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 water bodies, especially in small mountain streams, is transient storage zones. The main effects include temporary retention of pollutants and reduce its concentration at the downstream and indirect impact on sorption process in the streambed. This paper presented the TOASTS model (Third Order Accuracy Simulation of Transient Storage) to simulate the 1-D pollutant transport in rivers with irregular cross-sections under unsteady flow with transient storage zones. TOASTS model verified with analytical solution and comparison with 2-D model. In order to demonstrate the model application two hypothetical examples were designed and four sets of well-established tracer study data that frequently cited in the literature, used. These examples cover different processes governing transport, cross-section types and flow regimes. The results of the TOASTS model compared with two common contaminant transport model ones, show better accuracy and numerical stability.

1 Introduction

First efforts to understanding the solute transport issue, leading to the longitudinal dispersion theory, is often referred to as classical advection-dispersion equation (ADE) (Taylor, 1954). This equation is a parabolic partial differential equation obtained from a combination of continuity equation and Fick's first law. The one-dimensional ADE equation is as follows:

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

Where, A= flow area$\left[L^2\right]$, C=solute concentration$\left[ML^{-3}\right]$, Q= volumetric flow rate $\left[L^3T^{-1}\right]$, D= dispersion coefficient$\left[L^2T^{-1}\right]$, λ= first-order decay coefficient $\left[T^{-1}\right]$, S= source$\left[MT^{-1}\right]$, t=time $\left[T\right]$ and x=distance$\left[L\right]$.

When this equation is used to simulate the transport in prismatic channels and rivers with relatively regular and uniform cross-sections, good results can be expected. But field studies, particularly in mountain pool-and-riffle streams, indicates that observed concentration-time curves have a lower peak concentration and longer tails than 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 study results, stated that to accomplish more accurate simulation of solute transport in natural rivers and streams, ADE equation must be modified and some terms added to it for considering the impact of stagnant areas-that 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 includes eddies, stream poolside areas, stream gravel bed, streambed sediments, porous media of channel 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, by temporary retention and gradual release of solute, causing an asymmetric shape in the observed concentration-time profiles, that could not be explained by classical advection-dispersion theory and on the other hand by providing the opportunity for reactive pollutants to repeated contact with streambed sediments, indirectly affect solute sorption process and makes it more intensive, especially in low flow conditions (Bencala, 1983, Bencala, 1984, Bencala et al., 1990, Bencala and Walters, 1983).

So far, 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). The transient storage mathematical model has been developed to show solute movement from the main channel to stagnant zones and vice versa. The simplest form of TSM is One-dimensional advection-dispersion equation with an additional term to transient storage (Bencala and Walters, 1983). Since the introduction of TS model, transient storage processes have been studied in a variety of small mountain streams to big rivers and shown that simulation results of tracer study data considering the transient storage impact have good agreement with observed data. Also, interactions between the main channel and storage zone, especially in mountain streams have 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, able to obviate shortcomings of current models of contaminant transport simulation, is presented. The TOASTS model merges numerical schemes with higher order accuracy of the solution of advection-dispersion equation with transient storage zones kinetic sorption in rivers with irregular cross sections of unsteady flow regime. This model illustrates a comprehensive modeling framework that links three sub-models to achieve 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 TOASTS model, results of two hypothetical examples (designed by authors) and four set of well-established tracer study data, are compared with the results of two current solute transport models, the MIKE11 model (that uses classical ADE equation for solute transport simulation) and OTIS model that today is the only existed model for solute transport with transient storage (Runkel, 1998).The TOASTS model and two other models properties are given in Table 1.

From Table 1, it is notable that the TOASTS model has advantages with no disadvantages known for both models so far. For example, OTIS in simulating transport in irregular cross-sections under non-uniform or unsteady flow has to rely on an external stream routing program and geometric properties and flow data must enter into the model from another routing program in the form of text file. Where, in the TOASTS and MIKE11 models, geometric properties and unsteady flow data, are directly evaluated from river topography, bed roughness, flow initial and boundary condition data. Also the TOASTS model has the ability to simulate solute transport problem in both with and without transient storage conditions under steady and unsteady flow regimes and in rivers with irregular cross section-without limitation in section number- that from this aspect is unique among solute transport models presented so far.

Another important point is the numerical scheme that used in the model structure. The key and basic difference of the TOASTS model refers to spatial discretization of transport equations. TOASTS uses the control volume approach and QUICK scheme in spatial discretization of advection-dispersion equation with transient storage and kinetic sorption[1], whereas the two other models employ central spatial differencing[2]. The more detailed comparison of numerical schemes used in structure of three subjected models is given in Table 2. As many of researchers claims, central spatial differencing, is incapable in simulation of the pure advection problem and doesn't introduce good performance in this regard (it leads to non-convergent results with numerical oscillations) (Zhang and Aral, 2004, Szymkiewicz, 2010), while QUICK scheme is better than the central scheme one (Neumann et al., 2011).

It should be mentioned that, in recent years QUICK scheme has been widely used in spatial differencing for ADE equation, due to its high-order accuracy (from third order), very small numerical dispersion and having higher stability rang, in particular in the case of pure advection dominant transport than other numerical methods (Neumann et al., 2011, Lin and Medina Jr, 2003). Hence, usage of the QUICK scheme in the numerical discretization of the transport equation leads to significant superiority of the TOASTS model to two other models, especially in advection dominant problems.

2 Methodology

2.1 Governing differential equations

The transient storage model is a simplified mathematical framework of complex physical processes of transport in a natural river or stream. There are several equations for solute

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[1]Centered Time - QUICK Space (CTQS)

[2] Centered Time - Centered Space (CTCS) have been used in OTIS model and Backward Time – Centered Space (BTCS) scheme employed in MIKE11 software.

transport with transient storage, which among them, the transient storage model presented by Bencala and Walters (1983), due to its ability to consider the unsteady flow regime and irregular cross-sections, is used in this study. By writing conservation of mass equations for solute in the main channel and storage zone, a coupled set of differential equations for the main channel and storage zone is derived:

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

$$\frac{dC_S}{dt} = \alpha\frac{A}{A_S}\left(C - C_S\right) \tag{3}$$

Where A and A_S are the main channel and storage zone cross-sectional area $\left[L^2\right]$; C, C_L and C_S are the main channel, lateral inflow and storage zone solute concentration $\left[ML^{-3}\right]$, respectively; q_{LIN} is the lateral inflow rate $\left[L^2T^{-1}\right]$; α is the storage zone exchange coefficient $\left[T^{-1}\right]$. For reactive (or non-conservative) solute, with considering two types of chemical reactions; kinetic sorption and first-order decay, equations (2) and (3) are re-written as:

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

$$\frac{dC_S}{dt} = S\left(C_S\right) + \hat{\lambda}_S\left(\hat{C}_S - C_S\right) - \lambda_S C_S \tag{5}$$

Where $\hat{C}_S$ is the background storage zone solute concentration $\left[ML^{-3}\right]$; C_{sed} is the sorbate concentration on the streambed sediment $\left[M/M\right]$; K_d is the distribution coefficient $\left[L^3M^{-1}\right]$; λ and λ_S are the main channel and storage zone first-order decay coefficient; $\hat{\lambda}$ and $\hat{\lambda}_S$ are the main channel and storage zone sorption rate coefficient $\left[T^{-1}\right]$, respectively; ρ is the mass of accessible sediment/volume water $\left[ML^{-3}\right]$; $L(C)$ and $S(C_S)$ are the right-hand side of equations (2) and (3) respectively. There is another variable concentration in equation (4), C_{sed}, which a mass balance equation is required:

$$\frac{dC_{sed}}{dt} = \hat{\lambda}\left(K_d C - C_{sed}\right) \tag{6}$$

2.2 Numerical solution of 1-D advection-dispersion equation with transient storage and kinetic sorption

Numerical solution of the Eqs. (4)-(6), in this study are based on the control volume method and centered time-QUICK space (CTQS) scheme. The spatial derivatives are discrete by QUICK scheme and average of *n* and *n+1* time levels. QUICK scheme is based on quadratic upstream interpolation for discretization of advection-dispersion equation (Leonard, 1979). In this scheme, face values are obtained from quadratic function passing through two upstream nodes and a downstream node. In a uniform grid, the value of desired quantity at the cell face is given by following equations:

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

$$if \quad u_w > 0: \qquad \phi_w = \frac{6}{8}\phi_W + \frac{3}{8}\phi_P - \frac{1}{8}\phi_{WW} \tag{8}$$

$$if \quad u_e > 0: \qquad \phi_e = \frac{6}{8}\phi_P + \frac{3}{8}\phi_E - \frac{1}{8}\phi_W \tag{9}$$

Where *P* denotes to the unknown nodes with neighbor nodes to the west and east are identified by *W* and *E* respectively. The west side control volume face is referred to by *w* and the east side face of control volume by *e*. The dispersion terms are evaluated using the gradient of the approximating parabola. Since the slope of chord between two points on a parabola is equal to the slope of the tangent to the parabola at its midpoint, on a uniform grid with equal control volumes, dispersion terms are the same as expressions of central differencing for dispersion, therefore:

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

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

The discretized form of the Eqs (4)-(6) are written as Eq (12)- (14):

