context, and considering Fig. 1, it can be determined the condition of the mass flow inlet boundary of inlet 1 and inlet 2 channels and the condition of the pressure outlet boundary of the outlet channel. In order to set the velocity to zero at the solid boundaries, the condition of non-slip boundary must be set, as well as assuming that the walls and bed are rough. In all simulated scenarios, when the difference between successive iterations is less than 10^{-6} for all variables, the solution can be considered convergent.

Numerical methods

Ansys-Fluent is used in this study to perform the numerical computations because it relies on the finite volume approach and also provides flexibility in choosing discretization schemes for all governing equations. By using the segregated solution method, the discretized equations are solved beside the initial and boundary conditions, and the governing equations are also solved sequentially (segregated from one another) (Khaldi , et.al.,2014). The first-order upwind scheme, which is one of the simplest and most stable discretization schemes, was used to discretize the solution. In order to calculate the pressure-velocity coupling, the PISO (Pressure implicit with the splitting of the operator) method was adopted, which can maintain the pressure-velocity stability of the Navier-Stokes equations to calculate the unsteady free surface flow.

Results and Discussion

In order to investigate the influence flow rates on the dispersion behavior of the pollutant from Diyala River as a tributary and Tigris river, different scenarios were considered. The calibrated results are shown in Figure (3) In April 2021, the BOD concentration is 12 mg/L, flow rate of 30 m^3/s and 5 mg/L, flow rate 455 m^3/s in Diyala and Tigris rivers, respectively. As seen from Fig. 3, the BOD is dispersed downstream along the river bank. BOD dispersed from the side discharge (Diyala River) downstream, causing decreases in its concentration due to the dilution process. BOD concentration does not return to its original concentration of 5 mg/L at a distance of about 1 km downstream. The self-purification process is one of the most important indicators for the river health. It is clear that this process is very slow due to the high flow in Tigris river. Figure (4) shows the calibrated and observed results of BOD. The results have shown a good agreement between simulated and observed results in which the agreement between the prediction and the field observation is acceptable and the present model is reliable for the predictions of the impact of Diyala River as tributary on the Tigris River.

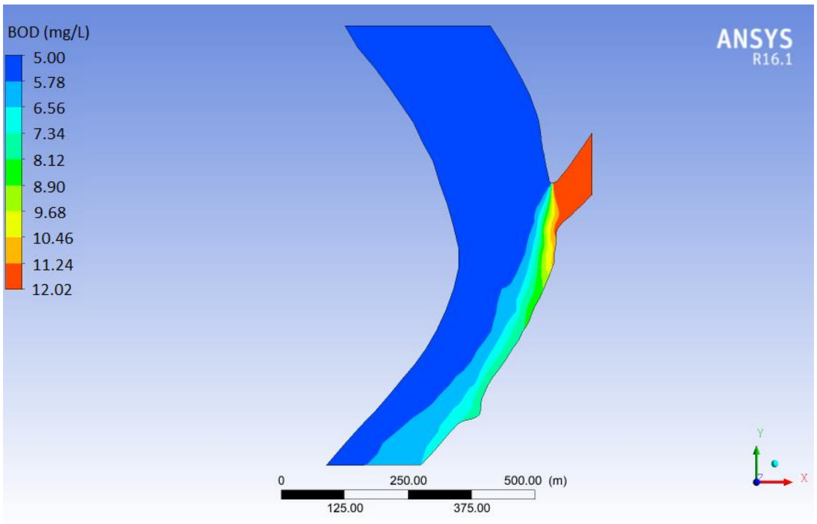

Figure (3) : Calibrated results of BOD dispersion along the confluence, Q_{Diyala} = 30 m^3/s, Q_{Tigris} = 455 m^3/s (April 2021).

