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Numerical Modeling of Instantaneous Spills in One-dimensional River Systems

Fatima M. A. Al-khafaji and Hussein A. M. Al-Zubaidi†
Department of Environmental Engineering, College of Engineering, University of Babylon, Babylon, Iraq
†Corresponding author: Hussein A. M. Al-Zubaidi; hussein.alzubaidi@uobabylon.edu.iq; alzubaidih10@gmail.com

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ABSTRACT

Modeling the fate and transport of spills in rivers is critical for risk assessment and instantaneous spill response. In this research, a one-dimensional model for instantaneous spills in river systems was built by solving the advection-dispersion equation (ADE) numerically along with the shallow water equations (SWEs) within the MATLAB environment. To run the model, the Ohio River's well-known accidental spill in 1988 was used as a field case study. The verification process revealed the model's robustness with very low statistic errors. The mean absolute error (MAE) and root mean squared error (RMSE) relative to the absorbed record were 0.0626 ppm and 0.2255 ppm, respectively. Results showed the spill mass distribution is a function of the longitudinal dispersion coefficient and the mass decay rate. Increasing the longitudinal dispersion coefficient reduces the spill impact widely, for instance after four days from the mass spill the maximum concentration decreased from 0.846789 to 0.486623 ppm, and after five days it decreased from 0.332485 to 0.186094 ppm by increasing the coefficient from 15 to 175 m^2/sec. A similar reduction was achieved by increasing the decay rate from 0.8 to 1.2 day^{-1} (from 0.846789 to 0.254274 ppm and from 0.332485 to 0.0662202 ppm after four and five days, respectively). Thus, field measurements of these two factors must be taken into account to know the spill fate in river systems.

INTRODUCTION

Many rivers especially populated ones are exposed to instantaneous spills of pollutants due to increasing industrialization and urbanization. Predicting the movement of pollutants in rivers is one area where water quality management is supported. Numerous things can poison rivers. Diffusion and advection transport processes have caused these pollutants to spread longitudinally, laterally, and vertically, resulting in a decline in the river's water quality (Ramezani et al. 2016, Ukpaka & Agunwamba 2023, Yip et al. 2021). In addition to instantaneous spills, the most frequent oil spills can have substantial, long-term detrimental effects on the ecosystem and river systems. Throughout the world in recent decades, there have been thousands of unintentional and intentional unlawful releases of pollutants into surface water. Large spatial distributions, limited capacities for dilution and dispersion, and a high potential for the formation of pollutant droplets and their interaction with suspended particles and sediments make spills in medium- and small-sized rivers more detrimental than spills in seas. The main factors influencing the river spill modeling are pollutant density, river movement, hydraulic structures, vegetation, and interaction with sediments. Also, the transport, spread, and fate of river spills are subject to complex physical and chemical processes that depend on the characteristics of the river, river hydraulics, and environmental conditions. The main instantaneous spill transport processes include the following: (i) advection brought induced by wind and river currents, (ii) Surface spreading is caused by the equilibrium of surface forces, gravitational forces, inertia, and viscous forces, and it results from both mechanical and turbulent diffusion. (iii) weathering mechanisms like oxidation, dissolution, emulsification, and evaporation, (iv) tumultuous mixing across the river's depth, (v) the way in which contaminants mix with river sediment and particle matter (vi) contact of pollutants with coastline (Kvočka et al. 2021, Kwon et al. 2021, Li et al. 2018, Zeunert & Meon 2020, Antonopoulos et al. 2015, Kargar et al. 2020, Tenebe et al. 2016, Al-Dalimy & Al-Zubaidi 2023).

There are different approaches for modeling pollutant spills in rivers. Ramezani et al. (2019) developed a one-dimensional model that simulates the fate of pollutant transport by solving the effect of several formulas for the longitudinal dispersion coefficient on ADE. The numerical solution was used to predict the transport of pollutants using MATLAB and Excel. The model used the finite differences to discretize the ADE explicitly. Results showed that the longitudinal dispersion coefficient is very essential and can impact the numerical solution accuracy extensively. In addition, the model results were close to the observations;

