A Comprehensive One-Dimensional Numerical Model for Solute Transport in Rivers

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Abstract

One of the mechanisms that greatly affect the pollutant transport in rivers, especially in mountain streams, is the effect of transient storage zones. The main effect of these zones is to retain pollutant temporarily and then release it gradually. Transient storage zones indirectly influence all phenomena related to mass transport in rivers. This paper presents the TOASTS[1] model to simulate 1D pollutant transport in rivers with irregular cross-sections under unsteady flow and transient storage zones. The proposed model was verified versus some analytical solutions and 2D hydrodynamic model. In addition, in order to demonstrate the model applicability, two hypothetical examples were designed and also four sets of well-established frequently-cited tracer study data were used. These cases cover different processes governing transport, cross-section types and flow regimes. The results of the TOASTS model, in comparison with two common contaminant transport model, show better accuracy and numerical stability.

1 Introduction

First efforts to understand the solute transport subject, led to longitudinal dispersion theory which is often referred to as classical Advection-Dispersion Equation (ADE) (Taylor, 1954).

[1] Third-Order Accuracy Simulation of Transient Storage

This equation is a parabolic partial differential equation derived from a combination of continuity equation and Fick's first law. The one-dimensional ADE equation is as follows:

$$\frac{\partial(AC)}{\partial t}=-\frac{\partial(QC)}{\partial x}+\frac{\partial}{\partial x}\left(AD\frac{\partial C}{\partial x}\right)-\lambda AC+AS \quad (1)$$

Where, A is the flow area, C the solute concentration, Q the volumetric flow rate, D the dispersion coefficient, λ the first-order decay coefficient, S the source term, t the time and x the distance. When this equation is used to simulate the transport in prismatic channels and rivers with relatively uniform cross-sections, accurate results can be expected; but field studies, particularly in mountain pool-and-riffle streams, indicate that observed concentration-time curves have a lower peak concentration and longer tails than the ADE equation predictions (Godfrey and Frederick, 1970, Nordin and Sabol, 1974, Nordin and Troutman, 1980, Day, 1975). Thus a group of researchers, based on field studies, stated that to accomplish more accurate simulations of solute transport in natural rivers and streams, ADE equation should be modified. They added some extra terms to it for consideration of the impact of stagnant areas that were so-called storage zones (Bencala et al., 1990, Bencala and Walters, 1983, Jackman et al., 1984, Runkel, 1998, Czernuszenko and Rowinski, 1997, Singh, 2003). Transient storage zones, mainly include eddies, stream poolside areas, stream gravel bed, streambed sediments, porous media of river bed and banks and stagnant areas behind flow obstructions such as big boulders, stream side vegetation, woody debris and so on (Jackson et al., 2013).

In general, these areas affect pollutant transport in two ways: On one hand, temporary retention and gradual release of solute, cause an asymmetric shape in the observed concentration-time curves, that could not be explained by the classical advection-dispersion theory and on the other hand by providing the opportunity for reactive pollutants to be frequently contacted with streambed sediments that indirectly affect solute sorption, especially in low flow conditions (Bencala, 1983, Bencala, 1984, Bencala et al., 1990, Bencala and Walters, 1983).

In the literature, several approaches have been proposed to simulate solute transport in the rivers with storage areas, that one of the most commonly used is the Transient Storage Model (TSM). TSM has been developed to consider solute movement from the main channel to stagnant zones and vice versa. The simplest form of the TSM is the one-dimensional advection-dispersion equation with an additional term to consider transient storage (Bencala and Walters, 1983). After the introduction of the TSM, transient storage processes have been studied in a variety of small mountain streams and also big rivers and it was shown that simulation results of tracer study data considering the transient storage impact, have good agreement with observed data. Also, it was shown that the interaction between the main channel and storage zones, especially in mountain streams, has a great effect on solute transport behavior (D'Angelo et al., 1993, DeAngelis et al., 1995, Morrice et al., 1997, Czernuszenko et al., 1998, Chapra and Runkel, 1999, Chapra and Wilcock, 2000, Laenen and Bencala, 2001, Fernald et al., 2001, Keefe et al., 2004, Ensign and Doyle, 2005, Van Mazijk and Veling, 2005, Gooseff et al., 2007, Jin et al., 2009).

In this study, a comprehensive model, called TOASTS, able to obviate shortcomings of current models of contaminant transport, is presented. The TOASTS model uses high-order accuracy numerical schemes and considers transient storage in rivers with irregular cross-sections under non-uniform and unsteady flow regimes. This model presents a comprehensive modeling framework that links three sub-models for calculating geometric properties of irregular cross-sections, solving unsteady flow equations and solving transport equations with transient storage and kinetic sorption.

To demonstrate the applicability and accuracy of the TOASTS model, results of two hypothetical examples (designed by the authors) and four sets of well-established tracer study data, are compared with the results of two existing frequently-used solute transport models, MIKE 11 model developed by the Danish Hydraulic Institute (DHI) and OTIS[1] model that today is the only existing model for solute transport with transient storage (Runkel, 1998). The TOASTS model and the two other model features are listed in Table 1. It should be noted that the OTIS model, in simulating solute transport in irregular cross-sections under unsteady flow regimes, has to rely on external stream routing and geometric programs. While, in the TOASTS and MIKE 11 models, geometric properties and unsteady flow data, are directly evaluated from river topography, bed roughness, flow initial and boundary conditions data. Another important point is in the numerical scheme which has been used in the TOASTS model solution. The key and basic difference of the TOASTS model refers to spatial

[1] One-Dimensional Transport with Inflow and Storage

discretization of the transport equation. This model uses the control-volume approach and QUICK[1] scheme in spatial discretization of the advection-dispersion equation considering transient storage and kinetic sorption; whereas the two other models employ central spatial differencing. More detailed comparison of numerical schemes used in the structure of three subjected models is given in Table 2.

As many researchers claim, central spatial differencing, is incapable of simulation of pure advection problems and does not introduce good performance in this regard (it leads to non-convergent results with numerical oscillations) (Zhang and Aral, 2004, Szymkiewicz, 2010). It should be mentioned that, in recent years the QUICK scheme has been widely used in numerical solutions of partial differential equations due to its high-order accuracy, very small numerical dispersion and higher stability range (Neumann et al., 2011, Lin and Medina Jr, 2003). Hence, usage of the QUICK scheme in numerical discretization of the transport equation leads to significantly better results especially in advection-dominant problems.

2 Methodology

2.1 Governing Equations

There are several equations for solute transport with transient storage, which among them, the TSM presented by Bencala and Walters (1983) is the most well-known one. Writing conservation of mass principle for solute in main channel and storage zone and doing some algebraic manipulation, a coupled set of differential equations is derived:

$$\frac{\partial C}{\partial t} = \frac{-Q}{A}\frac{\partial C}{\partial x} + \frac{1}{A}\frac{\partial}{\partial x}\left(AD\frac{\partial C}{\partial x}\right) + \frac{q_{LIN}}{A}\left(C_L - C\right) + \alpha\left(C_S - C\right) \tag{2}$$

$$\frac{\mathrm{d}C_S}{\mathrm{d}t} = \alpha\frac{A}{A_S}\left(C - C_S\right) \tag{3}$$

Where A and A_S are the main channel and storage zone cross-sectional area respectively, C, C_L and C_S the main channel, lateral inflow and storage zone solute concentration, respectively, q_{LIN} the lateral inflow rate and α the storage zone exchange coefficient. For

[1] Quadratic Upstream Interpolation for Convective Kinematics

reactive solute, with considering two types of chemical reactions; kinetic sorption and first-order decay, Equations (2) and (3) are rewritten as:

$$\frac{\partial C}{\partial t} = \mathrm{L}(C) + \rho\hat{\lambda}(C_{sed} - K_d C) - \lambda C \tag{4}$$

$$\frac{\mathrm{d}C_S}{\mathrm{d}t} = \mathrm{S}(C_S) + \hat{\lambda}_S(\hat{C}_S - C_S) - \lambda_S C_S \tag{5}$$

$$\frac{\mathrm{d}C_{sed}}{\mathrm{d}t} = \hat{\lambda}(K_d C - C_{sed}) \tag{6}$$

Where $\hat{C}_S$ is the background storage zone solute concentration, C_{sed} the sorbate concentration on the streambed sediment, K_d the distribution coefficient, λ and λ_S the main channel and storage zone first-order decay coefficients respectively, $\hat{\lambda}$ and $\hat{\lambda}_S$ the main channel and storage zone sorption rate coefficients respectively, ρ the mass of accessible sediment/volume water and L and S the right-hand side differential operator of Equations (2) and (3) respectively.

