Estimation of river Tigris dispersivities using a steady-state numerical model

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Received: 6 February 2018 / Accepted: 12 June 2018 / Published online: 26 June 2018
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Abstract

The present work suggests a simple approach for simulating the dispersion of pollutants in rivers and streams with the aid of computational fluid dynamics technique. The two-dimensional advection–dispersion equation was solved using FlexPDE code to predict the biochemical oxygen demand (BOD) and the total dissolved solids (TDS) concentrations at the confluence of Diyala with Tigris Rivers. In this model, two sets of data were used for calibration and validation processes. Various values of longitudinal and transverse dispersion coefficients were adopted in the model to determine the suitable value using the trial-and-error method. The results revealed that the best agreement between simulated and measured values was observed when the longitudinal and transverse dispersion coefficients are close to 10 and 5 m²/s, respectively. The results showed that the proposed methodology is more suitable for TDS, while for BOD, it needs an accurate representation of the chemical or biological transformations.

Keywords Pollutant transport · Diyala River · Tigris River · Water quality · FlexPDE

Introduction

Recently, attention has been paid to study the quality of the river water, given its importance as a major and vital source of many human activities such as agriculture, industry and water supply. Various anthropogenic factors have caused the increase in pollutant concentration in rivers such as urbanization and industrialization (Ismail et al. 2014). These pollutants are discharged into the rivers, sometimes without adequate treatment, and affect their quality adversely. River systems are very complex due to many processes (physical, chemical and biological) involved in their ecosystem. Numerous studies have been carried out concerning the river pollution issues, and perhaps the most prominent are those related to water quality modeling and simulation of the pollutant transport in the rivers (Sharma and Kansal 2013).

The majority of the pollutant transport simulation in surface waters depends on the advection–dispersion equation (ADE), a partial differential equation (PDE) (Ani et al.

2009). Numerical models have been extensively studied and developed in the literature to predict the pollutant spreading into rivers, and the most of them are one-dimensional. However, not every model is comprehensive enough and can provide all of the functionality required. On the other hand, analytical solutions have also been proposed for such cases (Zeng et al. 2015). Abderrezzak et al. (2015) stated that the application of analytical solutions to field cases is questionable.

The primary challenge of solving the ADE equation is the measurement of the dispersion coefficients, in which it is the major task for solving problems of pollutant transport in rivers. The suitable method to resolve the ADE equation is by providing estimates for all the involved terms in the equation to be known except the dispersion coefficients, which become the only unknown of the problem (Benedini and Tsakiris 2013). However, field tracer studies to obtain data on concentration profiles are an arduous process and can be costly and time-consuming, especially for deep and wide rivers (Kim 2012). Moreover, the estimated dispersion coefficients through a tracer experiment are valid for only the examined stream segment (Abderrezzak et al. 2015). Consequently, numerous studies were conducted to develop empirical formulas for the determination of both the longitudinal and transverse dispersion coefficients (Fischer 1967; Fischer

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et al. 1997; Seo and Cheong 1998; Baek and Seo 2013), or sometimes the coefficients are achieved by researcher's own experience (Velísková et al. 2014). Detailed and brief reviews and comparison of these empirical formulas can be found in Seo and Cheong (1998) and Baek and Seo (2016). Unfortunately, when applying these formulas on one river, the calculated dispersion coefficients may vary over several orders of magnitude (Abderrezzak et al. 2015; Benedini and Tsakiris 2013). Therefore, the issue of estimating the dispersion coefficients is still a challenge.

According to above, the present paper does not use the empirical formulas nor the field tracer experiment for the estimation of the dispersion coefficients. A simple approach was introduced by offering a simplified model through solving the ADE equation (two-dimensional forms) using CFD code. CFD technique has been widely used to provide valuable information relating to the description of the water flow hydrodynamics and the pollutant behavior along the river and stream (Khaldi et al. 2014). In this paper, an attempt has been undertaken to predict the pollutant concentration at the confluence of Diyala River with the Tigris River, southeast of Baghdad. The dispersion coefficients (longitudinal and transverse) were chosen as parameters to be calibrated by the trial-and-error method, whereas other input parameters were measured through field experiments. Two pollutants (conservative and non-conservative) were selected for simulation

process, namely biochemical oxygen demand (BOD) and total dissolved solids (TDS). BOD parameter is relatively complex in both assessment and simulation due to the fact that the organic matter is typically not uniformly dispersed in the water mass. Furthermore, BOD determination takes long time (5 days), according to the local practice and standards. In the present paper, the aim of selecting BOD was due to its importance in the Diyala River. Moreover, numerous studies have stated that the BOD concentration is relatively high in the river.