however, an inconsistent match with data was noticed in one of the case studies. Milišić et al. (2020) employed the MIKE11 model as a robust and successful numerical model in addition to the one-dimensional ADE model to compute the longitudinal dispersion coefficient mathematically and numerically. The results and the experimental data from the Nertevia River (in the northern region of Bosnia and Herzegovina) were found to be fairly consistent. The temporal and spatial variations of pollutants might also be predicted using this model. Thus, for calculating solute distribution in big rivers, one-dimensional modeling, and single-point measurement techniques are straightforward and reasonably reliable instruments that should be taken into consideration. Ritta et al. (2020) calculated the longitudinal dispersion coefficient for the ADE utilizing an analytical and numerical one-dimensional linear technique. The longitudinal dispersion coefficient was calculated utilizing a large number of parametric equations that can be predicted using partial differential equations. By comparing the analytical and numerical results, it was found that there was good agreement between them. They advanced from the top together, and suddenly they decreased sharply to almost zero. It was also observed that as the distance increased the concentration decreased. Camacho Suarez et al. (2019) investigated how concentration dynamics and adherence to river rules were affected by uncertainty in the longitudinal dispersion coefficient. To do this, six longitudinal dispersion regression equations were evaluated using the one-dimensional ADE and an analytical solution. The results showed that the Disley et al. equation (Disley et al. 2015) utilized efficiency metrics to determine which equation best described the dispersion coefficient. The results also showed that the effect of uncertainty varies greatly depending on the different characteristics of the rivers. Andallah & Khatun (2019) used numerical simulation by the one-dimensional ADE. Numerical and analytical solutions were used for the ADE. The Crank-Nicolson scheme was used in the numerical analysis and the relative error of three finite differences between FTBSCS and FTCSCS was compared. It was found that the Crank-Nicholson scheme was more accurate and the CNS and FTSCCS schemes were at a good rate of closeness. Thereby, many of these models try simplifying the solution to get results without linking the river flow continuity and momentums. In this research, the target numerical solution approach is to build a one-dimensional numerical model that simulates the fate of transport instantaneous pollutants spilled in rivers within the MATLAB environment using the analytical and numerical solution of the ADE simultaneously with SWEs to provide instant water depth and velocity at every numerical time step.

MATERIALS AND METHODS

Fig. 1 displays the general numerical development approach

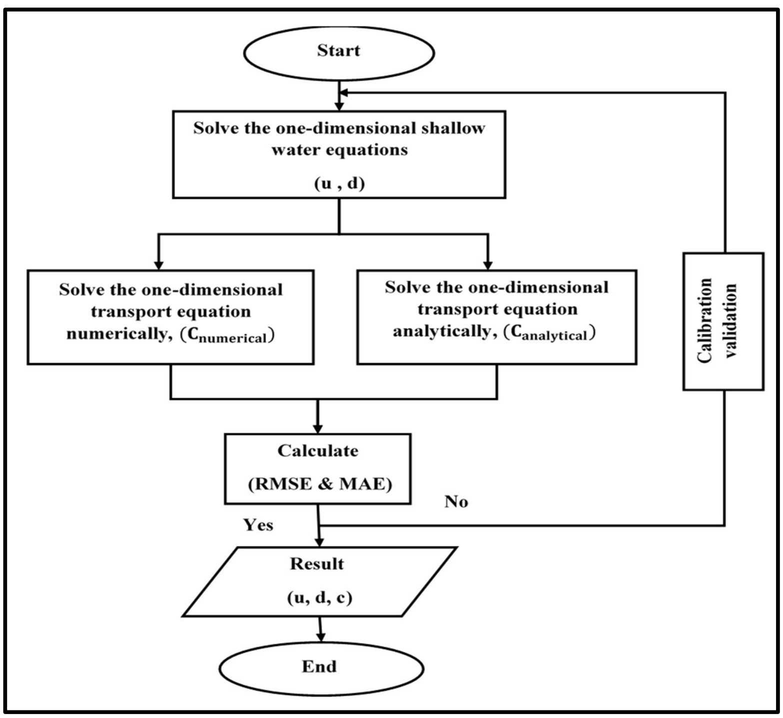

Fig. 1: Model development flow chart.

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used in the present model. The model starts by solving the SWEs to get the river longitudinal velocity (u) and the propagated water surface wave height (d) along the river length. Then, the ADE is solved analytically and numerically for the pollutant concentration (c) longitudinally and temporally. These solutions are repeated every numerical time step until the best calibrated and validated results are achieved with fewer statistical errors.

Numerical Solutions of the One-dimensional SWEs

SWEs consist of two fundamental equations of continuity equation (Eq.1) and momentum equation (Eq.2). The numerical solutions are found using the finite difference method by characterizing space and time as shown in Fig. 2. Accurate numerical solutions are obtained by relocating the grid points efficiently to reduce linearity error (Al-Zubaidi & Wells 2020, Delis & Nikolos 2021, Guinot 2013, Morel et al. 1996, Welahettige et al. 2018).

$$\frac{\partial d}{\partial t} + D\frac{\partial u}{\partial x} = 0 \quad \text{(continuity equation)} \qquad ...(1)$$

$$\frac{\partial u}{\partial t} + G\frac{\partial d}{\partial x} + \frac{(cf.u|u|)}{D} = 0 \quad \text{(momentum equation)} \qquad ...(2)$$

Where $D = d \pm d'$ as in Fig. 2, G is the acceleration of gravity (m/s^2), d is the height (m), u is the velocity (m/s), and cf is the friction coefficient.