2.2 Numerical Solution Scheme

Numerical solution of Equations (4) to (6), in this study are based on the control-volume method and centered time-QUICK space (CTQS) scheme. The spatial derivatives are discretized by the QUICK scheme which is based on quadratic upstream interpolation of discretization of advection-dispersion equation (Leonard, 1979). In this scheme, face values are computed using quadratic function passing through two upstream nodes and a downstream node. For an equally-spaced grid, the values of a desired quantity, φ, on the cell faces are given by the following equations:

$$\phi_{face} = \frac{6}{8}\phi_{i-1} + \frac{3}{8}\phi_i - \frac{1}{8}\phi_{i-2} \tag{7}$$

$$\varphi_w = \frac{6}{8}\varphi_W + \frac{3}{8}\varphi_P - \frac{1}{8}\varphi_{WW} \tag{8}$$

$$\varphi_e = \frac{6}{8}\varphi_P + \frac{3}{8}\varphi_E - \frac{1}{8}\varphi_W \tag{9}$$

Where P denotes an unknown node with neighbor nodes W (at left) and E (at right). It should be noted that the corresponding cell faces are denoted by the lowercase letters, w and e. Gradient at cell faces can be estimated using the following relationships:

$$\left(\frac{\partial\phi}{\partial x}\right)_w = \frac{\phi_P - \phi_W}{\Delta x} \tag{10}$$

$$\left(\frac{\partial\phi}{\partial x}\right)_e = \frac{\phi_E - \phi_P}{\Delta x} \tag{11}$$

Finally, the difference equations related to the Equations (4) to (6) can be derived as follows:

$$\begin{aligned}\frac{C_P^{n+1} - C_P^n}{\Delta t} = &\frac{1}{2}\left[\left(\frac{-Q_p}{A_p\Delta x}(C_e - C_w)\right)^{n+1} + \left(\frac{-Q_p}{A_p\Delta x}(C_e - C_w)\right)^{n}\right] + \\ &\frac{1}{2}\left\{\frac{1}{A_P^{n+1}\Delta x}\left[\left(AD\frac{\partial C}{\partial x}\right)_e - \left(AD\frac{\partial C}{\partial x}\right)_w\right]^{n+1} + \frac{1}{A_P^{n}\Delta x}\left[\left(AD\frac{\partial C}{\partial x}\right)_e - \left(AD\frac{\partial C}{\partial x}\right)_w\right]^{n}\right\} + \\ &\frac{1}{2}\left[\frac{q_{LIN}^{n+1}}{A_P^{n+1}}(C_L - C_P)^{n+1} + \frac{q_{LIN}^{n}}{A_P^{n}}(C_L - C_P)^{n}\right] + \frac{\alpha}{2}\left[(C_S - C_P)^{n+1} + (C_S - C_P)^{n}\right] + \\ &\frac{\rho\hat{\lambda}}{2}\left[(C_{Sed} - K_d C_P)^{n+1} + (C_{sed} - K_d C_P)^{n}\right] - \frac{\lambda}{2}\left(C_P^{n+1} + C_P^{n}\right)\end{aligned} \tag{12}$$

$$\frac{C_S^{n+1} - C_S^n}{\Delta t} = \frac{1}{2}\left[\begin{aligned}&\left(\alpha\frac{A_P}{A_S}(C_P - C_S) + \hat{\lambda}_S\left(\hat{C}_S - C_S\right) - \lambda_S C_S\right)^{n+1} \\ &+\left(\alpha\frac{A_P}{A_S}(C_P - C_S) + \hat{\lambda}_S\left(\hat{C}_S - C_S\right) - \lambda_S C_S\right)^{n}\end{aligned}\right] \tag{13}$$

$$\frac{C_{Sed}^{n+1} - C_{Sed}^{n}}{\Delta t} = \frac{1}{2}\left[\left(\hat{\lambda}(K_d\, C_P - C_{Sed})\right)^{n+1} + \left(\hat{\lambda}(K_d\, C_P - C_{Sed})\right)^{n}\right] \tag{14}$$

Writing Equations (12) to (14) for all control-volumes in the solution domain and applying the boundary conditions, a system of linear algebraic equations will be introduced:

$$a_{WW}C_{WW}^{n+1} + a_W C_W^{n+1} + a_P C_P^{n+1} + a_E C_E^{n+1} = R_P \tag{15}$$

Where a_{WW}, a_W, a_P, a_E and R_P are the corresponding coefficients and the right-hand side term. Solving this system, main channel concentrations in n+1 time level will be computed.

Having main channel concentration values, the storage zone and streambed sediment concentrations could be calculated.

2.3 Damköhler Index

Damköhler number is a dimensionless number that reflects the exchange rate between the main channel and storage zones (Jin et al., 2009, Harvey and Wagner, 2000, Wagner and Harvey, 1997, Scott et al., 2003). For a stream or channel this number is defined as:

$$\mathrm{DaI} = \alpha\left(1+\frac{A}{A_s}\right)\frac{L}{u} \tag{16}$$

Where L is the main channel length, u the average flow velocity and DaI the Damköhler number. When DaI is much greater than unity, e.g. 100, the exchange rate between the main channel and storage zone is too fast and could be assumed that these two segments are in balance. Accordingly, when DaI is much lower than unity, e.g. 0.01, the exchange rate between main channel and storage zone is very low and negligible. In other words, in such a stream where DaI is very low, practically there is no significant exchange between the main channel and storage zone and transient storage zones do not affect downstream solute transport. Therefore, for reasonable estimation of transient storage model parameters, the DaI value must be within 0.1 to 10 range (Fernald et al., 2001, Wagner and Harvey, 1997, Ramaswami et al., 2005).

3 Model Verification

In this section the TOASTS model is verified using several test cases. These test cases include analytical solutions of constant-coefficient governing equations for two types of upstream boundary condition (continuous and Heaviside) and also by comparing the model results with 2D model. Complementary explanations for each case are given below.

3.1 Verification by Analytical Solutions

In this section, model verification is carried out using analytical solutions presented by Kazezyılmaz-Alhan (Kazezyılmaz-Alhan, 2008). The designed example is a 200 m length channel with constant cross-sectional area equal to 1 m^2. The flow discharge, dispersion coefficient, storage zone area and exchange coefficient are 0.01 m^3/s, 0.2 m^2/s, 1 m^2 and

0.00002 s^{-1}, respectively. The DaI number can be calculated from the Equation (19) equal to 0.8. This example is implemented for two different types of upstream boundary conditions; a) continuous and b) Heaviside.

a) Continuous Boundary Condition

In this case, a solute concentration of 5 mg/m^3 is injected continuously for 10 hours at the inlet. The time and space steps are considered equal to 30 sec and 1 m, respectively. Figure 1 shows the TOASTS model results compared to the analytical solution at 50 m, 75 m and 100 m from the inlet. Note that both axes have been nondimensionalized with respect to the maximum values. Also, square of correlation coefficient (R^2), Root Mean Square Error (RMSE), Mean Absolute Error (MAE) and Mean Relative Error (MRE) are given in Table 3. According to Figure 1 and the error indices given in Table 3, it is clear that the trends of numerical and analytical solutions are similar and the TOASTS model shows a good accuracy in this example.

In order to show the model capability and assess the model accuracy in a case without transient storage, the model is executed for α=0 for this example and the result at the distance of 100 m from the inlet is compared to the analytical solution of the classical advection-dispersion equation. The results are shown in Figure 2 and Table 3. Figure 2 also illustrates that in the case of with transient storage, concentration-time curve has lower peak than the without storage one (α=0), that matches the previously-mentioned transient storage concept.

b) Heaviside Boundary Condition

In this case a solute concentration of 5 mg/m^3 is injected at the inlet for a limited time of 100 minutes. The time and space steps are considered equal to 30 seconds and 1 meter respectively. Comparison of the model results and the analytical solution at the distance of 50 m, 75 m and 100 m from the inlet is presented in Figure 3 and Table 4. Also, corresponding results at the distance of 100 m for the case without storage (α=0) are given in Figure 4 and Table 4. It is obvious that the TOASTS model results in both cases (with and without storage) have a reasonable agreement with the analytical solution.