Materials and methods

Study area

Diyala River (or Sirwan) is one of the major tributaries of Tigris River in Iraq. Diyala River arises in the Zagros Mountains in Iran and enters Iraq from the eastern part, and then it runs for 386 km until its confluence with Tigris River near Jisr Diyala area, southeast Baghdad (Fig. 1). Diyala River can be classified according to the topography of the area into four regions: upper Darbandikhan dam, upper Diyala, central Diyala and lower Diyala (Hamza 2012). The latter region is considered the most polluted one due to the presence of various drains and effluents which discharge their water in

Fig. 1 Map of the study area, **a** Iraq, **b** Baghdad governorate, **c** urban area of Baghdad, **d** sampling locations

the river such as Khalis North irrigation drainage outfall, Al-Nahrawan irrigation drainage outfall, Saria North irrigation drainage outfall, Khalis North irrigation drainage outfall, new Al-Rustamiyah wastewater treatment plant outfall, old Al-Rustamiyah wastewater treatment plant outfall and the Army canal (Dawood and Rasheed 2005).

The average annual flow discharge of the Tigris and Diyala Rivers is 672 and 200 m³/s, respectively (Al-Ansari and Knutsson 2012). Water flows of the Tigris River have decreased annually in a dramatic way for the past two decades, due to the major water impoundment projects constructed by the neighboring countries (Turkey, Syria and Iran) (Al-Ansari and Knutsson 2011). Furthermore, the climate conditions vary in the river catchments. The rainy season starting from November to April, with an annual amount of precipitation varies from 800 mm near the northern parts to 250 mm near southern limits of the basin (Al-Ansari et al. 1987).

Accordingly, the water quality of Diyala River has been deteriorated during the last decades (Abbas et al. 2016), especially when no proper management plan has been placed by the authorities to preserve the quality of the river. Since the river is the third largest tributary of the Tigris River, the present study attempts to explore the effect of the water quality of the river on the Tigris River water quality by solving a numerical model to predict the pollutant transport at the confluence region of the rivers.

Overview of the modeling approach

Generally, the water quality of rivers is defined in terms of concentrations of the various reactive and non-reactive substances in the water. The mathematical models for concentration prediction are based on the principle of mass conservation. The three-dimensional (3D) ADE equation can be written as

$$\frac{\partial \bar{C}}{\partial t} + \frac{\partial}{\partial x}(\bar{u}\bar{C}) + \frac{\partial}{\partial y}(\bar{v}\bar{C}) + \frac{\partial}{\partial z}(\bar{w}\bar{C}) = D_m \left[\frac{\partial^2 \bar{C}}{\partial x^2} + \frac{\partial^2 \bar{C}}{\partial y^2} + \frac{\partial^2 \bar{C}}{\partial z^2} \right] + \frac{\partial}{\partial x} \left[\epsilon_x \frac{\partial \bar{C}}{\partial x} \right] + \frac{\partial}{\partial y} \left[\epsilon_y \frac{\partial \bar{C}}{\partial y} \right] + \frac{\partial}{\partial z} \left[\epsilon_z \frac{\partial \bar{C}}{\partial z} \right] + S + Q + R, \quad (1)$$

where $\bar{C}$ = substance concentration, t = time, $\bar{u}$, $\bar{v}$, $\bar{w}$ = average velocity in the three directions, ϵ_x = longitudinal dispersion coefficient, ϵ_y = transversal dispersion coefficient, ϵ_z = vertical dispersion coefficient, D_m = mass diffusion coefficient, S = sources and sinks due to settling and resuspension, Q = external loadings to the aquatic system from point and nonpoint sources, and R = reactions due to chemical and biological processes. The upper bar means that the respective quantities are averaged due to the turbulence.

Applications of 3D models require extensive data set, and this can lead to very complex models. On the other hand, the use of one-dimensional (1D) models would be

straightforward, especially for moderate rivers (e.g., Diyala River). The main flaw of the 1D model is that they are not capable of simulating the pollution spreading until the mixing of pollutants across the stream section becomes complete (Velísková et al. 2014). Two-dimensional (2D) model seems valid, and therefore, a 2D model was chosen in this study since they can adequately describe the modeled system.