A sequence of time-stepped numerical solutions for the unknown height and velocity of a wave propagating through an incompressible medium with a given constant density is obtained using the initial and boundary conditions can be computed numerically in the form of Eq.4 and 5 based on the grid discretization in Fig. 3 in which Δx is the space increment and Δt is the time steps (Li & Chen 2019, Zhou et al. 2018):

$$\frac{d_j^{i+1} - d_j^i}{\Delta t} + \beta D^i \frac{u_{j+1}^{i+1} - u_{j-1}^{i+1}}{2\Delta x} + (1-\beta)D^i \frac{u_{j+1}^i - u_{j-1}^i}{2\Delta x} = 0 \qquad ...(3)$$

$$\frac{u_{j-1}^{i+1} - u_{j-1}^i}{\Delta t} + \beta G \frac{d_j^{i+1} - d_{j-1}^{i+1}}{2\Delta x} + (1-\beta)G\frac{d_j^i - d_{j-1}^i}{2\Delta x} + \frac{cf.|u^i|}{D^i}\left(\beta u_{j-1}^{i+1} + (1-\beta)u_{j-1}^i\right) = 0 \qquad ..(4)$$

If the β is between (0 > β > 1), the solution is semi-implicit, and If the β = 0, the solution is fully explicit, and the solution will be fully implicit when β = 1.

Numerical Solution of the One-dimensional ADE

To account for a variable cross-sectional area of the river, the one-dimensional ADE (Eq. 5) is discretized as shown in Eqs. 6 and 7 First-order forward difference method for the temporal derivative, Second-order Central Difference Scheme for the second spatial derivative, and First-order Upwind Strategy for the first spatial derivative are used.

$$\frac{\partial C}{\partial t} + \frac{1}{A}\frac{\partial uAC}{\partial x} = \frac{E}{A}\frac{\partial^2 AC}{\partial x^2} - kC \qquad ...(5)$$

Where C is the pollutant cross-sectional average concentration (ppm), E is the longitudinal dispersion

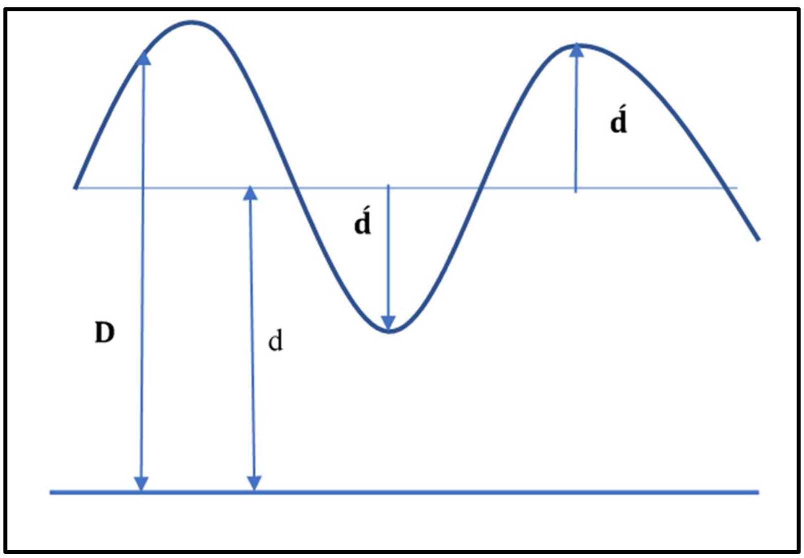

Fig. 2: Water depth presentation in the SWEs.

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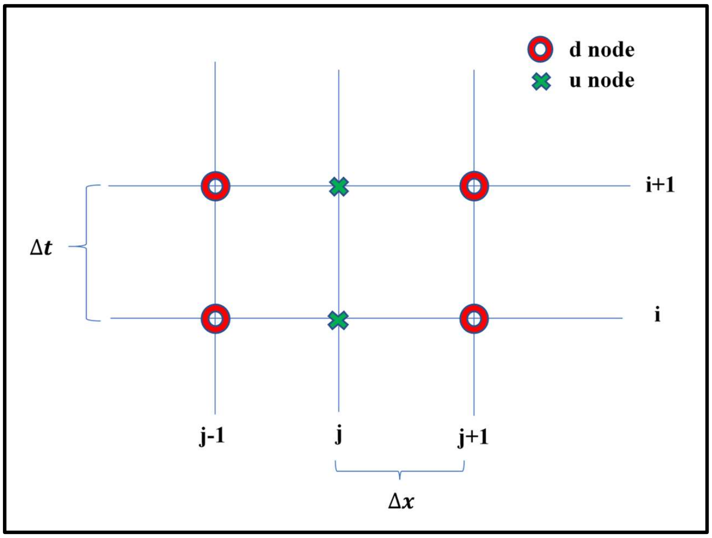