3.2 Verification by 2D Model

The main cause of transient storage phenomena is velocity difference between the main channel and storage zones. 2D depth-averaged models consider velocity variations in two dimensions and give more accurate predictions of solute transport behavior in reality. Hence, they could be used for verification of the presented 1D model as a benchmark. For this purpose, a hypothetical example was designed. To do so, a river of length of 1200 m, with irregular cross-sections, is considered. Figures 5 and 6 show bed topography of the hypothetical river. In order to take into account a hypothetical storage zone, the distance between 300 m to 600 m of the river has been widened. The flow conditions in the river considered to be non-uniform and unsteady. The solute concentration in the main channel and storage zone, at the beginning of the simulation (initial conditions), assumed to be zero. In calculations of both flow and transport models, space and time steps are considered equal to 100 m and 1 minute respectively. The dispersion coefficient, storage zone area and exchange coefficient are 10 m^2/s, 22 m^2 and 1.8×10^{-4} s^{-1} respectively. For this example the DaI number is calculated equal to 0.4. The upstream boundary condition for transport sub-model is a 3 hour lasting step loading pulse with 20 mg/m^3 pick concentration. The results of the TOASTS model for simulating with and without transient storage were compared to the 2D model at the distance of 800 m from the inlet. Figure 7 and Table 5 illustrates these results. This figure shows that with appropriate choice of As and α, concentration-time curves given by the TOASTS model are so close to those given by the 2D model. These results also imply the necessity of considering transient storage term in the advection-dispersion equation for more accurate simulation of solute transport especially in natural rivers and streams.

4 Application

In this section, the applications of the TOASTS model using a variety of hypothetical examples and several sets of observed data are presented. Some properties of these test cases are given in Table 6. As shown in this table, the test cases include a wide variety of solute transport simulation applications at different conditions.

4.1 Test Case 1: Pure Advection

In order to show the advantage of the numerical scheme used in the TOASTS model, for advection dominant problems, a hypothetical example was designed and three numerical schemes CTQS[1], CTCS[2] and BTCS[3] were applied. To do so, steady flow by velocity of 1 m/s was assumed. Total simulation time was 5 hours and space and time steps were 100 m and 10 seconds respectively. Note that advection is the only transport mechanism. The results of this test case are depicted in Figure 8. It is clear that, for the pure advection simulation, the CTQS scheme has less oscillation than the other two schemes. In particular, this figure represents that, the result of the CTCS scheme which is used in the OTIS model, shows high oscillations. Therefore, it can be concluded that for advection dominant simulation the TOASTS model has a better performance. It is interesting to note that in mountain rivers where the transient storage mechanism is more observed, due to relatively high slope, higher flow velocities occur which lead to advection dominant solute transport.

4.2 Test Case 2: Transport with First-Order Decay

This example illustrates the application of the TOASTS model in solute transport simulation by first-order decay. A decaying substance enters the stream with steady and uniform flow during a 2 hour period. The solute concentration at the upstream boundary is 100 mg/m^3. Also, in order to assess the TOASTS model capability in the case of high flow velocity and advection dominant transport, this example implemented for three cases with different Peclet numbers. The simulation parameters for different cases are given in Table 7. Figures 9 to 11 show simulation results of the three numerical models in comparison with analytical solution. Error indices are given in Tables 8 and 9. It is obvious from Figures 9(a) to 9(c) that in the first case (Peclet number less than 2), all methods simulated concentration-time curves accurately. Also, Figures 9(d) to 9(f) show that the MIKE 11 model cannot simulate concentration longitudinal profile accurately, because it does not consider the transient storage effect on solute transport.

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[1] Centered Time-QUICK Space (CTQS)

[2] Centered Time-Centered Space (CTCS)

[3] Backward Time-Centered Space (BTCS)

In the second case, by increasing the computational space step, all methods show a drop in the peak concentration, that its amount for the MIKE 11 model is more and for the TOASTS model is less than the others (Figures 10(a) to 10(c)). Figures 10(d) to 10(f) and Table 9 represent that the results of the models that use the central differencing scheme in spatial discretization of transport equations, show more discrepancy in comparison with the analytical solution.

In the third case, flow velocity increased about four times. As illustrated in Figure 11(c), by increasing the Peclet number, the OTIS model results show more oscillations. This model also shows very intense oscillations in the longitudinal concentration profile in the form of negative concentrations (Figure 11(e)), while observed oscillations in the TOASTS model are very small compared to the OTIS model (Figure 11(d)). However, the QUICK scheme oscillations in advection dominant cases are less likely to corrupt the solution. Also the MIKE 11 model results in comparison with the TOASTS model have greater difference with the analytical solution.

The main reason of the difference between the obtained results in the three cases, is actually related to how advection and dispersion affect the solute transport. The dispersion process affects the distribution of solute in all directions, whereas advection acts only in the flow direction. This fundamental difference manifests itself in the form of limitation in computational grid size.

4.3 Test Case 3: Conservative Solute Transport with Transient Storage

This example shows the TOASTS model application to field data, by using the conservative tracer (Chloride) injection experiment results, which was conducted in Uvas Creek, a small mountain stream in California (Figure 12). Details of the experiments can be found in Avanzino et al., 1984. Table 10 shows simulation parameters for the Uvas Creek experiment (Bencala and Walters, 1983). For assessing efficiency and accuracy of the three discussed models in simulation of the impact of physical processes on solute transport in a mountain stream, they are implemented for this set of observed data. Figures 13(a) to 13(c) illustrates simulated Chloride concentration in the main channel. It can be seen from these figures and Table 11 that the TOASTS model simulated the experiment results slightly better than the two other ones. Comparison of Figures 13(a) and 13(b) shows that the TOASTS and OTIS models have good accuracy in modeling the peak concentration and the TOASTS model has a slightly better performance in simulation of rising tail of concentration-time curve, particularly in 281 m station. Figure 13(c) shows MIKE 11 model results. It shows significant discrepancies with the observed data, particularly in peak concentrations. However, at 38 m station, where transient storage has not still affected solute transport, the results of the three models have little difference with the observed data (Table 11). Figure 14 depicts the TOASTS model results for Uvas Creek experiment for simulations with and without transient storage at 281 m and 433 m stations. This figure shows that in simulation with transient storage, the results have more fitness with the observed data in general shape of the concentration-time curve, peak concentration and peak arrival time. Figure 15 shows the simulated Chloride concentrations in the storage zone. The concentration-time curves in the storage zone have longer tails in comparison with the main channel. That means some portions of the solute mass remain in the storage zones and gradually return to the main channel.

4.4 Test Case 4: Non-Conservative Solute Transport with Transient Storage

The objective of this test case is to demonstrate the capability of the TOASTS model in non-conservative solute transport modeling in natural rivers. For this purpose, the field experiment of the three-hour reactive tracer (Strontium) injection into the Uvas Creek was used. The experiment conducted at low-flow conditions, so due to the high opportunity of solute for frequent contact with relatively immobile streambed materials, solute and streambed interactions and its sorption into bed sediments were more intense than during the high-flow conditions. Hence, the sorption process must be considered in simulation of this experiment (Bencala, 1983). Some of the simulation parameters are given in Table 12 and the other parameters are the same as those given in Table 10. Figures 16(a) to 16(c) and Table 13 show solute transport simulation results of the three subjected models in comparison with the observed data. According to these figures it could be said that the TOASTS model shows better fitness with the observed data. Figure 16(c) shows that simulation without taking into account the transient storage and kinetic sorption in the MIKE 11 model, leads to very poor results. The zero exchange coefficient at 38 m station causes reasonable results by this model at this station. Figure 17 illustrates the TOASTS and OTIS model results for sorbate concentrations on the streambed sediments versus the observed data at 105 and 281 m stations. It is clear from this figure and Table 13 that the TOASTS model is slightly better fitted to the observed data.

4.5 Test Case 5: Solute Transport with Transient Storage in a River with Irregular Cross-Sections

This test case shows the TOASTS model application for a river with irregular cross-sections under non-uniform flow conditions. The real data set for this test case was collected in a tracer experiment which has been done in the Athabasca River near Hinton, Alberta, Canada. Details of the experiments can be found in Putz and Smith, 2000. In this study, the simulation reach length is 8.3 km, between 4.725 km to 13.025 km of the river. The main reason in selecting this reach is that it has common geometric properties of rivers with storage zones. Total simulation time is 10 hours, space and time steps are considered equal to 25 meters and 1 minute, respectively. The exchange coefficient is assumed equal to 6×10^{-4} s^{-1} by calibration. According to the estimated parameters, DaI is calculated equal to 3.8 which is in the acceptable range and therefore transient storage zones affect downstream solute transport in the simulation reach. Since samples were collected only in four cross-sections downstream of the injection site, the observed concentration-time curve at 4.725 km was used as an upstream boundary condition of the transport model and the observed concentration-time curve at 11.85 km was used to compare the model results with the observed data. Figure 18 and Table 14 represent Athabasca experiment simulation results. It is clear that the concentration-time curves simulated by the TOASTS and OTIS models fit very well with the observed data; but again the MIKE 11 model failed to reproduce an accurate result which means a poor performance of the classical advection-dispersion equation in simulation of solute transport in natural rivers.

4.6 Test Case 6: Solute Transport with Hyporheic Exchange under Unsteady Flow Conditions

This test case shows an application of the TOASTS model to simulate solute transport in irregular cross-sections stream, under unsteady flow regime. In most of solute transport models, for simplification, flow is considered to be steady, while in most natural rivers, unsteady flow condition is common and neglecting temporal flow variations may lead to inaccurate results for solute transport simulation.