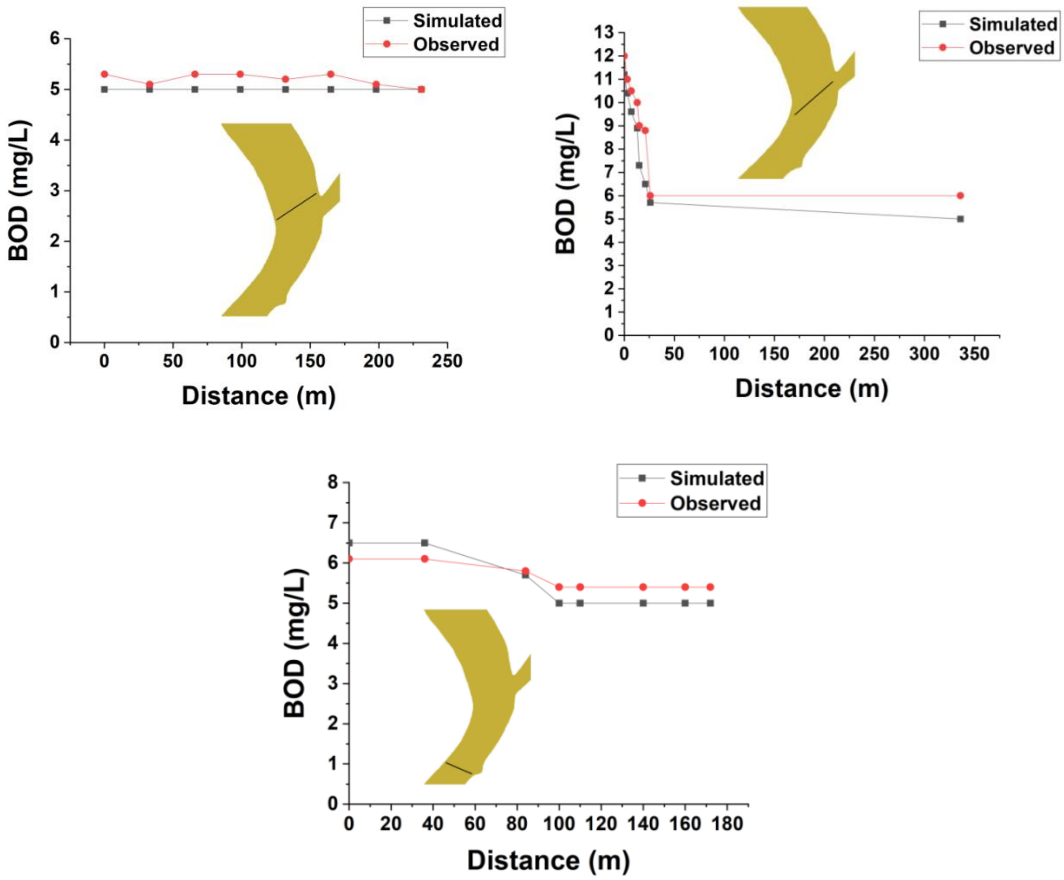

Figure (4) : Calibrated vs. Simulated results of BOD dispersion.

The validation results are shown in Figure (5) using field data observed in the dry season. The flow in Diyala river is very low and according to the high flow rate in the Tigris river (569 m^3/s), the dilution process of BOD concentration is quite clear in which the concentration of BOD is reduced downstream the channel. Moreover, BOD concentration is dispersed more closely along the bank of the channel when the flow rate in the Tigris river is high, i.e. the highest the flow rate in the Tigris river, the dispersion behavior tend to be along the bank of the channel as depicted in the Figure (5). Furthermore, it was observed that the BOD concentration returned to its original concentration of 4 mg/L at about less than 1 km downstream distance. The dilution process is obvious in this case. Figure (6) shows the validation and observed results of BOD. It should be noticed that in the validation process, the simulation was performed on data from August 2021 without changing the calibrated coefficients to examine the ability of the calibrated model. However, the validation results have shown a good agreement between simulated and observed results (Figure (6)).

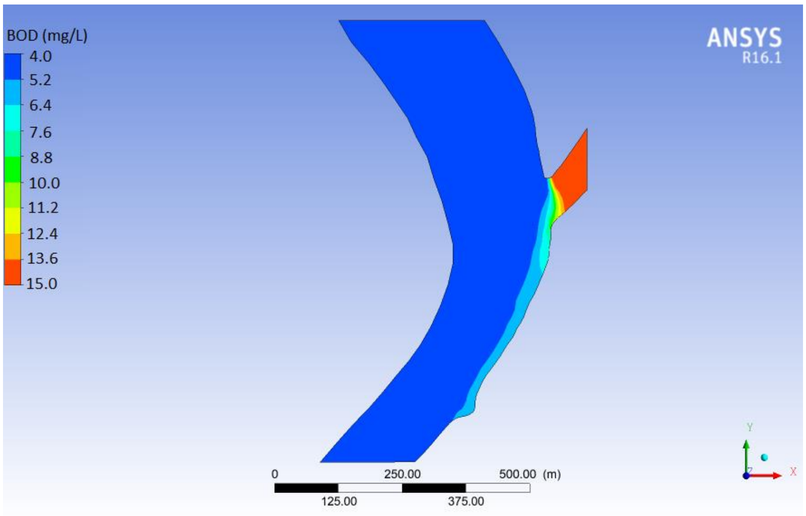

Figure (5) : Validation results of BOD dispersion along the confluence, Q_{Diyala} = 7.6 m^3/s, Q_{Tigris} = 569 m^3/s (April 2021).