Fig. 3: Grid discretization of SWEs numerical solution.

coefficient (m^2/s), k is the chemical degradation or decay rate (1/s), and A is the river cross-section area (m^2).

$$C_j^{i+1} = C^i - \Delta t[\mathrm{UPWIND}] + \frac{E\Delta t}{\Delta x^2 A_j^i}$$

$$\left[A^i_{i+\frac{1}{2}}\left(C^i_{j+1} - C^i_j\right) - A^i_{i-\frac{1}{2}}\left(C^i_j - C^i_{i-\frac{1}{2}}\right)\right] - KC^i_j\Delta t \quad \ldots(6)$$

$$\mathrm{UPWIND} = \begin{cases}\left(uAC\big|^i_j - uAC\big|^i_{j-1}\right)/\left(A^i_j\Delta x\right) & u^i_j \geq 0\\ \left(uAC\big|^i_j - uAC\big|^i_{j+1}\right)/\left(A^i_j\Delta x\right) & u^i_j < 0\end{cases} \quad \ldots(7)$$

Model Verification

Analytically, reactive pollutants instantaneously leaked into rivers by the advection and dispersion processes, passing through the first mixing zone can be described according to Eq.8 (Chin, 2006) which is the analytical solution of Eq. 5:

$$C = \frac{M}{A\sqrt{4\pi Et}}\exp -\left[\frac{[x-ut]^2}{4Et} + kt\right] \quad \ldots(8)$$

Where M is the spill mass (g).

The model was validated by comparing the one-dimensional ADE numerical solution with the analytical solution and calculating statistical errors. MAE and RMSE were used as statistical measures to measure and evaluate model performance in research studies. The RMSE and the MAE are calculated for model results as shown in Eqs. 9 and 10 (Al-Zubaidi & Wells 2018, Al-Zubaidi & Wells 2017, Chai & Draxler 2014, Chicco et al. 2021, Hodson 2022, Robeson & Willmott 2023, Wang & Lu 2018):

$$MAE = \frac{\sum_1^N \left|C_{numerical} - C_{analytical}\right|}{N} \quad \ldots(9)$$

$$RMSE = \sqrt{\frac{\sum_1^N \left(C_{numerical} - C_{analytical}\right)^2}{N}} \quad \ldots(10)$$

Where N is the number of comparisons.

Case Study

The Ohio River in the eastern United States of America as in Fig. 4 was chosen as a case study to test the performance of the established model. The Allegheny and Monongahela Rivers meet here, forming the Ohio River, a little below Pittsburgh (Clark et al. 1990). The river dimensions are (an average length of 480000 m, average width of 800 m, and average depth of the river 10 m) with an average discharge of 1500 m^3/s. Many intricate processes, like as mixing, exchange with storage zones, shearing advection, lateral mixing, hyporheic exchange, and effective diffusion in bottom sediment, affect the transport of pollutants in large rivers. On Saturday, January 2, 1988, over 3.8 million gallons of diesel oil collapsed in a storage tank in Pittsburgh. About 800,000 gallons spilled into the river at that time. This accident was chosen as a field case study to run the model based on. The river length was discretized using

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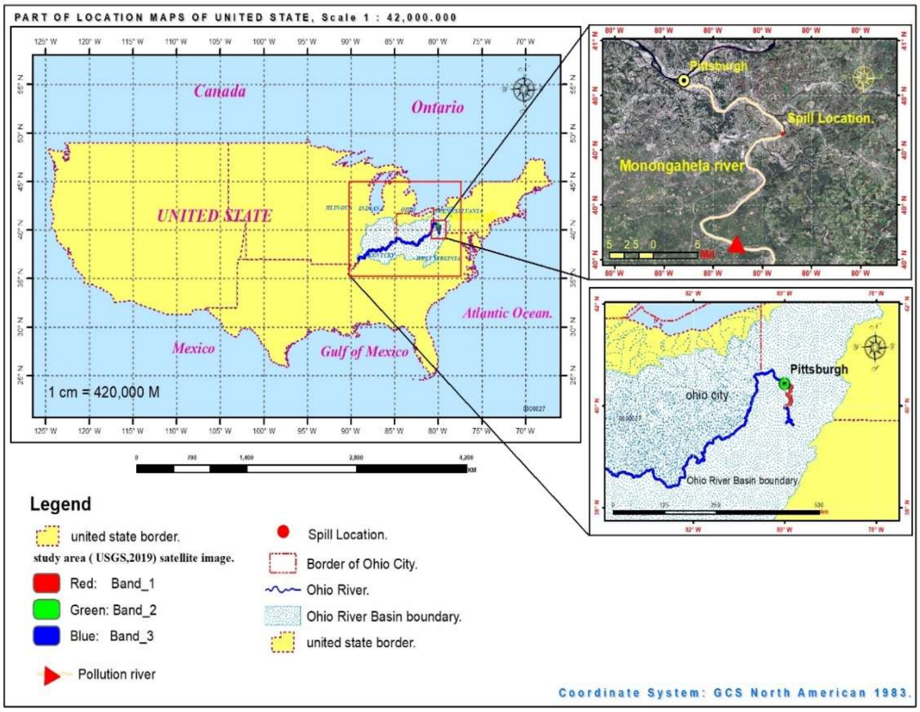