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

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

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

By substitution the values on the control face from Eqs.(8)-(11) and doing some algebraic operations, equation (12) can be written as:

$$a_{WW}C_{WW}^{n+1}+a_WC_W^{n+1}+a_PC_P^{n+1}+a_EC_E^{n+1}=R_P \tag{15}$$

For solving the resultant system of linear equations, all of the quantities that appear on the right hand side of equation (15) should be known, hence the quantities of storage zone concentration and the sorbate concentration in the streambed sediment at the advanced time level (C_{Sed}^{n+1} و C_S^{n+1}), should be evaluated by using Eqs.(13) and (14) as:

$$C_S^{n+1}=\frac{\gamma_P^{n+1}C_P^{n+1}+\gamma_P^nC_P^n+\left(2-\Delta t\lambda_S-\gamma_P^n\right)C_S^n}{2+\gamma_P^{n+1}+\Delta t\lambda_S} \tag{16}$$

$$\gamma=\frac{\alpha\Delta tA}{A_S}$$

$$C_{Sed}^{n+1}=\frac{\left(2-\Delta t\hat{\lambda}\right)C_{Sed}^n+\Delta t\hat{\lambda}\,K_d\left(C_P^n+C_P^{n+1}\right)}{2+\Delta t\hat{\lambda}} \tag{17}$$

If N refers to the number of control volumes in solution domain, writing equation (15) for each four successive control volumes, from third to N-1th control volume, results a set of equations with N-3 equation and N unknowns. For solving this set of equations three more equations are needed, which yield from upstream and downstream boundary conditions. In QUICK scheme the concentration quantities at control faces calculated by using of concentration values in three adjacent nodes, two nodes at upstream and one node at downstream. Nodes 1, 2 and N all for the reason of locating the proximity of domain boundaries and implementation of boundary conditions, need to be treated separately. Equation (18) shows the matrix form of the resultant system of equations. By solving this system of equations, main channel concentrations in n+1 time level are obtained. Having main channel concentration values, storage zone and streambed sediment concentrations could be evaluated from Eqs. (16) and (17) for all control volumes.

$$\begin{bmatrix} a_P & a_E & & & & & & & \\ a_W & a_P & a_E & & & & & & \\ a_{WW} & a_W & a_P & a_E & & & & & \\ & a_{WW} & a_W & a_P & a_E & & & & \\ & & & \vdots & \vdots & \vdots & \vdots & & \\ & & & \vdots & \vdots & \vdots & \vdots & & \\ & & & \vdots & \vdots & \vdots & \vdots & & \\ & & & & & a_{WW} & a_W & a_P & a_E \\ & & & & & & a_{WW} & a_W & a_P \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \\ \vdots \\ \vdots \\ \vdots \\ C_{N-1} \\ C_N \end{bmatrix} = \begin{bmatrix} R_1 \\ R_2 \\ R_3 \\ R_4 \\ \vdots \\ \vdots \\ \vdots \\ R_{N-1} \\ R_N \end{bmatrix} \tag{18}$$

2.3 Damköhler Index

For assuring that transient storage happens in designed hypothetical examples, Damköhler number was used. This criterion 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 with length L, DaI is written as:

$$DaI = \frac{\alpha\left(1 + A/A_S\right)L}{u} \tag{19}$$

Where A and A_S are the main channel and storage zone cross-sectional area $\left[L^2\right]$ respectively; L is the main channel length $\left[L\right]$, α is the storage zone exchange coefficient $\left[T^{-1}\right]$ and u is average flow velocity $\left[LT^{-1}\right]$.

When DaI is much greater than unity, for example 100, the exchange between the main channel and storage zone is too fast and could be assumed that these two segments are in balance. When DaI is much lower than unity, for example 0.001, the exchange rate between the 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 does not affect downstream solute transport. Therefore, for reasonable estimation of transient storage model parameters, the DaI value must be within 0.1 to 10 (Fernald et al., 2001, Wagner and Harvey, 1997, Ramaswami et al., 2005).

3 Model verification

The TOASTS model is verified by analytical solution of advection-dispersion equation with transient storage for two types of upstream boundary condition (continuous and Heaviside) and also by comparing the model results with 2-D model ones. The characteristics and simulation parameters of hypothetical examples for model verification have been given below.

3.1 Verification by analytical solution

In this section, model verification, carried out by using analytical solutions presented by Kazezyılmaz-Alhan (2008), (Kazezyılmaz-Alhan, 2008). Analytical solutions were developed for the transient storage model introduced by Bencala and Walters (1983), for both continuous and finite source boundary conditions, assuming that flow velocity, channel cross-sectional area and longitudinal dispersion coefficient do not change with respect to time, with no lateral inflows, and first order decay in the main channel and storage zone. The designed example is a 200 m length channel with regular cross sections and constant cross sectional area ($1 m^2$). 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 obtained from equation (19) as 0.8 (it is between 0.1 and 10), so transient storage can be considered in the downstream solute transport simulation. Also, this example is implemented for two different types of upstream boundary conditions; a) continuous and b) Heaviside.

a) Upstream boundary condition: continuous

In this case, a solute concentration of 5 mg/m^3 is injected continuously for 10 hours. Computational time and space steps assumed 30 seconds and 1 m, respectively. Figure 1 shows the TOASTS model results compared to analytical solution at 50, 75 and 100 meters from upstream. In this study, for assessing accuracy of models, four error indexes were used. The square of the correlation coefficient (R^2) which compares the trend of calculated data with exact ones, Root Mean Square Error (RMSE), Mean Absolute Error (MAE), which have the same dimension as the observed data, and Mean Relative Error (MRE), that expressed in percentage. Error indexes for the continuous contaminant boundary condition are given in Table 3. According to Figure 1 and error indexes of Table 3, it is clear that the trends of numerical and analytical solutions of transient storage equations are similar and also the TOASTS model shows acceptable precision in this example.

As previously mentioned the TOASTS model has the ability of solute transport simulation in both with and without storage cases. Hence, in order to show model capabilities and assess the model results accuracy in without transient storage case, the model is implemented with α=0 for this example and results compared to analytical solutions of classic advection-dispersion equation. For instance, the results are shown in Figure 2, in the form of comparative concentration-time curves in two cases of with and without storage at 100 m from upstream. The last column of Table 3 presents error indexes for continuous boundary condition simulation without transient storage. It can be seen from Figure 2 that the model results, in both cases, are very close to analytical solutions. Error indexes, also confirm these results. This figure also illustrates that in the case of with transient storage, concentration-time curves have lower peak than the without storage ones (α=0), that matches the previously mentioned transient storage concept.

b) Upstream boundary condition: Heaviside function

In this case, a solute concentration of 5 mg/m^3 is injected to the stream for a limited time of 100 minutes. Total time of simulation was 10 hours, also time and space steps assumed 30 seconds and 1 meter, respectively. Comparison of model results with analytical solutions illustrated in Figure 3. Table 4 shows error indexes for this simulation. Figure 3 and Table 4 confirm the reliability of TOASTS model results.

After assuring the correctness of simulation results in the case of Heaviside upstream boundary condition with transient storage, the TOASTS model is implemented for this example with α=0 and the obtained results are compared to analytical solution of classic advection-dispersion equation ones. Results are given in Figure 4, as comparative concentration- time curve at 100 meters from upstream. Error indexes for simulation with and without storage are presented in Table 4. According to Figure 4, it is obvious that the TOASTS model results in both cases (with and without storage) have reasonable fitness with analytical solution and both results follow a similar trend. This figure also clearly shows the difference between solute concentration-time curves in two cases. When storage affects downstream solute transport, these curves show lower peak and longer tail than without storage transport ones.

3.2 Verification by 2-D model

The main cause of occurrence of transient storage phenomena is velocity differences between the main channel and storage zones (areas that assumed to be stagnant relative to main channel). The 2D model considers velocity variations in two dimensions of a river and so gives more accurate predictions of solute transport behavior in reality. Which means that it takes into account the effects of TS zones automatically, and could be used for verification of the presented 1-D model as a reference. For this purpose, a hypothetical example was designed, a 1200 meter length river, with irregular cross-sections that the cross sectional area varied with space and time. Figure 5 illustrates bathymetry properties of the hypothetical river. As clear in the figure, for creation of a hypothetical storage zone, in the distance of 300 to 600 meters the river has been widened as unilateral.

The total time of the simulation is equal to 14 hours and the flow condition in the river is unsteady and non-uniform. Also in this example the flow assumed to be subcritical, thus for model implementation boundary conditions at each upstream and downstream points are needed. The boundary conditions of flow sub-model are volumetric flow rate and water level variations with respect to time at upstream boundary (x=0 m) and downstream boundary (x=1200 m), respectively. For creation of flow initial condition, flow sub-model was implemented for 14 hours with constant flow discharge and depth, that equals to their values at t=0 (cold-start). Implementation of transport model also needs initial condition and two boundary conditions. Upstream and downstream boundary conditions are step loading and zero-gradient concentration, respectively.

The solute concentration in the main channel and storage zone, at the beginning of the simulation, assumed to be zero. In calculations of both flow and transport models, space step (Δx) and time step (Δt) are 100 m and 1 minute, respectively. Dispersion coefficient (m^2/s), Storage zone area (m^2) and exchange coefficient are 10, 22 and 1.8×10^{-4} respectively. For this example the DaI number is obtained as 0.4, that is in the appropriate range (between 0.1 and 10), which means that transient storage is involved in downstream transport. The upstream boundary condition for transport sub-model is a three hour lasting step loading pulse with 20 mg/m^3 pick concentration. TOASTS model results for simulations with and without transient storage compared to 2-D model ones, at different distances from upstream, are illustrated in Figure 6. This figure shows that with appropriate A_S and α, concentration-time curves with transient storage are so close to the 2-D model results curve. These results also indicate the necessity of considering transient storage terms in advection-dispersion equation for more accurate simulation of solute transport especially in natural rivers and streams.