Tracer study that is used in this section, conducted in January 1992 at Huey Creek, located in McMurdo valleys, Antarctica (Figure 19). The flow rate was variable from 1 to 4 cfs[1] during the experiments. Since this stream does not have obvious surface storage zones, cross-sectional area of storage zones and exchange rate of this area, actually represent the rate of hyporheic exchange and interaction between surface and subsurface water (Runkel et al., 1998). Details of the experiments can be found in Runkel et al., 1998. Table 15 shows the simulation parameters. Figures 20(a) to 20(c) and Table 16 represent simulation results of Lithium concentration at 213 and 457 meter stations, by the three subjected models. The results of the TOASTS model have a slightly better fitness to the observed data than the two other models. This figure also indicates that the general shape of the concentration-time curve for this example is a little different from the other examples. Figure 20(c) represents the results of the MIKE 11 model. As seen in this figure, results have large differences with the observed data in peak concentrations and general shape of the curve. Figure 21 shows the corresponding storage zone concentrations at 213 and 457 m stations. It can be seen that solute concentration-time curves in the storage zone have lower peak and much longer tails that implies longer residence time of solute in these areas compared to the main channel.

5 Conclusion

In this study a comprehensive model was developed that combines numerical schemes with high-order accuracy for solution of the advection-dispersion equation considering transient storage zones term in rivers. In developing the subjected model (TOASTS), for achieving better accuracy and applicability, irregular-cross sections and unsteady flow regime were considered. For this purpose the QUICK scheme due to its high stability and low approximation error has been used for spatial discretization.

The presented model was verified successfully using several analytical solutions and 2D hydrodynamics and transport model as benchmarks. Also, its validation and applications were

[1] cubic feet per second

proved using several hypothetical examples and four sets of well-established tracer experiments data under different conditions. The main concluding remarks of this research are as the following:

- The numerical scheme used in the TOASTS model (i.e. CTQS scheme), in cases where advection is the dominant transport process (higher Peclet numbers), has less numerical oscillations and higher stability compared to the CTCS and BTCS numerical schemes.
- For a specified level of accuracy, TOASTS can provide larger grid size, while other models based on the central scheme face with step limitation that leads to more computational cost.
- As denoted by other researchers, classical advection-dispersion equation, in many cases, including transient storage and sorption cannot simulate accurate results.
- The TOASTS model is a comprehensive and practical model, that has the ability of solute transport simulation (reactive and non-reactive), with and without storage, under both steady and unsteady flow regimes, in rivers with irregular cross-sections that from this aspect is unique compared to the other existing models. Thus, it could be suggested as a reliable alternative to current popular models in solute transport studies in natural rivers and streams.

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Table 1. Comparison of the three model features used in this study

Model	Model features				
	Limitations on input parameters	Irregular cross-sections	Unsteady flow	Transient storage	Kinetic sorption
OTIS	Yes	No	No	Yes	Yes
MIKE 11	No	Yes	Yes	No	No
TOASTS	No	Yes	Yes	Yes	Yes

Table 2. Comparison of numerical methods used in the three models

Model	Numerical methods			
	Discretization scheme	Order of accuracy	Stability	Numerical dispersion
TOASTS	Centered Time-QUICK Space (CTQS)	2nd-order in time 3rd-order in space	$Pe < \frac{8}{3}$	0
OTIS	Centered Time-Centered Space (CTCS)	2nd-order in time 2nd-order in space	$Pe < 2$	0
MIKE 11	Backward Time-Centered Space (BTCS)	1st-order in time 2nd-order in space	$Pe < 2$	$\frac{U^2 \Delta t}{2}$

* $Pe = \frac{U \Delta x}{D}$

Table 3. Error indices of verification by the analytical solution for continuous boundary condition

Index	With storage			Without storage
	50 m	75 m	100 m	100 m
R^2 (%)	99.97	99.96	99.96	99.99
RMSE (mg/m^3)	0.021	0.026	0.033	0.009
MAE (mg/m^3)	0.017	0.023	0.029	0.006
MRE (%)	0.450	0.780	1.20	0.640

Table 4. Error indices of verification by the analytical solution for Heaviside boundary condition

Index	With storage			Without storage
	50 m	75 m	100 m	100 m
R^2 (%)	99.98	99.97	99.96	99.99
RMSE (mg/m^3)	0.034	0.045	0.058	0.0094
MAE (mg/m^3)	0.031	0.044	0.056	0.007
MRE (%)	3.5	4.2	5	1.49

Table 5. Error indices of verification by the 2D model

Index	With storage	Without storage
R^2 (%)	99.97	99.91
RMSE (mg/m^3)	0.095	1.88
MAE (mg/m^3)	0.066	0.77
MRE (%)	3.1	36.5

Table 6. Properties of the test cases used for the TOASTS model application

Example no.	Section type	Flow regime	Solute transport processes					
			Physical				Chemical	
			Advection	Dispersion	Transient storage		First-order decay	Kinetic sorption
					Surface	Hyporheic exchange		
1	Regular	Steady Uniform	Yes	No	No	No	No	No
2	Regular	Steady Uniform	Yes	Yes	No	No	Yes	No
3	Irregular	Steady Non-uniform	Yes	Yes	Yes	No	No	No
4	Irregular	Steady Non-uniform	Yes	Yes	Yes	No	No	Yes
5	Irregular	Steady Non-uniform	Yes	Yes	Yes	No	No	No
6	Irregular	Unsteady Non-uniform	Yes	Yes	No	Yes	No	No

Table 7. Simulation parameters related to test case 2

L (m)	*D* (m^2/s)	λ (s^{-1})	Case	Space step (m)	Peclet number
2200	5	0.00002	1	10	0.24
			2	100	2.4
			3	100	10

Table 8. Error indices of concentration time-series in test case 2

	Index	Model		
		TOASTS	OTIS	MIKE 11
Pe=0.24	R^2 (%)	99.93	99.93	99.98
	RMSE (mg/m^3)	0.460	0.460	0.850
	MAE (mg/m^3)	0.236	0.238	0.480
	MRE (%)	0.9	1.0	1.7
Pe=2.4	R^2 (%)	98.26	97.82	97.75
	RMSE (mg/m^3)	2.66	2.98	3.24
	MAE (mg/m^3)	1.42	1.55	1.73
	MRE (%)	3.77	4.11	4.93
Pe=10	R^2 (%)	98.8	98.2	98.24
	RMSE (mg/m^3)	3.60	4.41	4.46
	MAE (mg/m^3)	0.80	1.12	1.17
	MRE (%)	1.25	1.95	2.15

Table 9. Error indices of concentration longitudinal profiles in test case 2

	Index	Model		
		TOASTS	OTIS	MIKE 11
Pe=0.24	R^2 (%)	99.9	99.9	99.9
	RMSE (mg/m^3)	0.146	0.154	0.360
	MAE (mg/m^3)	0.105	0.108	0.280
	MRE (%)	1.91	1.97	3.20
Pe=2.4	R^2 (%)	98.6	98	96
	RMSE (mg/m^3)	0.53	0.65	0.86
	MAE (mg/m^3)	0.40	0.47	0.64
	MRE (%)	5.40	6.56	11.20
Pe=10	R^2 (%)	95.7	92	88.4
	RMSE (mg/m^3)	5.46	7.24	7.88
	MAE (mg/m^3)	3.02	4.47	5.05
	MRE (%)	6.27	12.44	13.50

Table 10. Simulation parameters for Uvas Creek experiment (test case 3)

Reach (m)	Flow discharge (m^3/s)	Dispersion coefficient (m^2/s)	Cross- sectional areas		Exchange coefficient (s^{-1})
			Main channel	Storage zone	
0-38	0.0125	0.12	0.30	0	0
38-105	0.0125	0.15	0.42	0	0
105-281	0.0133	0.24	0.36	0.36	3×10^{-5}
281-433	0.0136	0.31	0.41	0.41	1×10^{-5}
433-619	0.0140	0.40	0.52	1.56	4.5×10^{-5}

Table 11. Error indices of simulation of Uvas Creek experiment (test case 3)

Index	38 m			281 m			433 m		
	TOASTS	OTIS	MIKE 11	TOASTS	OTIS	MIKE 11	TOASTS	OTIS	MIKE 11
R^2 (%)	94.30	94.20	94.10	99.40	99.31	99.10	98.84	98.8	97.82
RMSE (mg/m^3)	0.727	0.728	0.730	0.180	0.183	0.340	0.203	0.205	0.440
MAE (mg/m^3)	0.202	0.203	0.212	0.108	0.109	0.205	0.121	0.125	0.280
MRE (%)	3.50	3.55	3.68	2.07	2.08	3.60	2.27	2.40	5.30