Fig. 4: Ohio River study area, US.

longitudinal increments (Δx) of 3000 m and time steps (Δt) of 303 s to ensure the model stability. The spill location is located at i = 2 and that happened on day 2 from the start of the simulation. In addition, a first-order decay rate (k) of 0.8 1/day and dispersion coefficient (E) of 15 m^2/s were known for the river.

RESULTS AND DISCUSSION

The model was run using the available input data of the Ohio River spill to simulate and predict the pollutant fate and transport along the river. Fig. 5 displays the model simulation results after different days from the mass spill initial date. The model shows that the highest concentrations occur within the mixing zone at the source of the instantaneous spill and decrease with river distance. Also as travel time increases, the maximum pollutant concentration decreases as the instantaneous spill flows downstream the river length. This means that the relationship between pollutant travel distance and time with concentration is opposite. The pollutant plume moves with distance taking the bell shape, and as it travels along the river distance its amplitude decreases and becomes wider similar to the model behavior developed (Ramezani et al. 2019). A comparison was made between the analytical and numerical solutions for the presented case study of the Ohio River to verify the model performance. Fig. 6 shows the comparison results of the model predictions compared to the analytical solution. Very good agreement was accomplished by the model based on the same case study in which the MAE value was 0.0626 ppm and the RMSE value was 0.2255 ppm. In addition, another comparison was made to check the differences at various selected locations along the river length as shown in Fig. 7. The statistical errors were very good reflecting the model's robustness. For example, at a river distance of 45 miles, the RMSE=0.3959 ppm and the MAE=0.021 ppm, at a river distance of 56.25 miles, the RMSE=0.1907 ppm, and the MAE=0.0077 ppm, and at a river distance of 65.625 miles, the RMSE=0.0984 ppm and MAE=0.0034 ppm.

Two parameters are responsible for the pollutant's final fate within the river, the longitudinal dispersion coefficient and the pollutant decay rate. In other words, how the plume amplitude and width decay and vanish eventually. Fig. 8 shows the evaluation of the model sensitivity to longitudinal dispersion coefficient variation. Several values of the longitudinal dispersion coefficient were selected (E=15,55,95,135, and 175 m^2/s) on two different days (t=4 and 5 days) to run the model for the same Ohio River hydraulic and geometric properties along the river. The impact is very clear. A gradual decrease in the pollutant concentrations happens as the longitudinal dispersion coefficient increases. For example, on day number 4, the maximum pollutant concentration decreased from 0.846789

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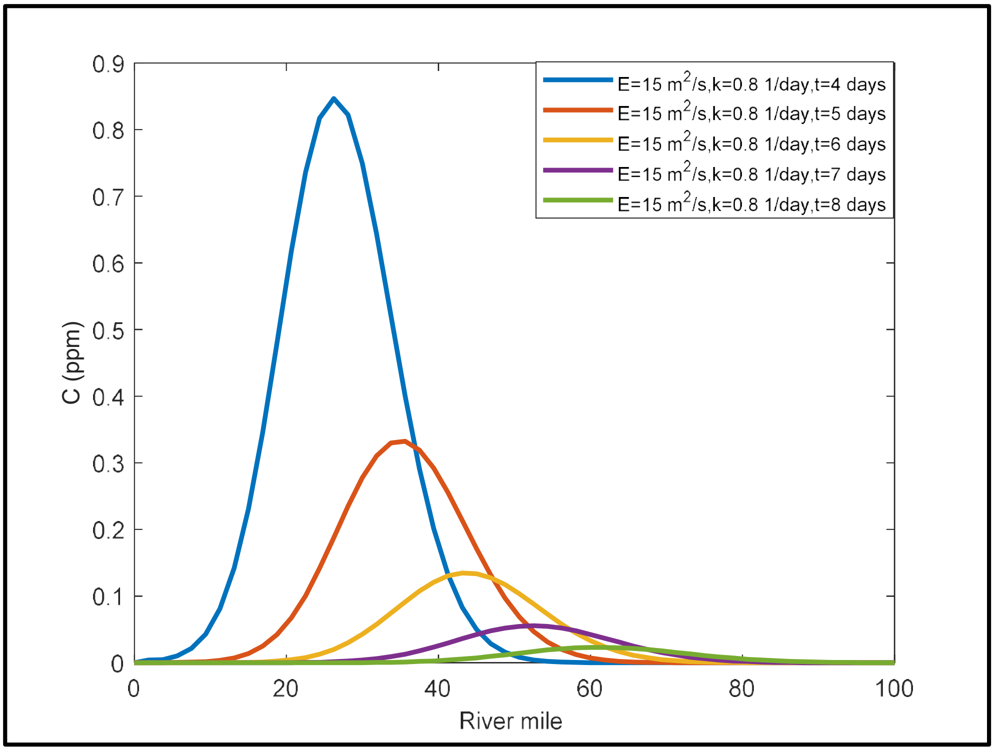