As previously mentioned, the 2-D model due to consideration of velocity variations in two dimensions of river reach, gives more accurate predictions of solute transport behavior in rivers with TS zones, so the results of three models (TOASTS, OTIS and BTCS with TS[1]) compared to 2-D model ones, to assess their accuracy in simulation of solute transport with transient storage. Figure 7 (a) and (b) shows the results of two different models (OTIS and BTCS with TS) in comparison to 2-D and TOASTS models. It should be noted that due to proximity of results and to facilitate the comparison, the results have been presented in separate figures. These figures indicate that the TOASTS model results are closer to 2-D model results compared to two other model ones. That means that with considering appropriate parameters for the storage zone area and exchange coefficient, the TOASTS model is capable of estimating observed concentration-time curves in natural rivers and streams with sufficient and reasonable precision. For detailed comparison, error indexes are

[1] For this method a computer code is written.

given in Table 5. These error indexes show that among all three mentioned models, TOASTS has less error percentage and more accuracy than the two other ones. Also the trend of TOASTS results is closer to the 2-D model ones than the others.

4 Application

In this section, the application of the TOASTS model and a comparison of the results with the ones of OTIS and MIKE11 models are presented by using designed hypothetical examples and several sets of observed data (well-established tracer study data). General characteristics of these examples are given in Table 6. As shown in the table, the chosen examples include a wide variety of solute transport simulation applications at different flow regimes in various cross-section types (regular and irregular) and physical and chemical transport processes.

4.1 Example 1: Pure advection

In order to demonstrate the advantages of numerical method used in the TOASTS model, for advection dominant problems, a hypothetical example designed and three numerical schemes CTQS, CTCS and BTCS were implemented for this purpose. The results are shown and compared in the form of concentration-time curves. Steady flow with 10 m^3/s volumetric rate and regular cross-sections with10 m^2 area were assumed. Total time of simulation was 5 hours, space and time steps were 100 m and 10 seconds, respectively. Due to that advection is the only affective process in transport, the effect of dispersion and transient storage were ignored (dispersion coefficient assumed to be very small and near to zero).

According to Figure 8 it is clear that, for pure advection simulation, the CTQS scheme has a less oscillation than the two other ones. In particular, this figure shows that, the results of CTCS scheme that also used in OTIS numerical model structure have very high oscillations, while the CTQS scheme results show very little oscillations and higher numerical stability. Therefore, it can be concluded that for advection dominant simulation the TOASTS model has better performance than two other models. It is interesting to note, that in mountain rivers where the transient storage mechanism is also more observed, due to relatively high slope, have higher flow velocities than plain rivers, and as a result advection is the dominant process in solute transport. Thus, these results somehow confirm the superiority of the TOASTS model for simulation of solute transport with transient storage compared to the common models.

4.2 Example 2: Transport with first-order decay

This example illustrates the application of the TOASTS model in solute transport simulation undergoing first-order decay without transient storage and kinetic sorption in the form of a hypothetical problem. A decaying substance enters the stream with steady and uniform flow during a two hour period. The solute concentration at the upstream boundary is 100 concentration units. Also, in order to assess TOASTS model capabilities in the case of high flow velocity and advection dominant transport, this example implemented for three cases with different Peclet numbers (as the Peclet number is the measure of advection relative power). The simulation parameters and properties of three model implementation cases are given in Table 7. Figure 9 to Figure 11 show simulation results of three numerical models in comparing to analytical solution. Error indexes are given in Table 8 and Table 9. It is obvious from Figure 9 (a) to (c) that in the first case (Peclet number less than 2), all methods simulated concentration time profile with the same accuracy. Also, Figure 9 (d) to (f) show that MIKE11 model cannot simulate concentration-space accurately, because it does not consider the transient storage effect on transport, as Table 9 indexes confirm it. In the second case, by increasing computational space step, all methods show a drop in peak concentration, that its amount for MIKE11 model is more and for the TOASTS model is less than the others (see Figure 10 (a) to (c)). Figure 10 (d) to (f) and Table 9 indexes demonstrate that the results of models that used a central differencing scheme in spatial discretization of transport equations, show more discrepancy to the analytical solution ones.

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

The reason of the difference among 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 spreads influence only in the flow direction. This fundamental difference manifests itself in the form of limitation in computational grid size. Numerical schemes with central spatial differencing produce spurious oscillations for certain problems such as high flow velocities and advection dominant transport. One way to overcome these oscillations is the use of finer grids, with the choice of space step based on the dimensionless Peclet number. Spatial discretization in a Peclet number smaller than 2 can eliminate numerical oscillations and Peclet number less than 10 can reduce such oscillation, greatly. However the more computational cost due to extensively fine grid may become impractical in some applications, particularly in natural rivers and streams. While quadratic upstream interpolation schemes such as QUICK scheme that used in the TOASTS model, is designed in the way that overcomes this oscillatory behavior. These schemes simulate the problem with reasonable accuracy even with greater space steps in comparison to central differencing ones(Versteeg and Malalasekera, 2007).

4.3 Example 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). Injection of concentrated NaCl solution started at 8 AM on 26 September 1972 and continued for 3 hours. During the experiment, flow discharge in Uvas Creek was near to seasonal base-flow, approximately to 12.5 lit/s, non-uniform and steady flow. Chloride background concentration recorded 3.7 mg/lit. Five sampling sites established in 38, 105, 281, 433 and 619 meters downstream of the injection point, respectively (Avanzino et al., 1984). Table 10 shows simulation parameters for the Uvas Creek experiment such as reach length, dispersion coefficient, discharge, main channel and storage zone cross sectional area and exchange coefficient for each reach (Bencala and Walters, 1983). For assessing of efficiency and accuracy of three discussed models in simulation of the impact of physical processes (advection, dispersion and transient storage) on solute transport in a mountain stream, they are implemented for this set of observed date.

Figure 13 (a) to (c) illustrates simulated chloride concentration in the main channel. It can be seen from this figure and Table 11 indexes, that the TOASTS model simulated the experiment results more accurate than the two other ones. Comparison of Figure 13 (a) and (b) show that the TOASTS and OTIS models have good precision in modeling the peak concentration and the TOASTS model has better performance in simulation of rising tail of concentration-time curve, particularly in 281 m station. Figure 13 (c) shows MIKE11 model results. Due to using classical AD equation and ignoring the effect of transient storage process, its results show significant discrepancies with observed data, particularly in peak concentrations. However, at 38 m station, where transient storage doesn't affect solute transport ($\alpha=0$), the results of three models have little difference with observed data (Table 11).

Figure 14 demonstrates the model results for Uvas Creek experiment for simulation with and without transient storage at 281 and 433 m stations. This figure shows that in simulation with transient storage, the results have more fitness with observed data in the general shape of the concentration-time curve, peak concentration and peak arrival time. Figure 15 shows the simulated chloride concentrations in storage zone. As it is obvious from the figure, the concentration- time curves in storage zone have longer tails in comparing with main channel ones. That means some portions of solute mass remain in storage zones, after passing the solute pulse and when completely passage of the pulse from stream occurs, gradually return to the main channel takes place. Because of these mechanisms the concentration- time curves in main channel have lower peak and longer tails than the predicted ones from classical advection-dispersion equation.

Figure 16 indicates the transient storage concept that mentioned later, in the form of observed data. This figure shows that gradually from the beginning of the simulation, the main channel solute concentrations decrease and add to storage zone concentrations. In the next example, the combined effect of physical and chemical processes on solute transport will be discussed.

4.4 Example 4: Non-conservative solute transport with transient storage

The objective of this example is a demonstration of the TOASTS model capabilities in non-conservative solute transport modeling in natural rivers and showing how physical and chemical processes affecting transport. For this purpose, the characteristics of a field experiment of the three-hour reactive tracer (Strontium) injection into the Uvas Creek were used. The experiment conducted at low-flow condition, 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 was more intense than during the high flow conditions. Hence the sorption process must be considered in simulation of this experiment (Bencala, 1983).

Simulation parameters are given in Table 12. The interesting point about this table data is the significant difference between the value of the sorption rate coefficient in the main channel and storage zone due to their completely different features of these two zones. The mass of accessible sediment/volume water (ρ) assumed at first and last reach is 4×10^4 and at other reaches 2×10^4. Other simulation parameters such as reach length, dispersion coefficient, flow discharge, cross-sectional area of main channel and storage zone and exchange coefficients, are the same as Table 10 parameters.

Figure 17 (a) to (c) shows solute transport simulation results in this stream by Three examined models in compare to observed data. According to Figure 17 it could be said that the TOASTS model results show better and more reasonable compatibility with observed data in general shape, peak concentration and peak arrival time. Presented error indexes in Table 13 also confirm it. Figure 17 (c) clearly shows that simulation without transient storage and kinetic sorption in MIKE11 model, leads to very different results from observed data. This model results, especially at 38 m station, which the exchange coefficient with storage zone assumed to be zero, demonstrate the direct effect of sorption on transport in the form of drop in peak concentration.