Moreover, the turbulent diffusion in rivers is more predominant than the molecular diffusion (Ji 2008), and thus, the effect of molecular diffusion can be neglected ($D_m = 0$), in comparison with the turbulent dispersion. The term S in Eq. (1) refers to the settling and resuspension in the river. This term can be ignored due to relatively high river flow velocity in the river. The term Q in Eq. (1) indicates the external waste loadings which are joining the river as a point or nonpoint sources in the study region. Since there is no external loadings subjected to the river in the study area, the term $Q = 0$. According to the conditions mentioned above, the steady-state ADE equation becomes

$$\frac{\partial}{\partial x}(\bar{u}\bar{C}) + \frac{\partial}{\partial y}(\bar{v}\bar{C}) = \frac{\partial}{\partial x} \left[\epsilon_x \frac{\partial \bar{C}}{\partial x} \right] + \frac{\partial}{\partial y} \left[\epsilon_y \frac{\partial \bar{C}}{\partial y} \right] + R. \quad (2)$$

This study explores the dispersion behavior of two pollutants, namely BOD and TDS. The latter is a conservative pollutant, and therefore, there are no chemical or biological reactions. Hence, the term R is equal to zero and Eq. (2) will become

$$\frac{\partial}{\partial x}(\bar{u}\bar{C}) + \frac{\partial}{\partial y}(\bar{v}\bar{C}) = \frac{\partial}{\partial x} \left[\epsilon_x \frac{\partial \bar{C}}{\partial x} \right] + \frac{\partial}{\partial y} \left[\epsilon_y \frac{\partial \bar{C}}{\partial y} \right]. \quad (3)$$

BOD (non-conservative pollutant) requires a long time to be oxidized biologically, and according to the short distance of the modeled area (short residence time), the BOD kinetics may be ignored logically. However, the BOD outcome of the present model was not acceptable when neglecting

the transformation of BOD. Therefore, the last right term of Eq. (2) takes into account the BOD decay rates. It is considered first-order decay term for BOD kinetics:

$$\frac{\partial}{\partial x}(\bar{u}\bar{C}) + \frac{\partial}{\partial y}(\bar{v}\bar{C}) = \frac{\partial}{\partial x} \left[\epsilon_x \frac{\partial \bar{C}}{\partial x} \right] + \frac{\partial}{\partial y} \left[\epsilon_y \frac{\partial \bar{C}}{\partial y} \right] - K_r \bar{C}, \quad (4)$$

where K_r is the overall decay coefficient and involves both deoxygenation rates (k_d) and settling of carbonaceous organic matter (k_s)

$$K_r = k_d + k_s. \quad (5)$$

The effect of settling k_s has been neglected as it is more important for shallow water bodies with less than 1 m depth (Chapra 1997) and thus, $K_r = k_d$. The value of k_d in the Diyala River was estimated by long-term BOD analysis, since the organic matter required 20 days to be oxidized. The methodology of sampling and analysis is discussed in the next section.

Data requirement for the modeling

Two types of data are required for simulation process: water quality data and river's hydraulic characteristics. Grab water samples were collected in nine points (30 cm depth) at two different months June 2016 and February 2017 (Fig. 1). The samples for TDS analysis were collected in polypropylene bottles and analyzed using temperature-controlled oven method. Water samples for BOD estimation were collected in non-reactive borosilicate glass BOD bottles (300 mL capacity) and measured using standard Winkler method. Water temperature was measured in situ using the mercury thermometer. It should be noticed that the greater the number of samples taken from the river, the more accurate the calibration and validation process. The samples considered in this study may not be quite sufficient for simulation process; however, they can be reasonable for calibrating and validating the model.

Another set of samples were collected to estimate the river deoxygenation rate k_d by long-term BOD analysis using Thomas method (Thomas 1950). The estimated BOD bottle rates are often not similar to river deoxygenation rate because the river includes processes (e.g., bio-sorption and turbulence) not existing in the BOD bottle (Haider and Ali 2010). However, Wright and McDonnel (1979) have proved that the river deoxygenation rates are similar to the bottle