Fig. 5: Model simulation results at different days along the river.

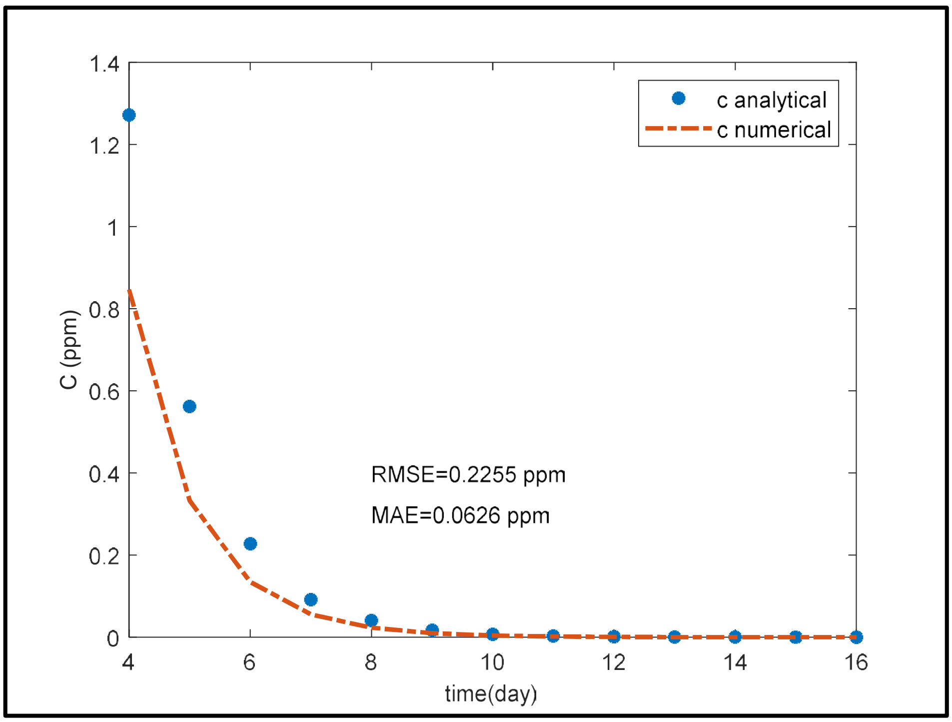

Fig. 6: Comparison between analytical and numerical solution results on different days after the initial spill date along the river.

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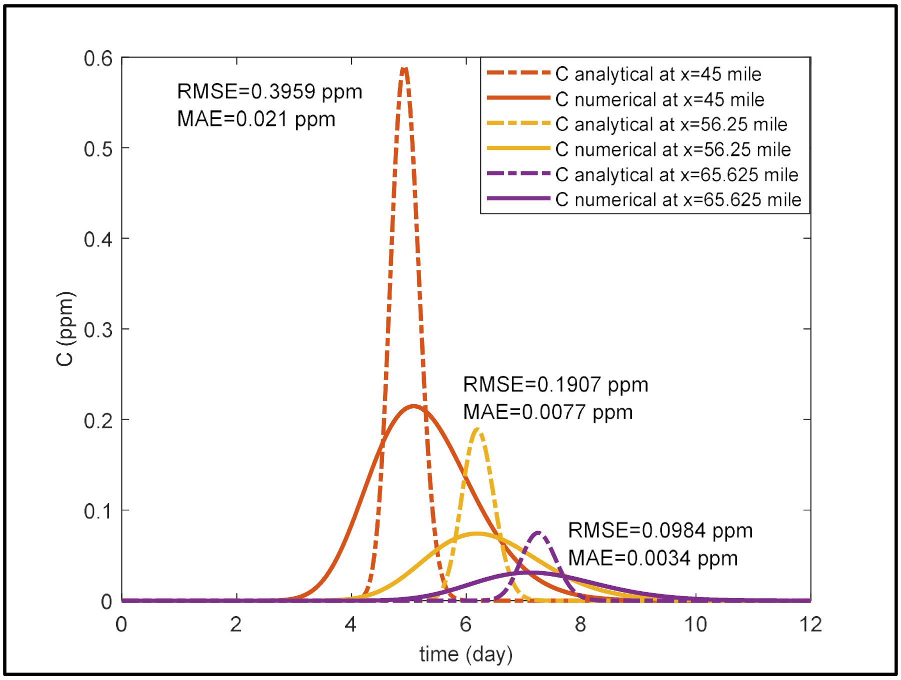