Figure 18 illustrates TOASTS and OTIS model results for sorbate concentrations on the streambed sediments versus observed data at 105 and 281 m stations. As it is clear from Figure 18 and Table 13 indexes, the TOASTS model results better fitted to observe data, which could be related to difference in numerical methods that used in models structure. Figure 19 presented Strontium sorbate concentrations at three various times of simulation (beginning, middle and the end of it) at all sampling stations. This figure clearly shows the solute sorption to and desorption from the bed sediments. At 38 and 105 m stations, which do not have storage zones (α=0), variation in concentration levels between the middle of simulation to the end of it, is too high. It means that a lot of amount of sorbate Strontium rapidly returns to the stream water during this period of time, however, in other station which have storage zones, this process is slower. Particularly at 619 m station that exchange with storage zone is more than others (due to greater exchange coefficient and storage cross - sectional area than other stations), it can be seen that even with to the end of the simulation, amount of sorbate concentration increased while desorption does not occur yet. In other words, presence of storage zones delays Strontium desorption from bed sediments. This happens because of the longer time combination of Strontium transport into the storage zone, its desorption and returns to main channel, compared to the solute pulse passage duration.

4.5 Example 5: Solute transport with transient storage in a river with irregular cross-sections

This example shows the model application for a river with irregular cross-sections under unsteady flow condition. Putz and Smith (2000) describe properties of two field injection experiments at a 26 km length reach from the Athabasca River near Hinton, Alberta, Canada. At first injection, 20% Rhodamin WT continuously injected to the river for 5.25 hours with constant discharge and at second one, a slug input tracer test was conducted and the samples were collected in four cross- sections downstream of the injection point; 4.725, 11.85, 16.275 and 20.625 kilometers (Putz and Smith, 2000). In this study the data of slug tracer injection experiment have been used. The simulation reach length is 8.3 km, between 4.725 km to 13.025 km of river. The geometric parameters between two cross-sections, where the survey data do not exist, calculated from linear interpolation of two adjacent sections for a known water level.

The fundamental point in selecting this reach, is it must have common geometric features of rivers with storage zones, such as pool-and-riffle consequently and significant and sudden width variations. Total time of the simulation is 10 hours, space and time step are 25 meters and 1 minute respectively. Cross sectional area and exchange coefficient of 5.5 to 6.250 km interval, assumed 40 m^2 and6×10^{-4}, respectively. Transient storage parameters obtained from trial and error and visually determining of simulation results to experimental data. According to estimated parameters, DaI obtained as 3.8, which are in acceptable domain, therefore it could be said that transient storage affects downstream solute transport in simulation reach.

The flow model boundary conditions are constant flow discharge 334 m^3/s at upstream and constant water surface elevation of 952.6 meters, according to the Environment Canada gauging station. Since samples were collected just in four cross-sections downstream of the injection site, given concentration-time curve at 4.725 kilometers used as the upstream boundary condition of transport model and the concentration-time curve taken at 11.85 kilometers were used to compare the model results with observed data. Downstream boundary condition of transport model was zero-gradient concentration.

Figure 20 shows Athabasca experiment simulation results at 11.85 kilometers from upstream by using three models. Error indexes also are given in Table 14. According to Figure 20 (a) and Table 14, it can be said that concentration-time curve resulted from implementation of TOASTS and OTIS models, fit very well with the observed tracer concentration-time curve, but the concentration-time curve simulated using the MIKE 11 model has great difference with the observed data. Higher MRE index indicates a poor performance of the classical ADE equation in simulation of solute transport in natural rivers. Thus, in order to more accurate simulation of solute transport in natural rivers, it is necessary that the impact of transient storage on solute downstream transport be considered.

4.6 Example 6: Solute transport with hyporheic exchange under unsteady flow condition

This example 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, in order to simplify the work process, flow is considered to be steady. While in most natural rivers, unsteady flow conditions are common and ignoring spatial and temporal flow rate variations and consequently a change in the geometry properties of cross-sections, may lead to incorrect results from the solute transport simulation. Tracer study that used in this section, conducted in January 1992 at Huey creek located in the of McMurdo valleys, Antarctica (Figure 21). The stream has a complex hydrological system, because the flow rate changes with respect to temperature and radiation variations, either daily or seasonally (Runkel et al., 1998). So, the flow rate was variable from 1 to 4 cubic feet per second during the experiment. Since this stream does not have obvious surface storage zones, cross-sectional area of storage zone and the exchange rate with this area, actually represents the rate of hyporheic exchange and interaction of surface and subsurface water. LiCl tracer at the rate of 8.7 ml/s was injected into the stream for a period of 3.75 hours. Samples were taken at various points downstream and flow was measured at the same time. Table 15 shows the simulation parameters.

Figure 22 (a) to (c) demonstrate simulation results of Li concentration at 213 and 457 meter stations, by three models. The figure and error indexes of Table 16 show that the results of the TOASTS model have a better fit to 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; the reason for this can be attributed to the extreme changes in flow rate during the experiment. Figure 22 (c) presents the results of the MIKE 11 model. As seen in the figure, results have great discrepancies with observed data in peak concentrations and general shape of concentration-time curve. Figure 23 shows storage zone concentration at 213 and 457 m stations. As demonstrated in the figure, solute concentration-time curves in storage zone have lower peak and much longer tails than main channel ones that indicates longer residence time of solute in these areas compared to main channel.

5 Conclusions

In this study a comprehensive model is presented, that merges numerical schemes with higher order accuracy for the solution of advection-dispersion equation with transient storage zones in rivers with irregular cross sections of unsteady flow regime, to obviate the flaws in current models of contaminant transport simulation. For this purpose QUICK scheme due to the high stability and law approximation errors have been used in the spatial discretization of the transport equation with transient storage and kinetic sorption. The presented model (TOASTS) is verified by analytical solution for two types of boundary conditions and with considering transient storage and the 2D model. The results of verification implied that the presented model has reasonable accuracy in simulation of solute transport in natural rivers and streams with transient storage zones.

Then the TOASTS model application was shown, compared to current common models in the form of two hypothetical examples (designed by the authors) and four sets of well-established tracer study data with different conditions (such as channel geometry, flow regime and the processes involved in transport). The results of the first example, showed that the numerical scheme used in the TOASTS model (e.g. CTQS scheme), in cases where advection is the dominant transport process, have less numerical oscillations and higher stability compared to CTCS and BTCS numerical schemes. The results of the second example, indicate that quadratic upstream interpolation schemes such as QUICK scheme, expand the stability domain of numerical solution of solute transport equations (higher Peclet numbers) while maintaining an acceptable level of accuracy, can provide a larger grid size. While the central spatial differencing method faced with step limitation and to achieve a stable solution the calculation time step must be selected carefully, that in some practical applications will result in a rise of computational cost.

The results of the third example for non-reactive tracer (chloride) showed that in addition to the standard mechanisms of advection and dispersion, the transient storage mechanism also affects solute concentration levels at downstream. The results of the fourth example, show that the absorption of reactive tracer (strontium) in streambed sediments played role in reduction of concentration levels at downstream. This is especially important in cases where pollution from fertilizers and pesticides occur, because the sorption of these substances into streambed sediments may greatly influence aquatic organisms and environment. Hence, in order to achieve reliable prediction of pollutant transport the impact of storage zones and contaminant sorption into the streambed sediments must be considered. The fifth example presented to demonstrate the capability of TOASTS model to accurate calculation of geometric properties of irregular cross- sections; the results indicate higher accuracy of TOASTS model in simulation of solute transport in a river with irregular cross-sections and transient storage than two other models.

In the sixth example, the most complex possibility was considered. This example shows the TOASTS model application and its results compared to the results of two other models (OTIS and MIKE11) in simulating solute transport under unsteady flow in a river with irregular cross-sections. This time, the results show again the higher accuracy of the TOASTS model compared to other models. Overall, considering all the mentioned points and obtained results, it can be said that the TOASTS is a comprehensive and practical model, that has the combined 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, without restrictions on the number of sections, that from this aspect, is unique compared to the other models that have been presented so far. Thus, it could be suggested as an appropriate alternative to the current popular models in solute transport studies in natural river and streams.

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Table1. Qualified comparison of three model characteristics

Model	Model features				
	No limitations on the number of input parameters	Calculation of irregular cross-sections geometric properties	Unsteady flow sub-model	Transient storage	Kinetic sorption
TOASTS	+	+	+	+	+
OTIS	-	-	-	+	+
MIKE 11	+	+	+	-	-

(Note: The + sign means having a characteristic and symbol - means lack of it)

Table 2- comparison of numerical methods used in structures of three models.