Table 12. Simulation parameters related to test case 4

Distribution coefficient (m^2/s)	Sorption rate coefficient (s^{-1})		Background concentration (mg/l)			Input concentration (mg/l)
	Main channel	Storage zone	Main channel	Storage zone	Bed sediments	
70	56×10^{-6}	1	0.13	0.13	9.1×10^{-3}	1.73

Table 13. Error indices of simulation of the Uvas Creek experiment (test case 4)

Index	Main channel concentration						Sorbate concentration			
	38 m			281 m			105 m		281 m	
	TOASTS	OTIS	MIKE 11	TOASTS	OTIS	MIKE 11	TOASTS	OTIS	TOASTS	OTIS
R^2 (%)	99.30	93.17	93.00	99.00	96.00	90.80	99.40	99.30	99.16	98.6
RMSE (mg/m^3)	0.05	0.12	0.17	0.055	0.070	0.200	1.05	1.64	2.67	2.86
MAE (mg/m^3)	0.021	0.044	0.086	0.048	0.055	0.115	0.75	1.50	2.40	2.41
MRE (%)	6.40	11.80	24.60	13.60	18.00	27.40	3.04	5.66	10.50	10.80

Table 14. Error indices of Athabasca River experiment (test case 5)

Index	Distance from upstream, 1850 m		
	TOASTS	OTIS	MIKE 11
R^2 (%)	99.75	99.8	62.5
RMSE (mg/m^3)	0.030	0.047	0.50
MAE (mg/m^3)	0.020	0.025	0.260
MRE (%)	1.70	4.77	28.60

Table 15. Simulation parameters related to test case 6

Reach (m)	Dispersion coefficient (m^2/s)	Storage zone area (m^2)	Exchange coefficient (s^{-1})
0-213	0.50	0.20	1.07×10^{-3}
213-457	0.50	0.25	5.43×10^{-4}
457-726	0.50	0.14	1.62×10^{-2}

Table 16. Huey Creek experiment error indices (test case 6)

Index	213 m			457 m		
	TOASTS	OTIS	MIKE 11	TOASTS	OTIS	MIKE 11
R^2 (%)	68.6	67	84	78	63.5	94
RMSE (mg/m^3)	0.673	0.674	0.740	0.48	0.63	0.62
MAE (mg/m^3)	0.28	0.30	0.54	0.23	0.28	0.52
MRE (%)	7.14	7.32	20.40	6.46	7.60	15

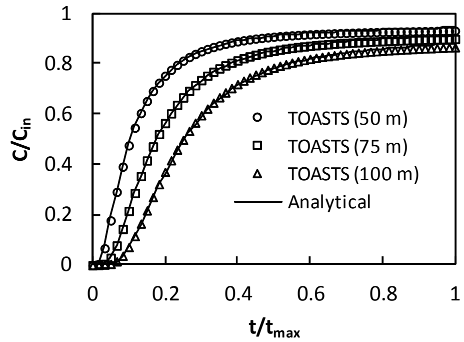


Figure 1. Results of the TOASTS model verification by the analytical solution for continuous boundary condition ($\alpha \neq 0$)

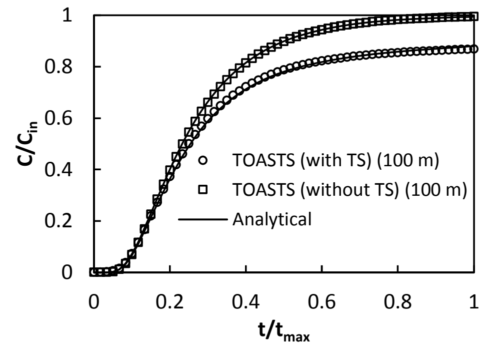


Figure 2. Results of the TOASTS model verification by the analytical solution for continuous boundary condition (α=0)

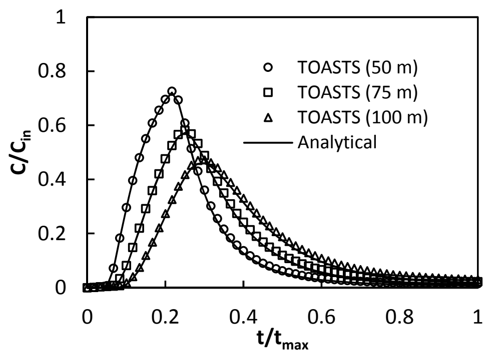


Figure 3. Results of the TOASTS model verification by the analytical solution for Heaviside boundary condition ($\alpha \neq 0$)

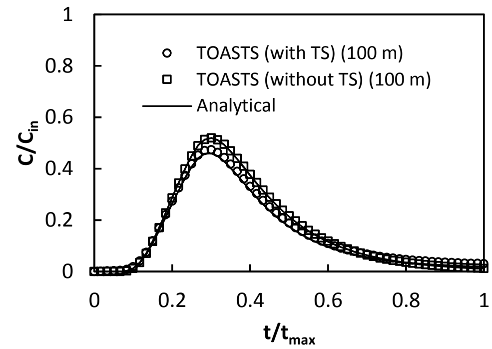


Figure 4. Results of the TOASTS model verification by the analytical solution for Heaviside boundary condition (α=0)

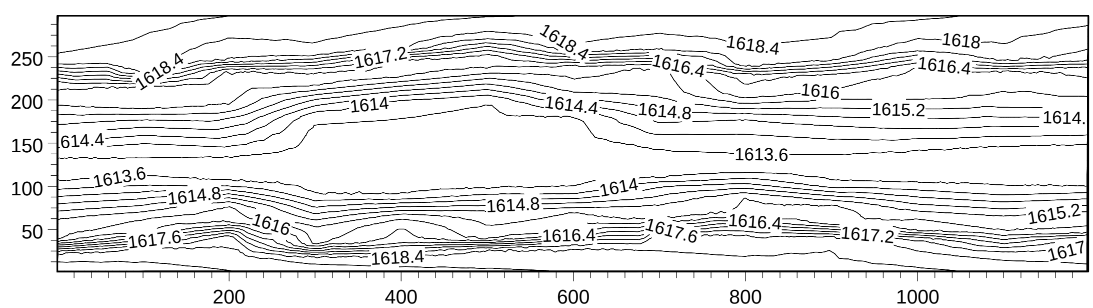


Figure 5. Bed elevation contours of the 2D hypothetical example

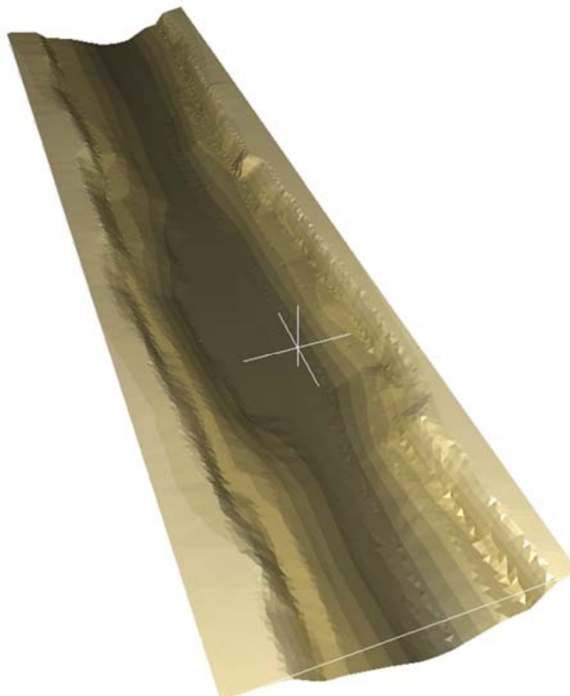


Figure 6. Bed elevation three-dimensional view of the 2D hypothetical example

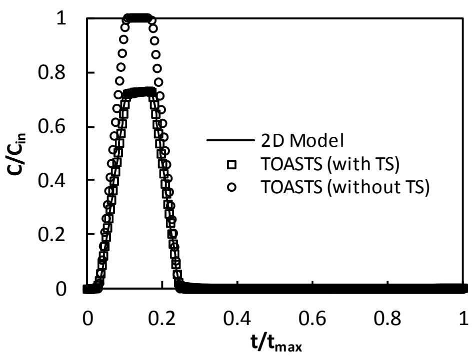


Figure 7. Results of the TOASTS model verification using the 2D model

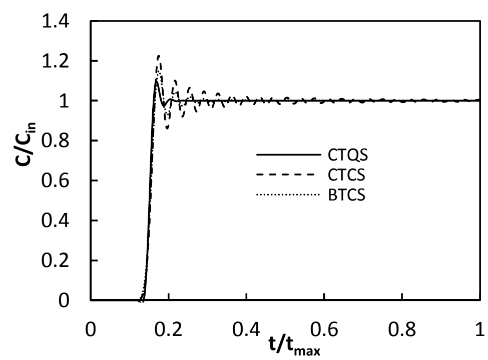


Figure 8. Comparison of the CTQS, CTCS and BTCS schemes for the pure advection test case