Fig. 7: Analytical solution plume of concentration compared to the numerical solution results of the model at different distances along the river.

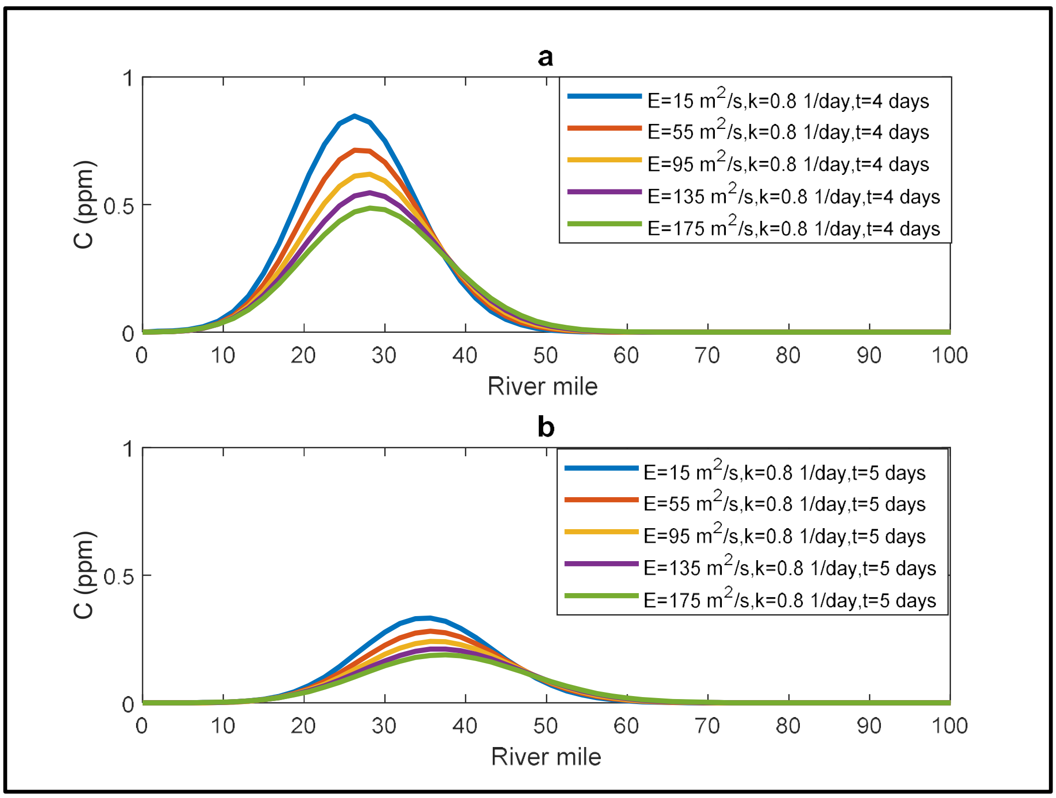

Fig. 8: Pollutant concentration distribution based on different longitudinal dispersion coefficients (a) at a time of 4 days and (b) at a time of 5 days from the spill date.