Model	Numerical methods			
	Discretization scheme	Accuracy order	Stability	Numerical dispersion
TOASTS	Centered Time - QUICK Space (CTQS)	Second order in time Third order in space	$Pe < 8/3$	_
OTIS	Centered Time - Centered Space (CTCS)	Second order in time Second order in space	$Pe < 2$	_
MIKE 11	Backward Time – Centered Space (BTCS)	First order in time Second order in space	$Pe < 2$	$U^2 \Delta t/2$

$(Pe = u.\Delta x / D)$ *

Table 3. Error indexes of verification by analytical solution, for continuous boundary condition, in simulations with and without transient storage

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 indexes of verification by analytical solution for Heaviside boundary condition, in simulations with and without transient storage

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 indexes for TOASTS, OTIS and BTCS with TS model for verification with 2-D model

Index	Distance from upstream, 500 m		
	OTIS	BTCS with TS	TOASTS
R^2 (%)	99.36	99.37	99.43
RMSE (mg/m^3)	0.36	0.37	0.35
MAE(mg/m^3)	0.16	0.18	0.15
MRE (%)	8.6	12.15	6.09

Table 6. The examples used for demonstration of model application

Example	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	+	–	–	–	–	–
2	Regular	Steady uniform	+	+	–	–	+	–
3	Irregular	Steady non-uniform	+	+	+	–	–	–
4	Irregular	Steady non-uniform	+	+	+	–	–	+
5	Irregular	Steady uniform	+	+	+	-	–	–
6	Irregular	Unsteady non-uniform	+	+	–	+	–	–

(Note: + sign means that the process affects transport and – sign means no effect)

Table 7- simulation parameters and characteristics three cases of models implementation for example 2

	L (m)	Q (lit/s)	A(m^2)	D (m^2/s)	λ (s^{-1})	Case	Space step (m)	Flow velocity (m/s)	Peclet number
Parameter	2200	0.12	1	5	0.00002	1	10	0.12	0.24
						2	100	0.12	2.4
						3	100	0.5	10

Table 8- Error indexes for concentration- time profiles in 500 m from upstream (example 2)

	Index	Distance from upstream, 500 m		
		TOASTS	OTIS	MIKE11
Case 1	R^2 (%)	99.93	99.93	99.98
	RMSE	0.460	0.460	0.850
	MAE	0.236	0.238	0.480
	MRE (%)	0.9	1.0	1.7
Case 2	R^2 (%)	98.26	97.82	97.75
	RMSE	2.66	2.98	3.24
	MAE	1.42	1.55	1.73
	MRE (%)	3.77	4.11	4.93
Case 3	R^2 (%)	98.8	98.2	98.24
	RMSE	3.60	4.41	4.46
	MAE	0.80	1.12	1.17
	MRE (%)	1.25	1.95	2.15

Table 9- Error indexes for concentration space profile (example 2)

	Index	Model		
		TOASTS	OTIS	MIKE11
Case 1	R^2 (%)	99.9	99.9	99.9
	RMSE	0.146	0.154	0.360
	MAE	0.105	0.108	0.280
	MRE (%)	1.91	1.97	3.20
Case 2	R^2 (%)	98.6	98	96
	RMSE	0.53	0.65	0.86
	MAE	0.40	0.47	0.64
	MRE (%)	5.40	6.56	11.20

Case 3	R^2 (%)	95.7	92	88.4
	RMSE	5.46	7.24	7.88
	MAE	3.02	4.47	5.05
	MRE (%)	6.27	12.44	13.50

Table 10- Simulation parameters for Uvas Creek experiment

Reach (m)	Flow discharge (m^3/s)	Dispersion coefficient (m^2/s)	Cross- sectional areas		Exchange coefficient
			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 indexes of simulation of Uvas Creek experiment

Index	38 m			281 m			433 m		
	TOASTS	OTIS	MIKE11	TOASTS	OTIS	MIKE11	TOASTS	OTIS	MIKE11
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 of example 4

Distribution coefficient, K_d (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 indexes of example 4 for both main channel and sorbate concentration at some stations

Index	Main channel concentration									Sorbate concentration			
	38 m			281 m			433 m			105 m		281 m	
	TOASTS	OTIS	MIKE11	TOASTS	OTIS	MIKE11	TOASTS	OTIS	MIKE11	TOASTS	OTIS	TOASTS	OTIS
R^2 (%)	99.30	93.17	93.00	99.00	96.00	90.80	93.60	90.00	80.20	99.40	99.30	99.16	98.6
RMSE (mg/m^3)	0.05	0.12	0.17	0.055	0.070	0.200	0.060	0.067	0.260	1.05	1.64	2.67	2.86
MAE(mg/m^3)	0.021	0.044	0.086	0.048	0.055	0.115	0.05	0.06	0.15	0.75	1.50	2.40	2.41
MRE (%)	6.40	11.80	24.60	13.60	18.00	27.40	17.40	20.70	40.00	3.04	5.66	10.50	10.80

Table 14- error indexes of Athabasca River experiment

Index	Distance from upstream, 1850 m		
	TOASTS	OTIS	MIKE11
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 of Huey Creek

Reach (m)	Dispersion coefficient (m^2/s)	Storage zone cross-sectional area	Exchange coefficient
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 indexes

Index	213 m			457 m		
	TOASTS	OTIS	MIKE11	TOASTS	OTIS	MIKE11
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

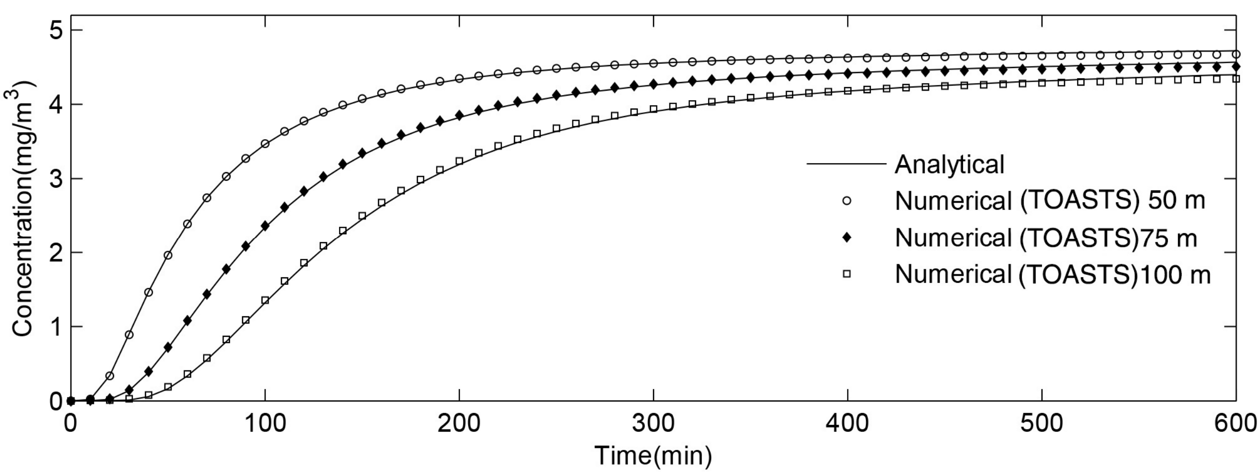


Figure 1. Results of TOASTS model verification by analytical solution for continuous boundary condition, at 50, 75 and 100 m from upstream.

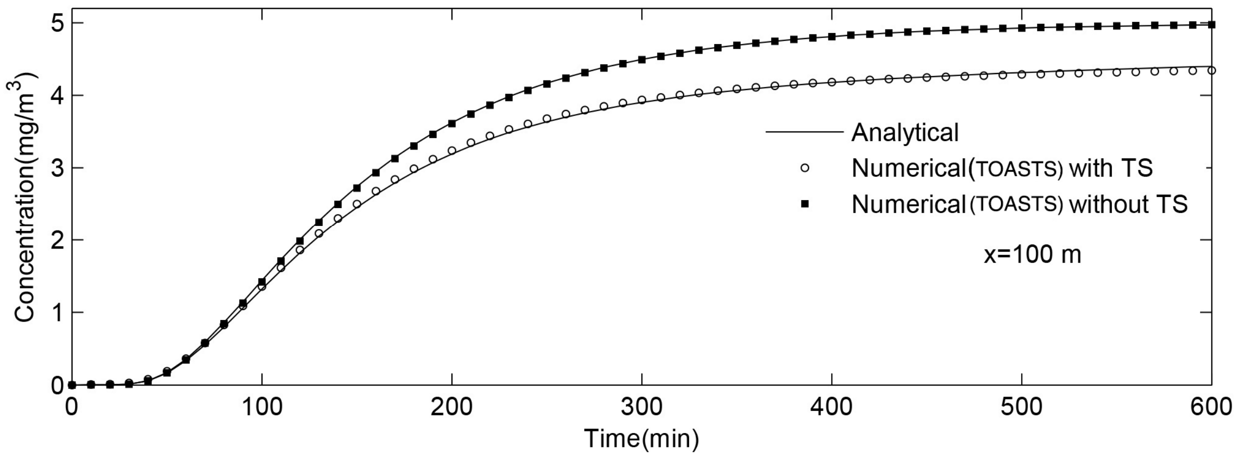


Figure 2. TOASTS model verification results with analytical solution for continuous boundary condition, for simulations with and without transient storage, at 100 m from upstream.