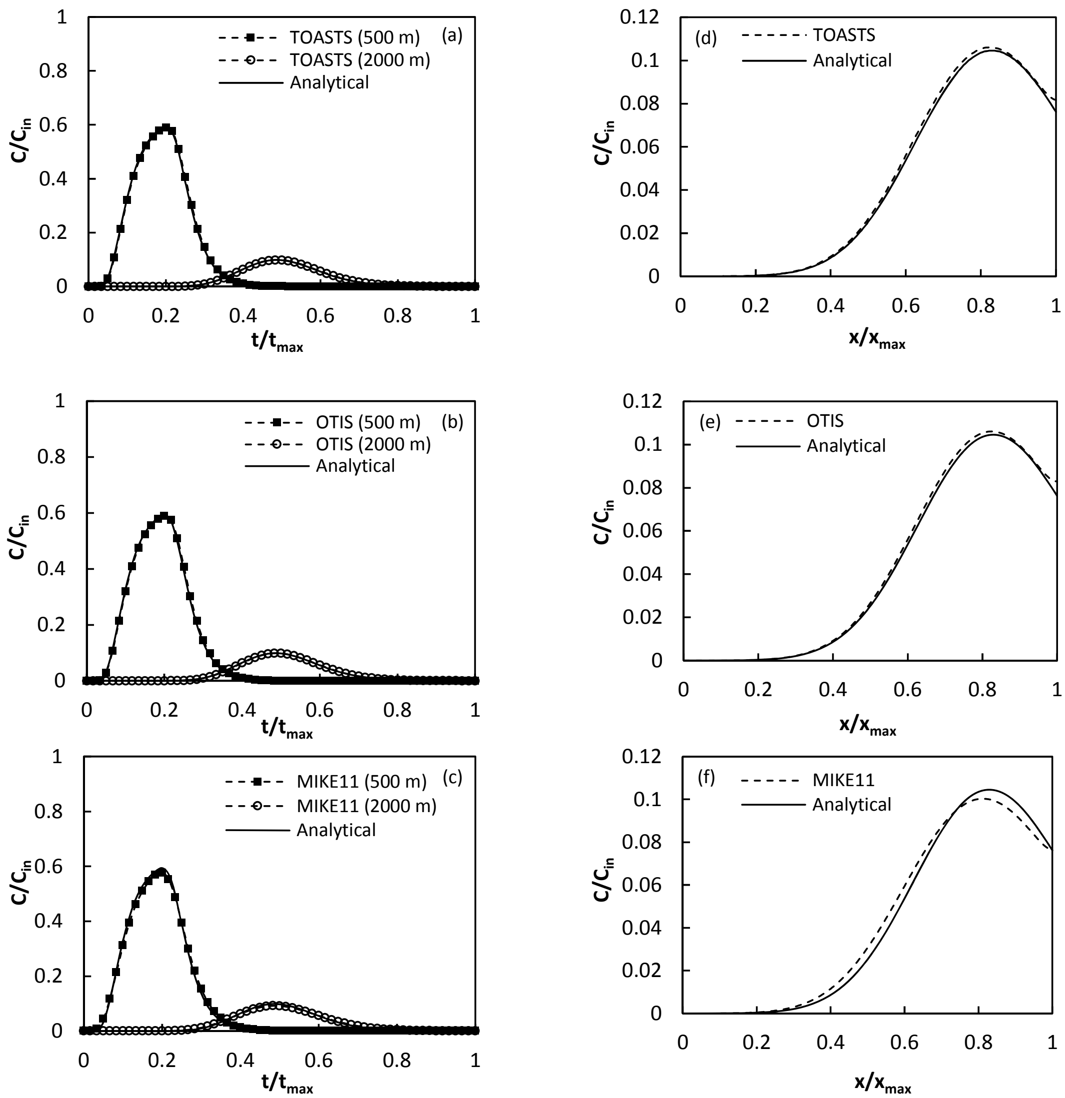


Figure 9. Comparison of the TOASTS, OTIS and MIKE 11 models in test case 2 for Pe=0.24

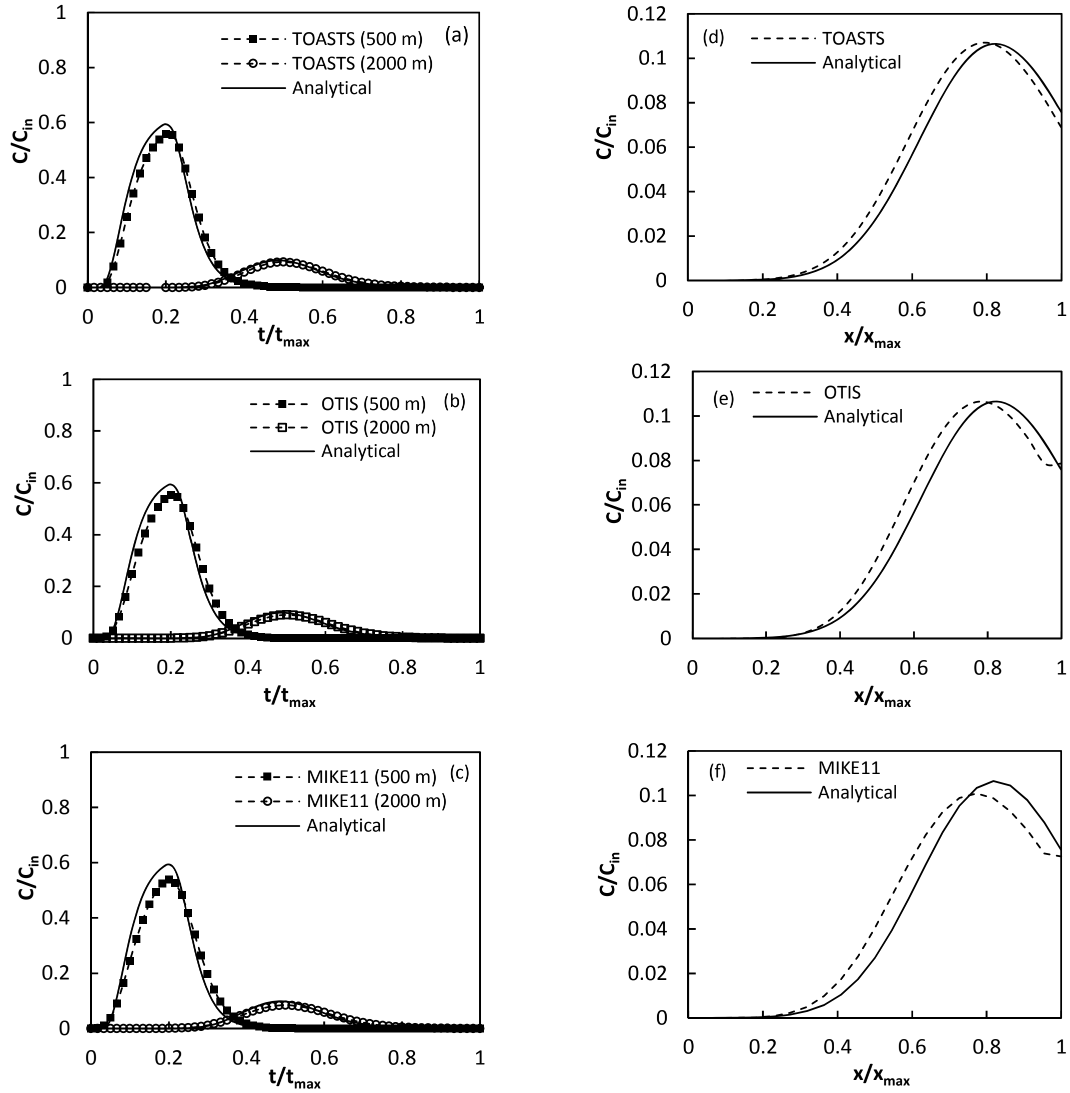


Figure 10. Comparison of the TOASTS, OTIS and MIKE 11 models in test case 2 for Pe=2.4