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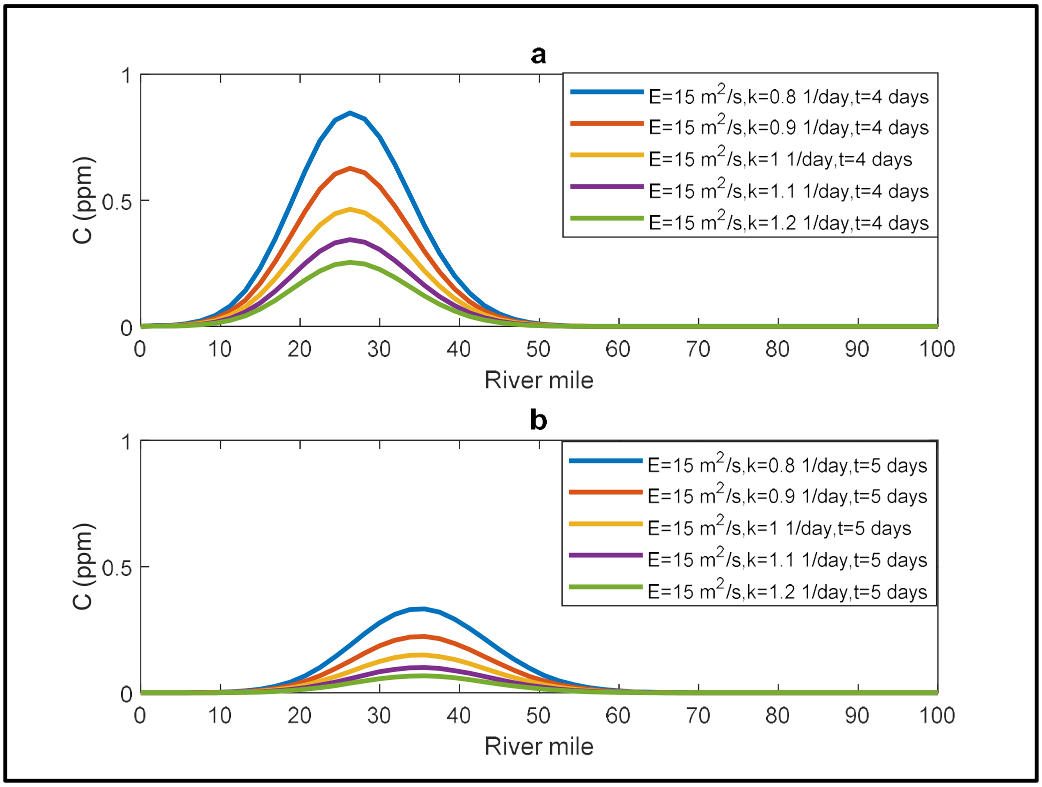

Fig. 9: Pollutant concentration distribution based on different decay rates (a) at the time of 4 days and (b) at the time of 5 days from the spill date.

to 0.486623 ppm, and on day number 5 day, the maximum pollutant concentration decreased from 0.332485 to 0.186094 ppm. Implying that there is an inverse association between them. Therefore, the longitudinal dispersion coefficient is very important and greatly affects the accuracy of the numerical solution. As conducted by Andallah & Khatum (2020), it is the main parameter that determines the transport of pollutants in one-dimensional river systems.

The latter parameter depends on the mass type itself. In general, the decay coefficient has the opposite impact on the pollutant residence time. Accordingly, different values of the decay rate were taken to determine the influence on the pollutant concentration distribution to assess the model capability of the decay rate variation. The decay rate values were taken on two different days too. The range for the chosen decay rate was from 0.8 to 1.2 1/day. At day number 4, the maximum pollutant concentration decreased from 0.846789 to 0.254274 ppm, and at day number 5, the maximum pollutant concentration decreased from 0.332485 to 0.0662202 ppm. Similar plume concentration reduction behavior compared to the longitudinal dispersion coefficient effect in which increasing the rate of decay with time reduces the concentration distribution longitudinally and temporally. Comparing the results in Fig. 8 and 9 leads to conclude that the effect of the longitudinal dispersion coefficient is very small compared to the decay rate. Also, the plume takes a bell shape as it travels from the source of the instantaneous mass spill. Consequently, the pollutant concentration distribution around the plume center decreases and its amplitude becomes lower and wider as the plume moves away from the spill source. Finally, by constructing a one-dimensional model including the numerical and analytical solution of ADE based on the available data to simulate the fate and transport of pollutants in the rivers, it was found it is necessary to model the case numerically rather than solving the case analytically only for better representation and realistic predictions (Fry et al. 1993).

CONCLUSION

In this study, a one-dimensional numerical model was developed to simulate the fate and transport of instantaneous spills in rivers by solving the ADE in conjugate with SWEs. It was found that the maximum pollutant concentrations occur within the mixing zone and decrease with increasing distance from the spill location. Also, as travel time increases the maximum concentration decreases as the pollutant plume flows downstream the river, spreading

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the pollutant distribution with less concentration until vanishing. In addition, it was concluded that whenever either the longitudinal dispersion coefficient or the decay rate increases during the model run, the pollutant concentration plume distribution decreases with distance. This property plays a major role in the pollutant fate and transport in the river, impacting the pollutant residence time. Furthermore, the numerical modeling along with the analytical solution gave the case study more applicability since it can control the river characteristics broadly.

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ORCID DETAILS OF THE AUTHORS

Fatima M. A. Al-khafaji: https://orcid.org/0009-0008-0616-9604
Hussein A. M. Al-Zubaidi: https://orcid.org/0000-0001-8746-8543

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