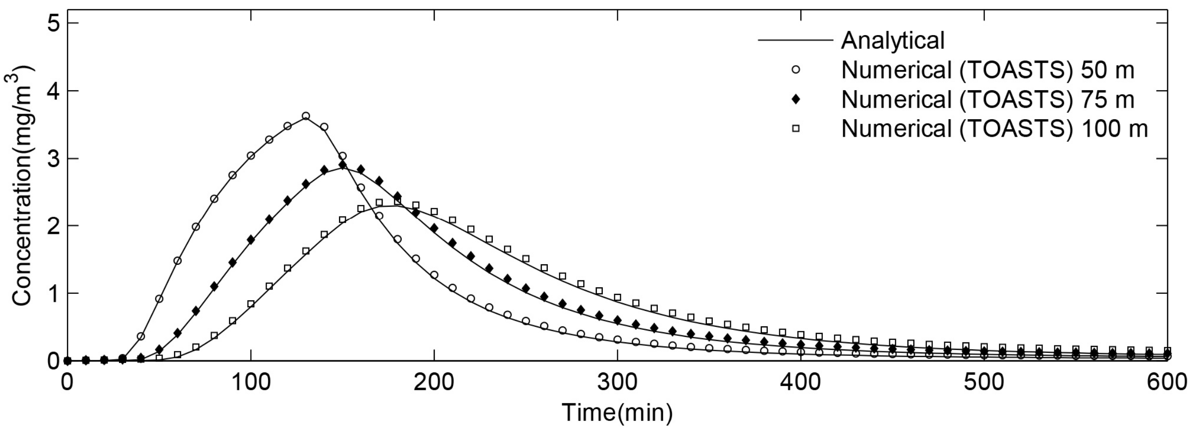


Figure 3. Results of TOASTS model verification with analytical solution for Heaviside boundary condition, at 50, 75 and 100 m from

upstrea

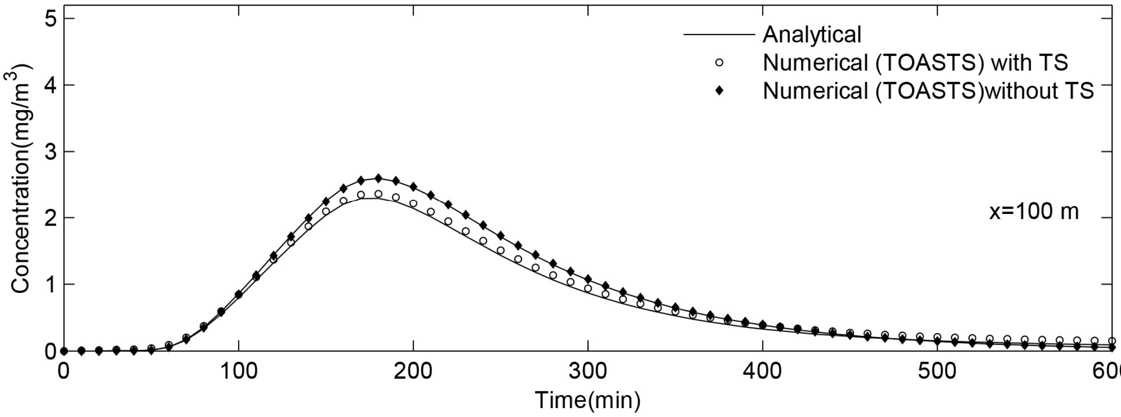


Figure 4. TOASTS model verification results with analytical solution for Heaviside boundary condition, for simulations with and without transient storage, at100 m from upstream.

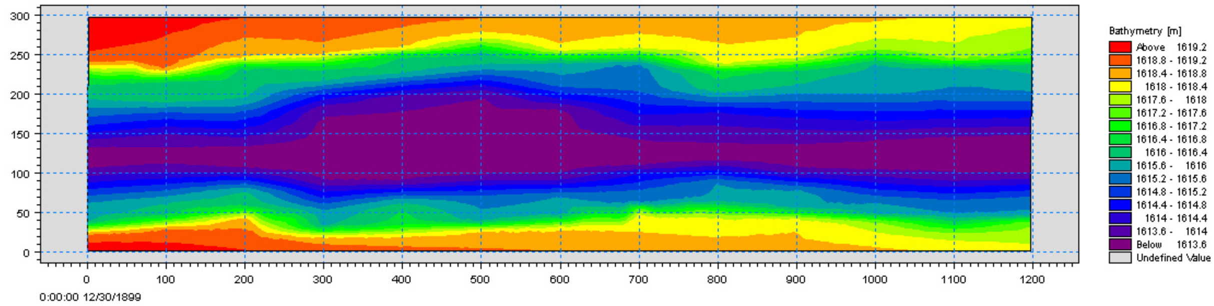
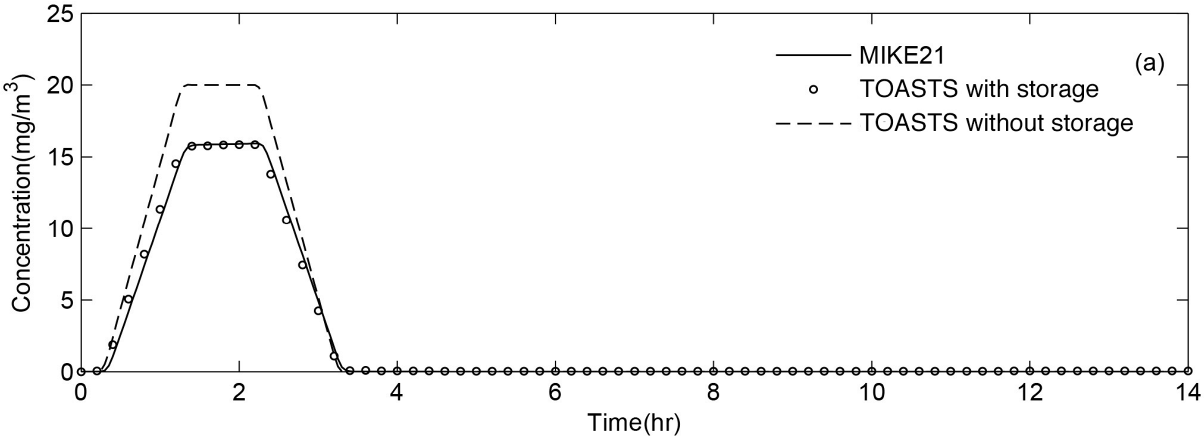


Figure 5. Bathymetry properties of the hypothetical river.



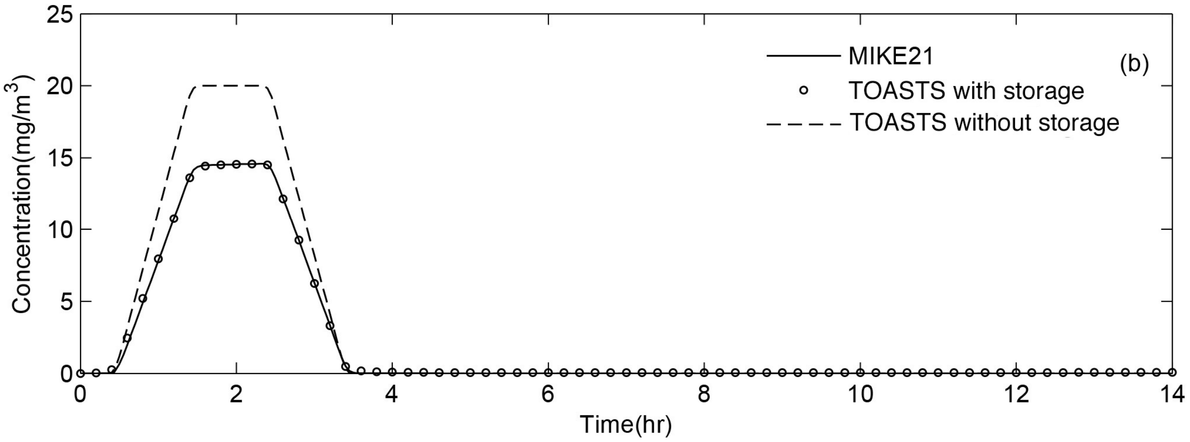


Figure 6. Simulation results of TOASTS model for simulation with and without storage in comparison with 2-D model results at (a) 500 m and (b) 800 m from channel upstream.

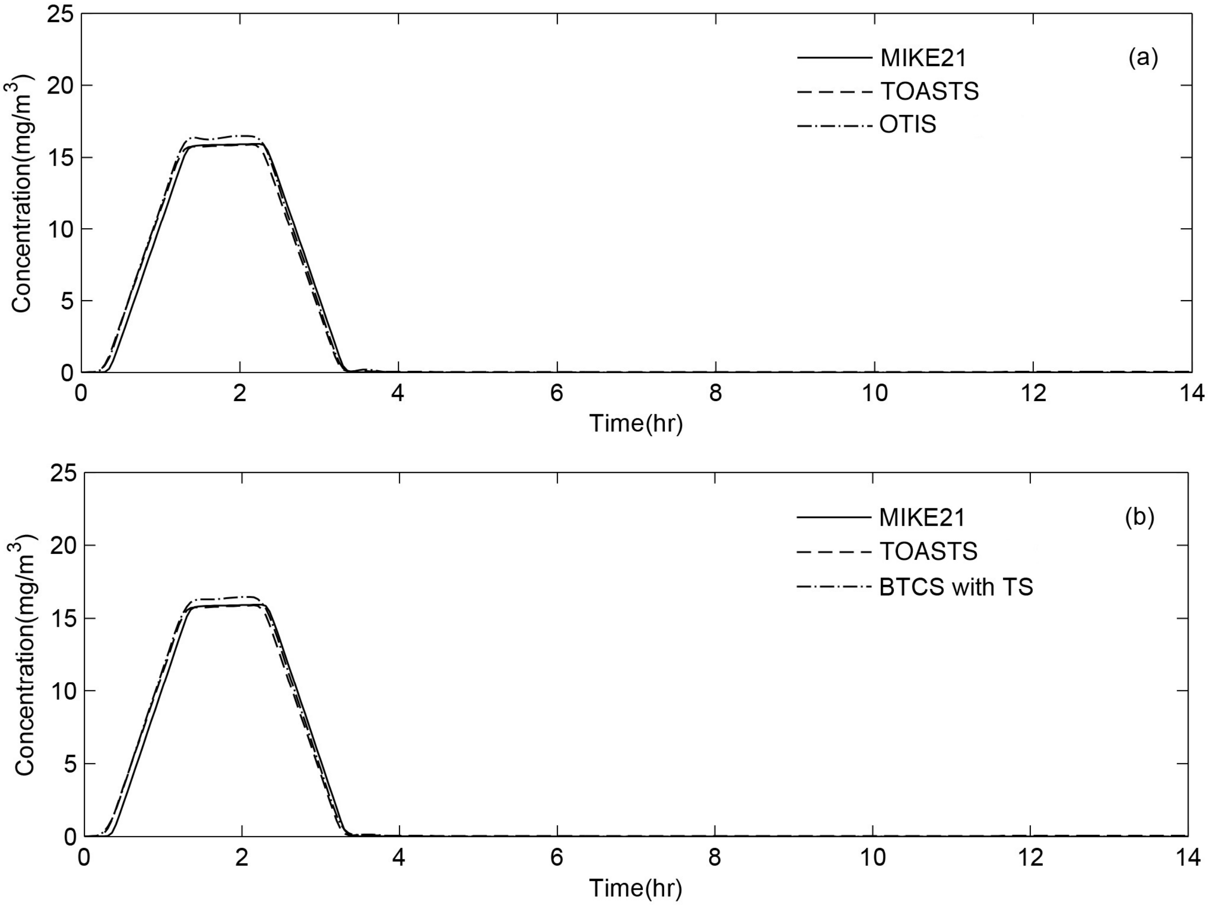


Figure 7. Comparison of results of (a) TOASTS and OTIS, (b) TOASTS and BTCS with TS models with 2-D model ones at 500 m from upstream.