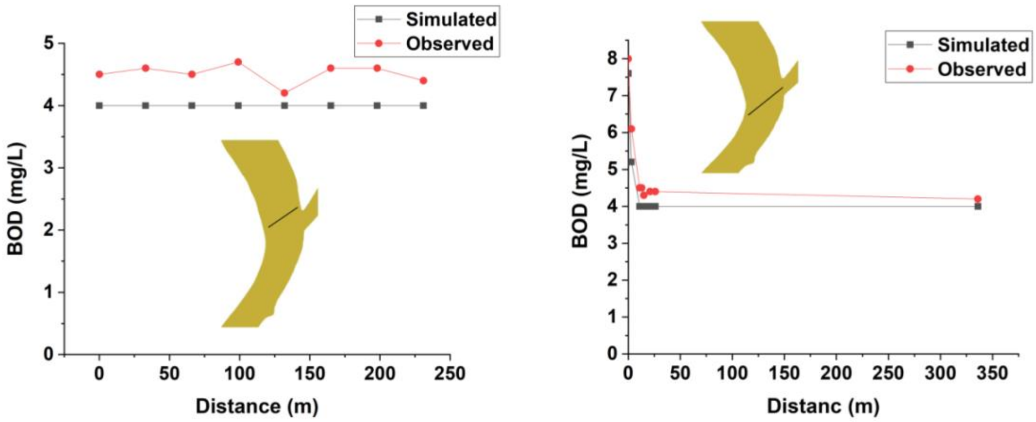

Figure (6) : Validated vs. Simulated results of BOD dispersion.

Three more scenarios were explored in order to provide a good basis and information about the relationship between the concentrations of pollutants and flow rate at the confluence of Diyala river with Tigris river. Table 2 shows the scenarios adopted for high, average and low flow along with BOD concentrations recorded by National Center for Water Resources Management during the last two decades (MOWR, 2021). Figure (7,8 and 9) demonstrate the BOD dispersion behavior during high, low and average flow, respectively. It can be seen from Figure (7) that the self-purification process in the river is very slow due to the high flow season in both rivers. This case rarely occurs, however, the BOD concentrations recorded are very low due to the dilution process.

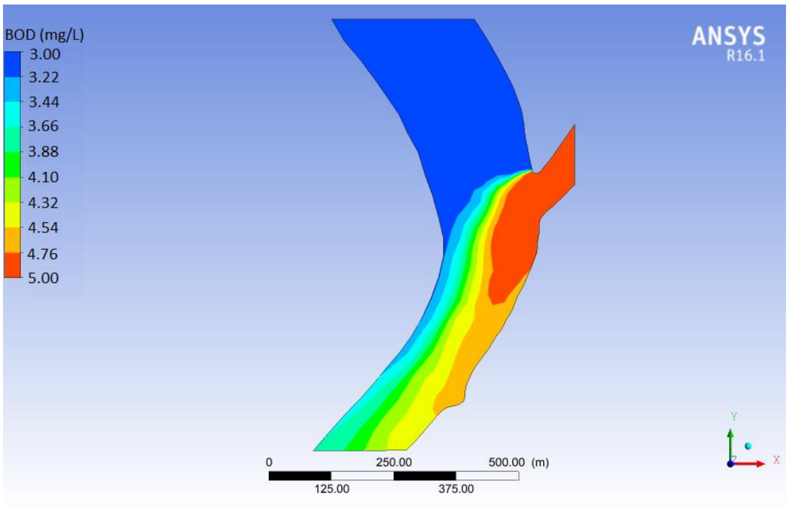

Figure (7) : High flow, Q_{Diyala} = 850 m^3/s, Q_{Tigris} = 870 m^3/s.

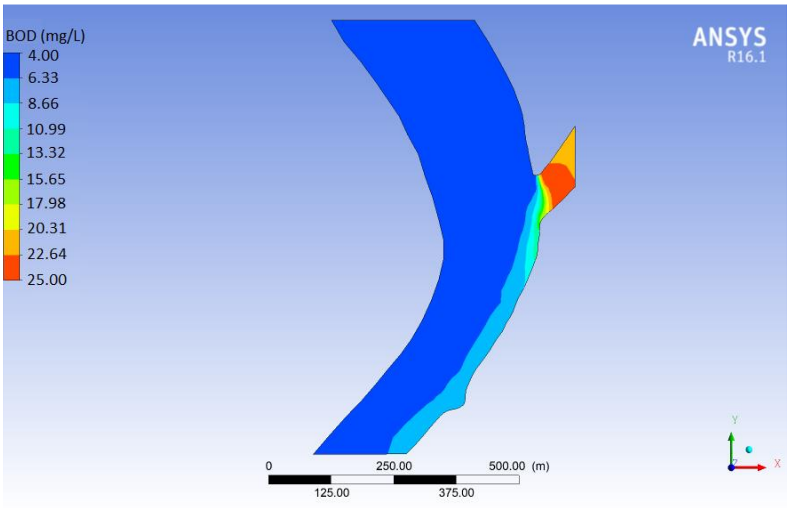

Figure (8) : Low flow, Q_{Diyala} = 5 m^3/s, Q_{Tigris} = 355 m^3/s.