Fig. 2 Meshing and the geometry of the study area

rates when the river flow rate is $22.7 \text{ m}^3/\text{s}$ or higher. Since the average flow in the Diyala River is $200 \text{ m}^3/\text{s}$ (more than the mentioned value) (Al-Faraj and Scholz 2014), the measured BOD bottle rates are considered to be the same with that of the river. The temperature correction has been applied using the following equation:

$$(k_d)_T = (k_d)_{20}(\theta)^{T-20}, \quad (6)$$

where $(k_d)_T$ and $(k_d)_{20}$ are decay coefficients at any temperature “ T ” and 20°C , respectively, and $\theta = 1.047$. As for river's hydraulic characteristics, the mean velocity in two directions was obtained using floating method at the same

Table 1 Results of the analyses used for model input, calibration and validation

Variables	Sampling points								
	S1	S2	S3	S4	S5	S6	S7	S8	S9
June 2016									
TDS (mg/L)	791	2118	1485	1273	1257	1490	1310	1290	2130
BOD (mg/L)	4.2	18.4	11.5	8.5	6.5	10.6	7.8	4.9	18.5
BOD rates, k_d (day^{-1}) at 20°C	0.09	0.09	0.09	0.13	0.13	0.13	0.13	0.10	0.12
T ($^\circ\text{C}$)	26	26	26	26	26	26	26	26	26
u (m/s)	0.32	0.32	0.32	0.35	0.35	0.35	0.35	0.36	0.33
v (m/s)	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.08
February 2017									
TDS (mg/L)	590	1720	1150	1010	933	1180	990	985	1724
BOD (mg/L)	3.1	14.5	9.5	7	6.1	9	6.1	4.9	15.2
BOD rates, k_d (day^{-1}) at 20°C	0.10	0.10	0.10	0.11	0.11	0.11	0.11	0.14	0.12
T ($^\circ\text{C}$)	16	16	16	16	16	16	16	16	16
u (m/s)	0.39	0.39	0.39	0.38	0.38	0.38	0.38	0.42	0.41
v (m/s)	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09	0.09

Fig. 3 Calibration results of TDS concentrations along Diyala River confluence with Tigris (June 2016)

points chosen to measure water quality parameters. The surface longitudinal and transverse velocities were measured in downstream flow and west directions, respectively. Thereafter, the mean river velocity was approximated by:

$$\text{velocity}_{\text{Mean}} \approx 0.85 \times \text{velocity}_{\text{Surface}} \quad (7)$$

Each velocity experiment was repeated at least three times. The water quality data along with deoxygenation rates and river velocities are shown in Table 1.

Numerical algorithm

A numerical solution has been achieved of Eqs. (3) and (4) by writing a customized program using the FlexPDE code. The software is based on finite element method for numerically solving partial differential equations (PDEs) (Robescu et al. 2008). Moreover, it has several features that make it applicable for different types of problems such as the ability to solve nonlinear PDEs of second order or less and eliminating the need for manually determining an appropriate mesh (the grid refinement automatically). FlexPDE is user-friendly software and does not include a pre-defined problem domain or equation list. The option of PDEs is entirely up to the user (FlexPDE 2005). However, the user required a

good knowledge of the program in the complex modeling conditions.

Model calibration

The model was calibrated using data from June 2016. In this study, longitudinal ϵ_x and transverse dispersion coefficients ϵ_y are chosen to be calibrated by the trial-and-error method. A lot of simulations were made by adjusting these coefficients until the outputs of the simulation have reasonable agreement with the observed data sets. The model was validated using data from February 2017 without adjusting the calibrated coefficients to examine the ability of the calibrated model.

Boundary and initial conditions

The mesh and geometry of the study are shown in Fig. 2. The boundary conditions adopted for the whole section are Neumann type (flux of BOD and TDS is zero). The data sets shown in Table 1 were used to provide the values of the constants in Eqs. (3) and (4). Various scenarios were examined by setting different values of dispersion coefficients. These

Fig. 4 Calibration results of BOD concentrations along Diyala River confluence with Tigris (June 2016)

values were proposed based on the literature studies given in the past for various rivers and streams.

Results and discussion

For both pollutants (TDS and BOD), different values of longitudinal and transverse dispersion coefficients have been adopted as $\epsilon_x = \epsilon_y$ and $\epsilon_x > \epsilon_y$ or $\epsilon_x < \epsilon_y$. The results of TDS dispersion at the confluence of Diyala River with Tigris River are shown in Fig. 3 for longitudinal and lateral distances. The concentration of TDS at S1 (before confluence) was 791 mg/L as shown in Table 1. The best agreement between simulated and measured TDS values was observed when the dispersion coefficients: $\epsilon_x = 10 \text{ m}^2/\text{s}$ and $\epsilon_y = 5 \text{ m}^2/\text{s}$. The estimated relative errors were ranged from 0.56 to 1.00%. Furthermore, it was found that the TDS concentration was 2118 mg/L at the confluence point and reduced to 1300 mg/L at 0.5 km downstream distance.