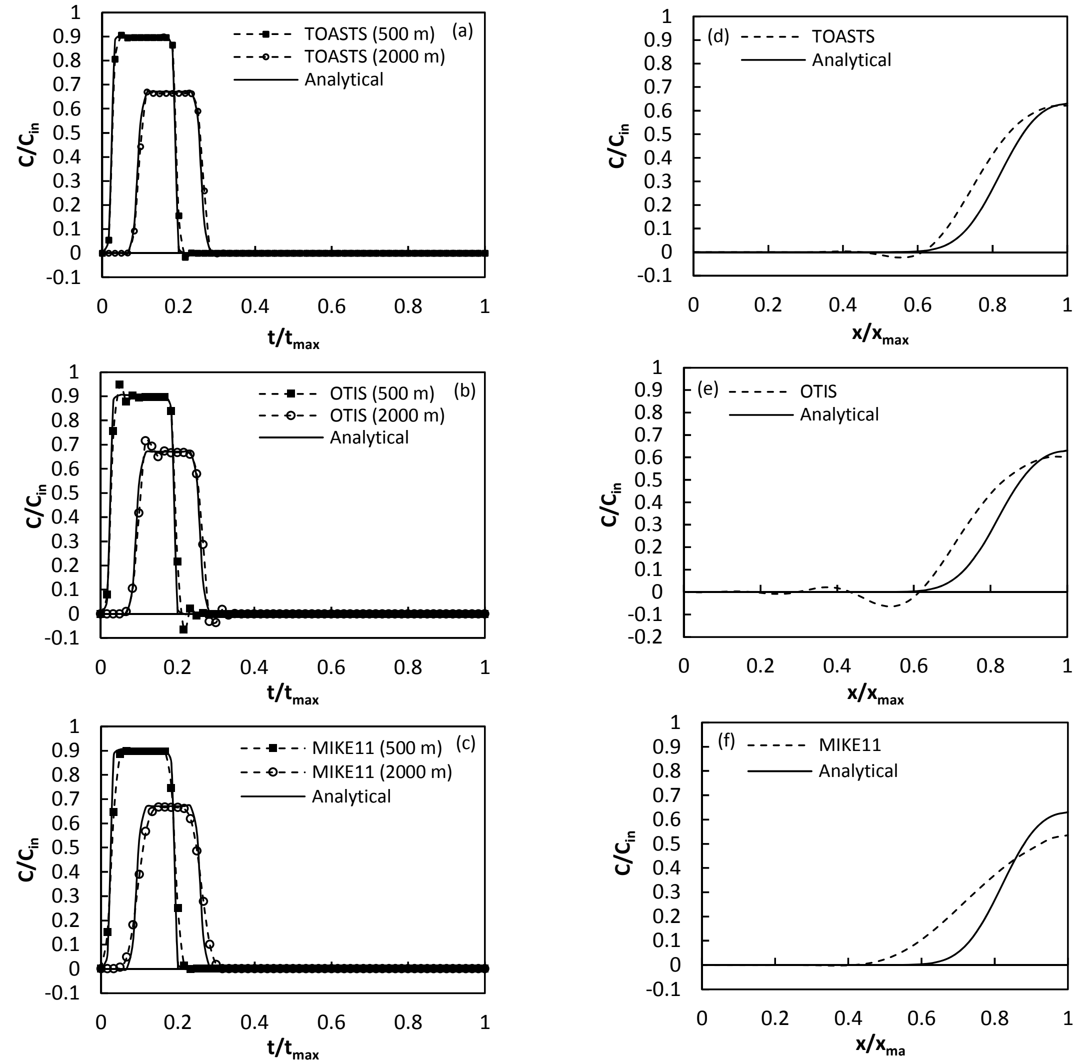


Figure 11. Comparison of the TOASTS, OTIS and MIKE 11 models in test case 2 for Pe=10

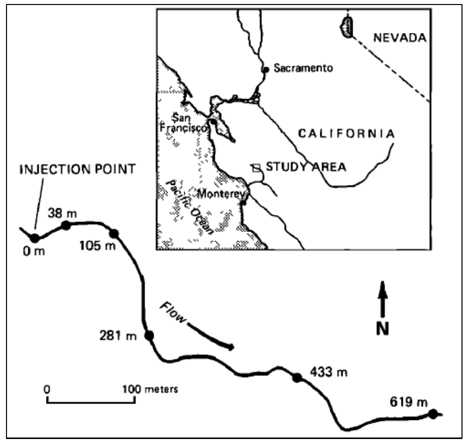


Figure 12. Uvas Creek (Santa Clara County, California) tracer study site map (Bencala and Walters, 1983)

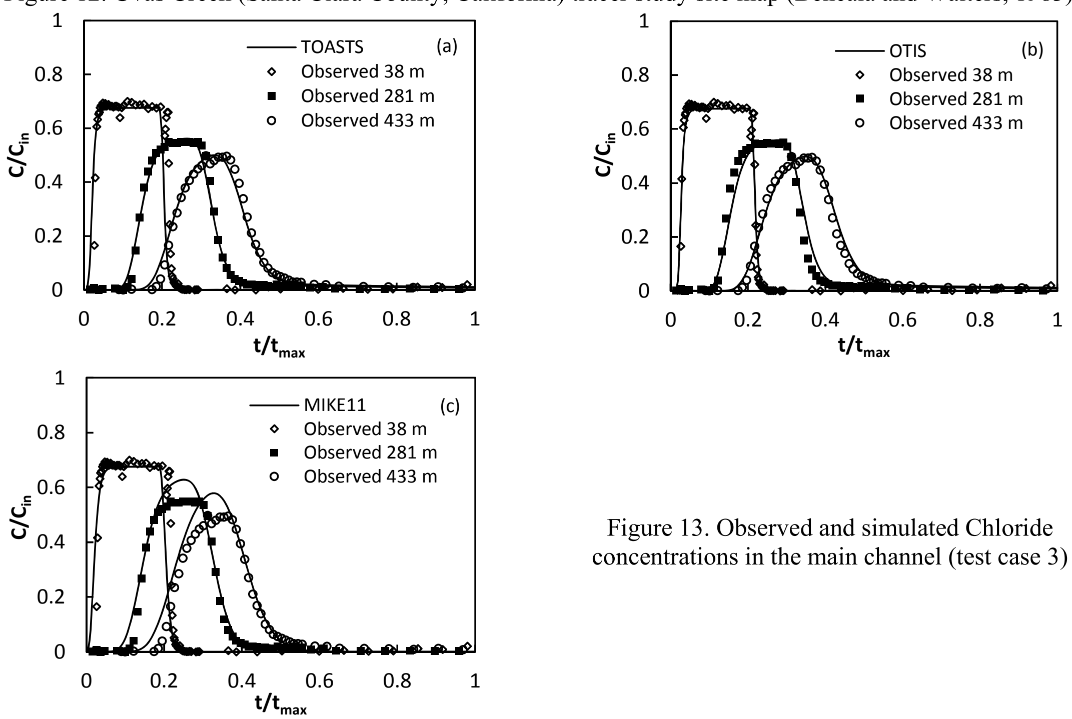


Figure 13. Observed and simulated Chloride concentrations in the main channel (test case 3)

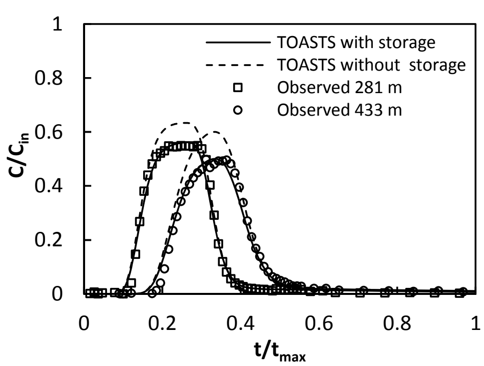


Figure 14. The TOASTS model results for simulation with and without transient storage (test case 3)

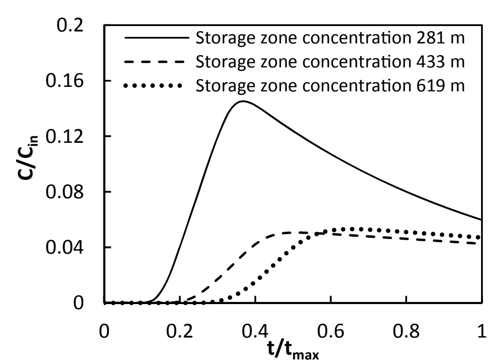
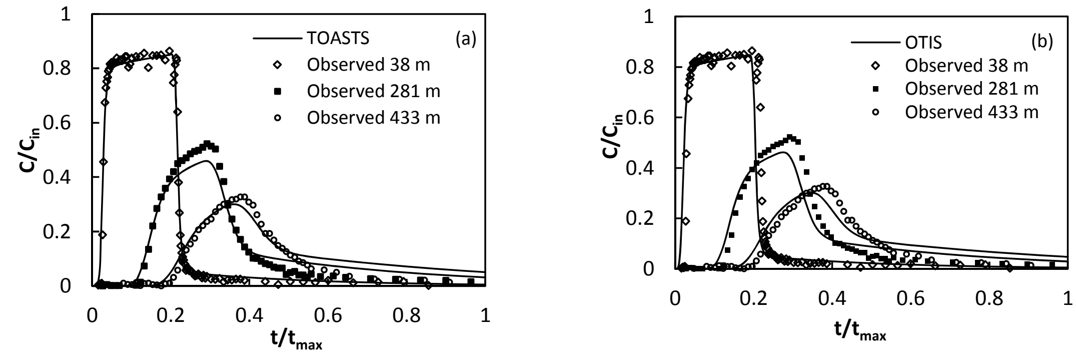