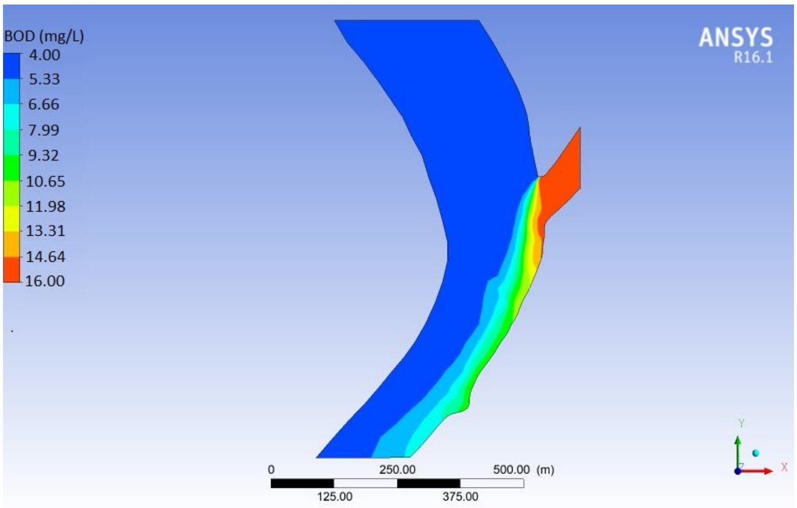

Figure (9) : Average flow, Q_{Diyala} = 62 m^3/s, Q_{Tigris} = 520 m^3/s.

In low flow case (Fig. 8), the concentration of BOD has been dispersed to a least distance than the previous case (i.e. the dispersion behavior tends to be along the bank of the rivers due to low flow condition in Diyala river). The same is true with average flow (Figure (9)). Generally, BOD concentration does not return to its original concentration in all simulated cases. Less downstream BOD concentration was observed to be close to 8 mg/L. Ismail and Muntasir ,2018 have used FlexPDE CFD code to solve a two-dimensional advection-dispersion equation to predict the pollutant concentration at the confluence of the Diyala river with the Tigris River. However, they stated that some errors in the simulation results, especially for the simulation of BOD. FlexPDE relies on the finite element method rather than the finite volume method used in the present study. Accordingly, the results of this study are more precise in describing the behavior of BOD dispersion in the study area.

In general, the water quality of Diyala river is deteriorated due to the high concentration of BOD which ranges from 12 to 15 mg/L during April 2021 and August 2021, respectively. Diyala River is characterized by low dissolved oxygen and high BOD concentration in the lower reach (south Baghdad). Various outflows are discharged to the river without adequate treatment. Besides, there is no existing plan to maintain the quality of the river (Abbas , et.al.,2016; Ismail and Muntasir 2018). Kannel , et.al.,2007) stated that the BOD concentration in rivers should not exceed 4 mg/L. This is not the case in the Diyala river and preparing an action plan is extremely important by authorities in order to preserve the rivers from organic pollution. Furthermore, the Tigris river is highly affected by the organic load from the Diyala river, in which BOD concentrations ranged from 4 to 9 mg/L at the left bank for a distance of more than one kilometer in all cases except for validation results.

Conclusions

Pollutant dispersion using the CFD technique has been investigated employing a 2D numerical model. Numerical computations were carried out using Ansys-Fluent, which is based on the finite volume approach. The study comprised the effect of flow rate and diffusivity coefficient on the dispersion behavior of BOD at the confluence of Diyala river with Tigris river. The simulated results showed a good agreement with the observed field data. BOD dispersion is mostly controlled by the dilution process and the self-purification process in the rivers. The water quality of the Diyala river is deteriorated and BOD concentration ranges from 12 to 15 mg/L due to various outflows being discharged to the river without adequate treatment. BOD values should be kept at more than 4 mg/L to preserve the aquatic life in the river and to be suitable for other uses. On the other hand, preserving the Tigris river from organic pollution as the Diyala river is a tributary. Moreover, it is concluded that the Tigris river is highly affected by the organic load from the Diyala river, in which BOD concentrations ranged from 4 to 9 mg/L at the left bank for a distance of more than one kilometer in all cases except for validation results. The findings of this study may provide a proper basis for decision-makers in order to sustain the water quality in the study area. Moreover, this study may serve as a basis for understanding the effect of the flow rate on the concentration of pollutants from the polluted tributary on the river.

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