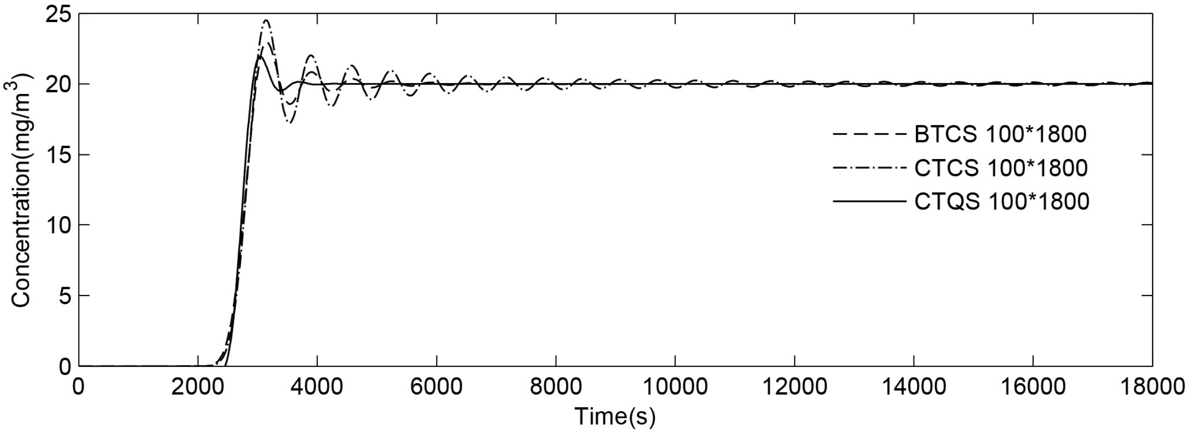


Figure 8. Comparison of CTQS, CTCS and BTCS scheme results for pure advection simulation at 100×1800 computation grid

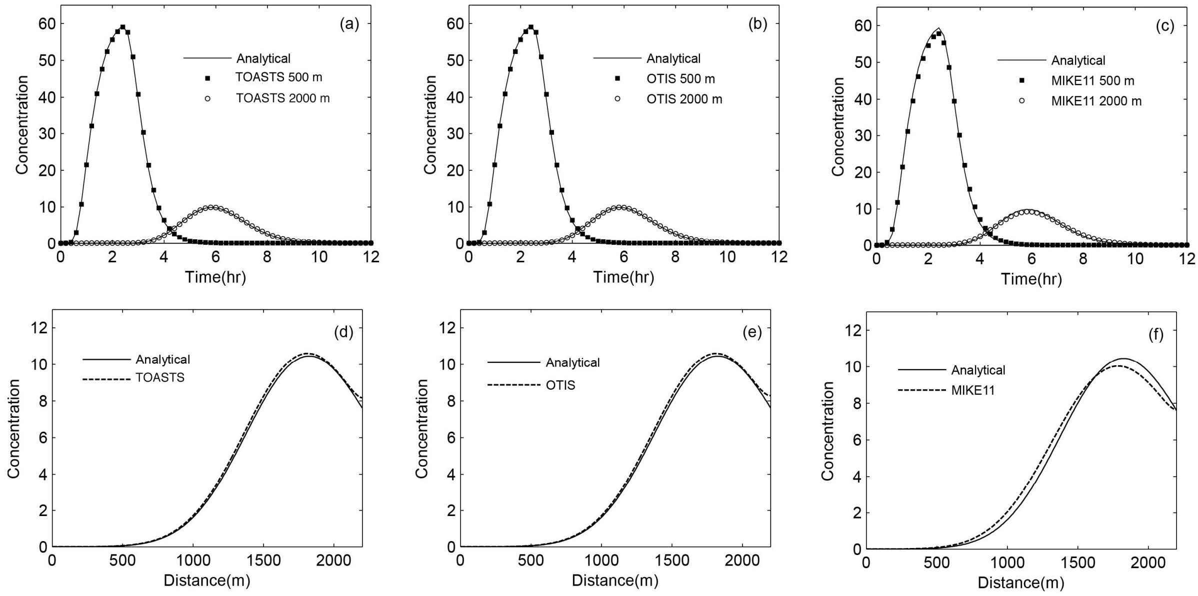


Figure 9. Comparison of various numerical schemes (TOASTS, OTIS and MIKE11) with analytical solution for the first case

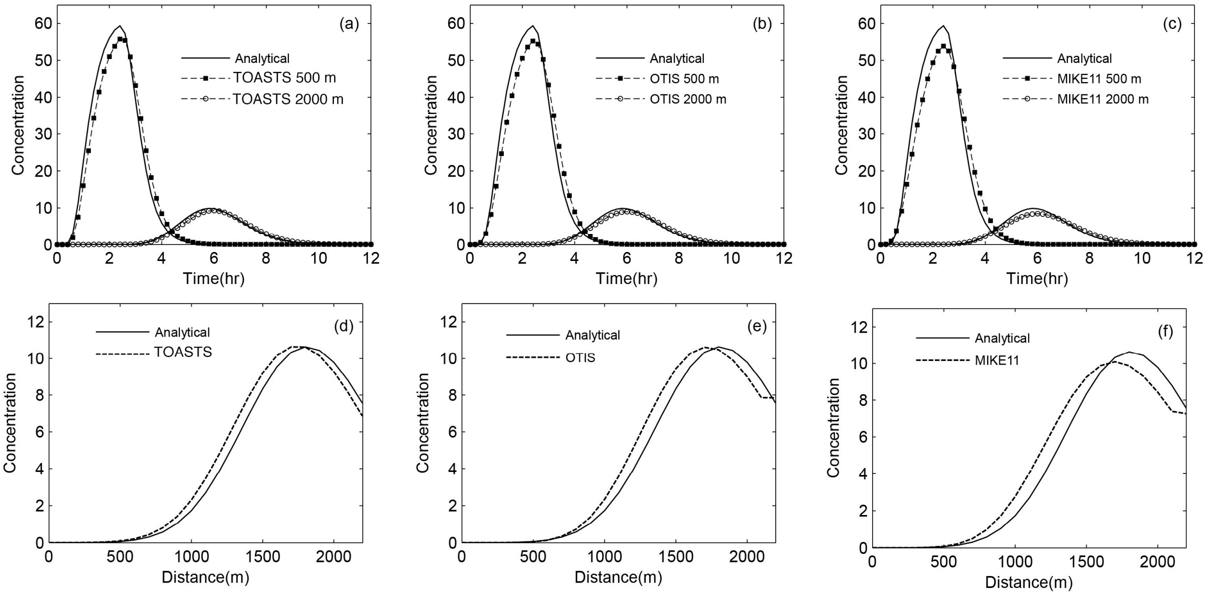


Figure 10. Comparison of various numerical schemes (TOAST, OTIS and MIKE11) with analytical solution for the second case

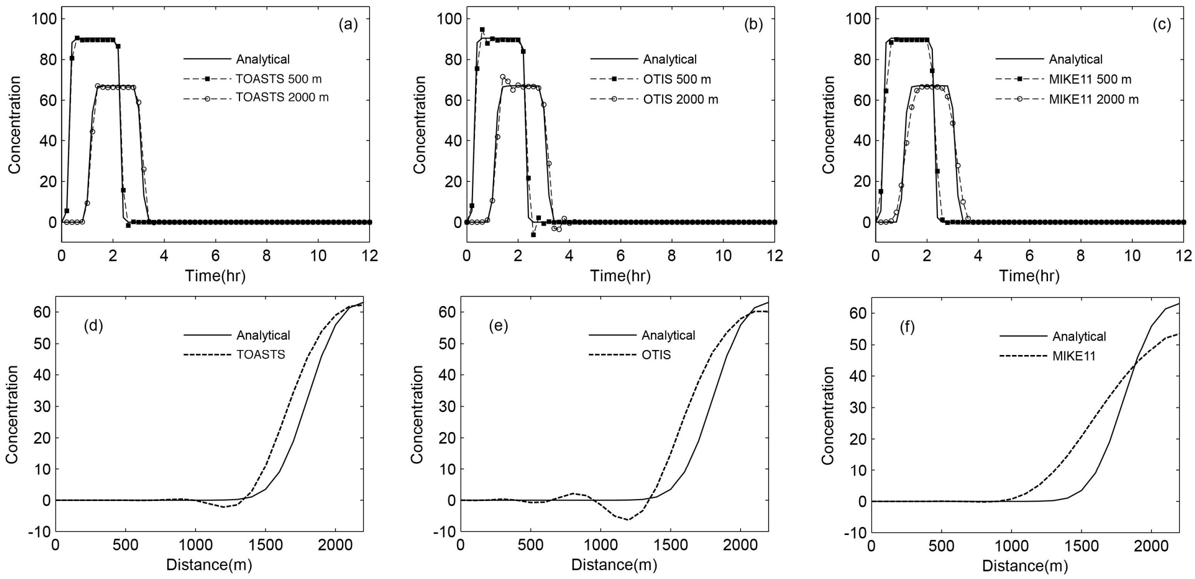


Figure 11. Comparison of various numerical schemes (TOASTS, OTIS and MIKE11) with analytical solution for the third case