Figure 15. Observed and simulated storage zone concentrations computed by the TOASTS model (test case 3)



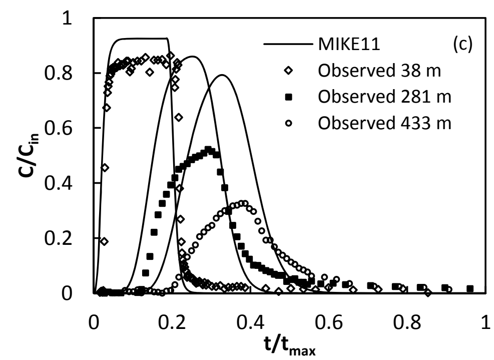


Figure 16. Observed and simulated Strontium concentrations in the main channel (test case 4)

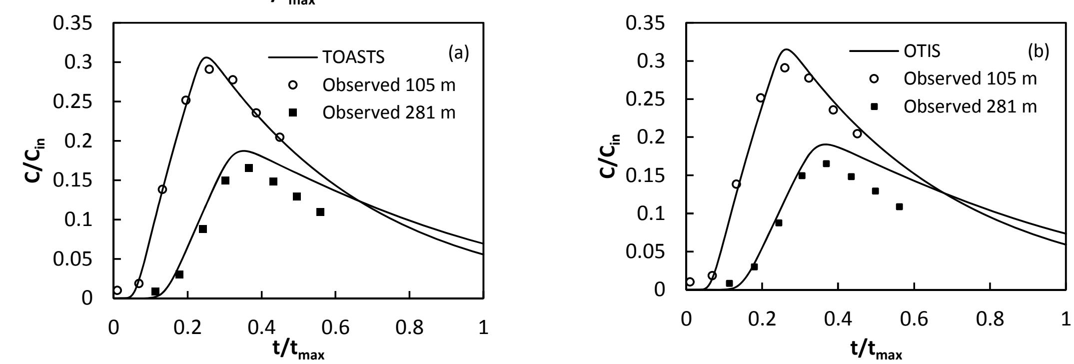


Figure 17. Observed and simulated sorbate Strontium concentrations in Uvas Creek experiment (test case 4)

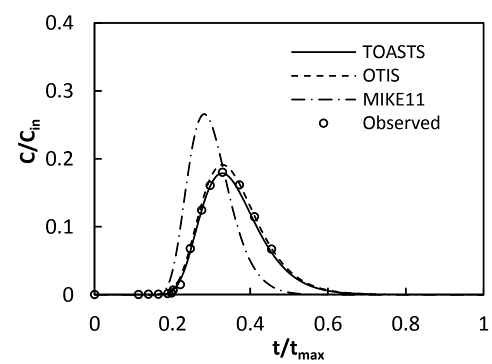


Figure 18. Simulation results for Athabasca River experiment (test case 5)

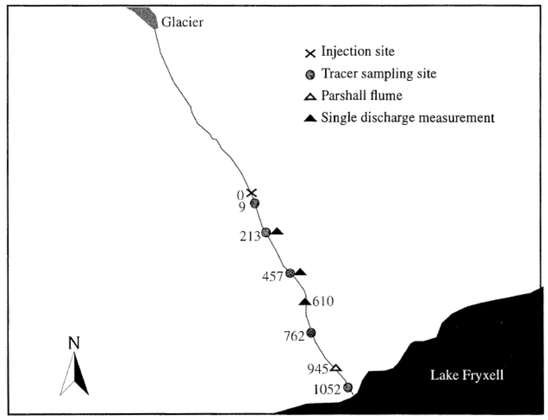


Figure 19. Huey Creek tracer study site map (Runkel et al., 1998)

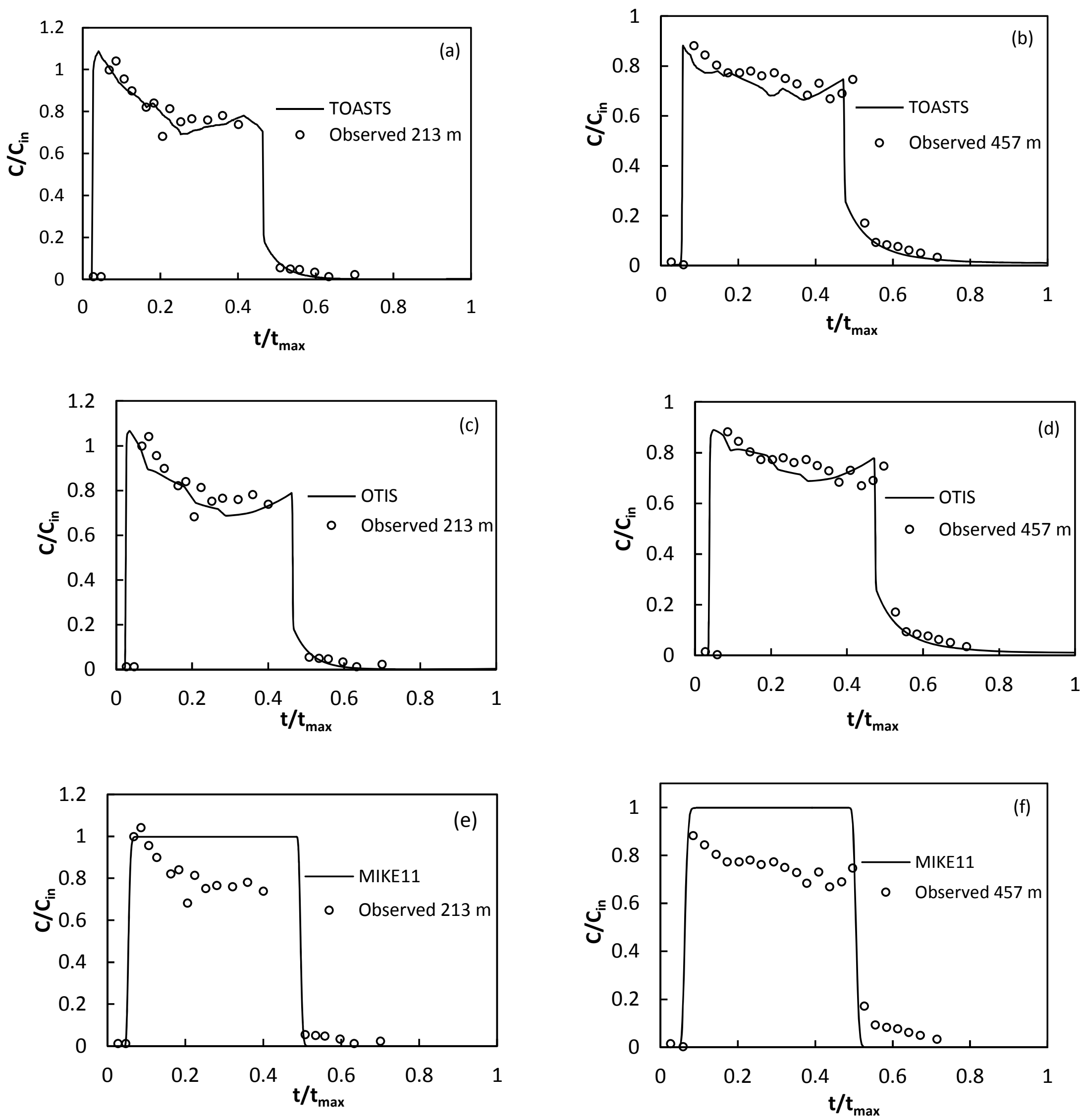


Figure 20. Observed and simulated main channel Lithium concentrations (test case 6)

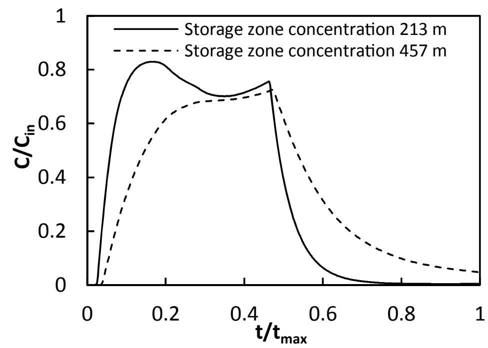


Figure 21. Storage zone concentrations (test case 6)