The BOD (non-conservative pollutant) concentration at S1 (before confluence) was 4.8 mg/L (Table 1). The results of BOD dispersion at the confluence of Diyala River with Tigris River are shown in Fig. 4 for longitudinal and lateral distances. As same for TDS, the best fitting between simulated and measured BOD values was observed when

$\epsilon_x = 10 \text{ m}^2/\text{s}$ and $\epsilon_y = 5 \text{ m}^2/\text{s}$. The estimated relative errors for BOD were extremely higher than those of TDS and were ranged from 4.34 to 18.40%.

For model validation, data from February 2017 were used without changing the calibrated dispersion coefficient values ($\epsilon_x = 10 \text{ m}^2/\text{s}$ and $\epsilon_y = 5 \text{ m}^2/\text{s}$). The results of model validation for TDS and BOD are shown in Figs. 5 and 6, respectively. The estimated relative errors for TDS and BOD were ranged from 1.69 to 3.96% and 1.63 to 25.73%, respectively.

The simulated results of TDS for both calibration and validation processes showed a good agreement with the observed values. The maximum relative errors were 1.00 and 3.96% for calibrated and validated results, respectively. In case of BOD, the results demonstrate that there is a high error between the simulated and observed values. This error may be attributed to the complex biological transformations process of BOD (e.g., oxidation of carbonaceous BOD, oxidation of nitrogenous BOD and sediment oxygen demand "SOD") that need to be included in the model with great accuracy. Another reason is that usually the organic matter is not uniformly dispersed in the water mass as mentioned earlier. It can be agglomerates of organic substances, flakes, chunks, settleable matter, etc. In certain cases, the samples should be prepared (homogenized, settled or filtered) in order to avoid the problem of BOD dispersion in water. The

Fig. 5 Validation results of TDS (February 2017)

above reasons may explain the errors in the results of BOD. The BOD concentration was 18.4 mg/L at the confluence point and reduced to 5.2 mg/L at 0.5 km downstream distance of the Tigris River.

The methodology of the proposed model can be deemed as a simple approach in comparison with other conventional methods which have been used for estimation of dispersion coefficients such as experimental and field tracer studies. On the other hand, this method can be effortless, time-saving and inexpensive. Moreover, the model required only the river flow velocity to be determined, in addition to the water quality data. This model can be applied only for steady-state and uniform flow conditions. In spite of some errors between the simulated results of reactive pollutant and the experimental data, the results of non-reactive pollutant were acceptable. The model has some limitations such as ignoring the effect of side inflow velocities of the Diyala River. However, the model can give an initial impression of the water quality status of the river.

This paper does not compare the estimated values of longitudinal and transverse dispersion coefficients with the empirical formulas that already have been developed previously by different authors. This because of lack of data required for the calculation of dispersion coefficients such as discharge, shear velocity, depth, and slope. The performance

evaluation of these formulas versus the approach adopted in this study is the next stage of this work.

Generally, FlexPDE code can be used as an effective tool for simulating the pollutant spreading into rivers and streams. The idea of proposing different values for dispersion coefficients was the absence of a precise empirical equation to evaluate these coefficients in spite of the development of several equations previously. On the other hand, the process of calculating these coefficients on the ground is costly and requires effort. Although the proposed methodology of this study is not very accurate, it enables us to estimate the dispersion coefficients with less effort and cost compared to laboratory or field methods. The results showed that the method is more suitable for conservative pollutants, while non-conservative pollutants need an accurate representation of the chemical or biological transformations.

Conclusions

Simulation of TDS and BOD dispersion at the confluence of Diyala River with Tigris River has been investigated in this study. The present model can be used for modeling the dispersion phenomenon in the rivers and streams. In spite of some errors in the simulation results, the outcomes from this

Fig. 6 Validation results of BOD (February 2017)

model were realistic to the actual situation of the river. It was observed that the model was more effective for conservative pollutants (TDS), while non-conservative pollutants (BOD) need an accurate representation of the chemical or biological transformations.

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