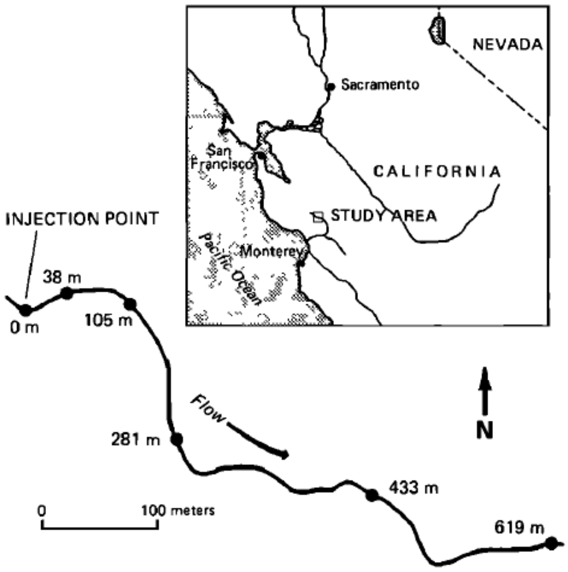
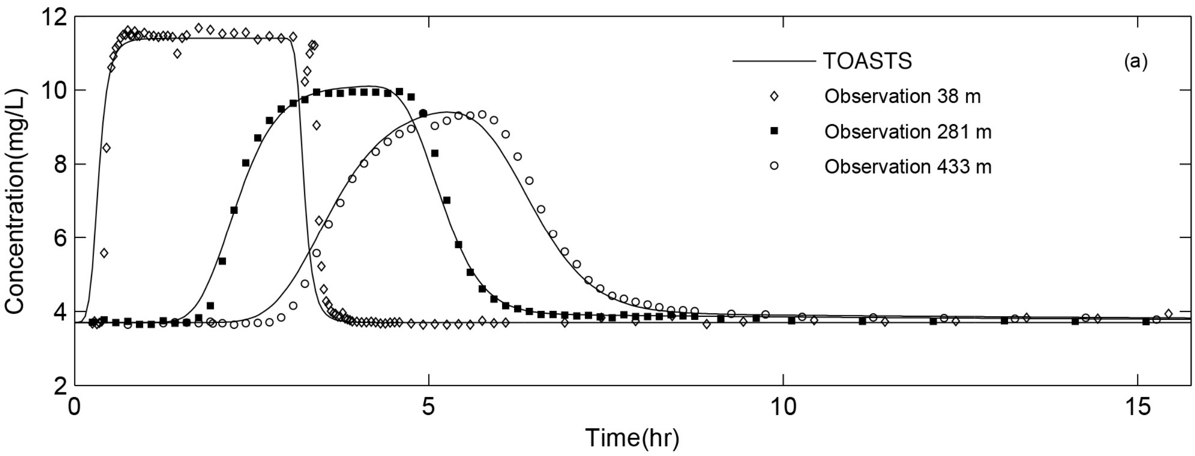


Figure 12-Experimental reach of Uvas Creek (Santa Clara County, California). The injection point and five monitoring locations are indicated (Bencala and Walters, 1983).



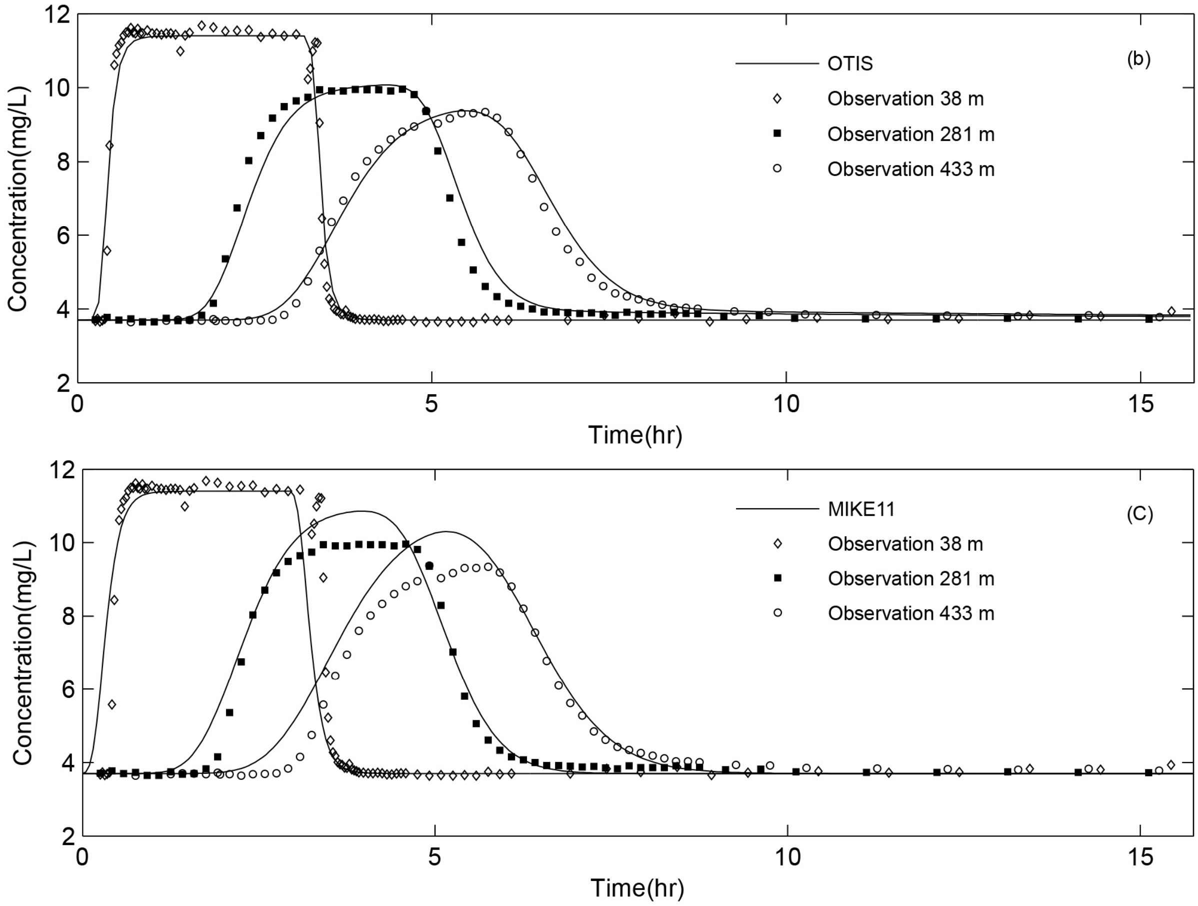


Figure 13. Observed and simulated chloride concentrations in main channel at 38, 281 and 433 m Uvas Creek by (a) TOASTS, (b) OTIS and (c) MIKE11 models.

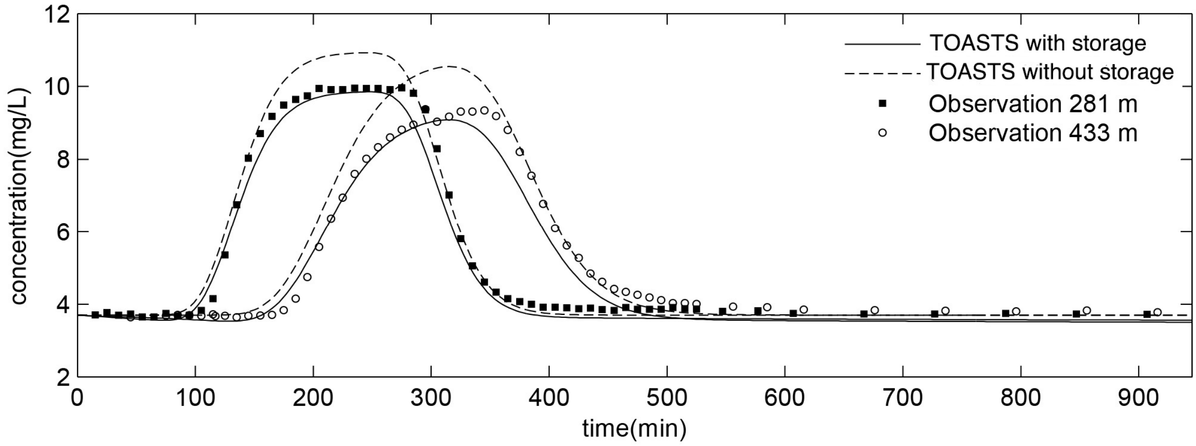


Figure 14. TOASTS model results for simulation with and without transient storage at 281 and 433 m stations.

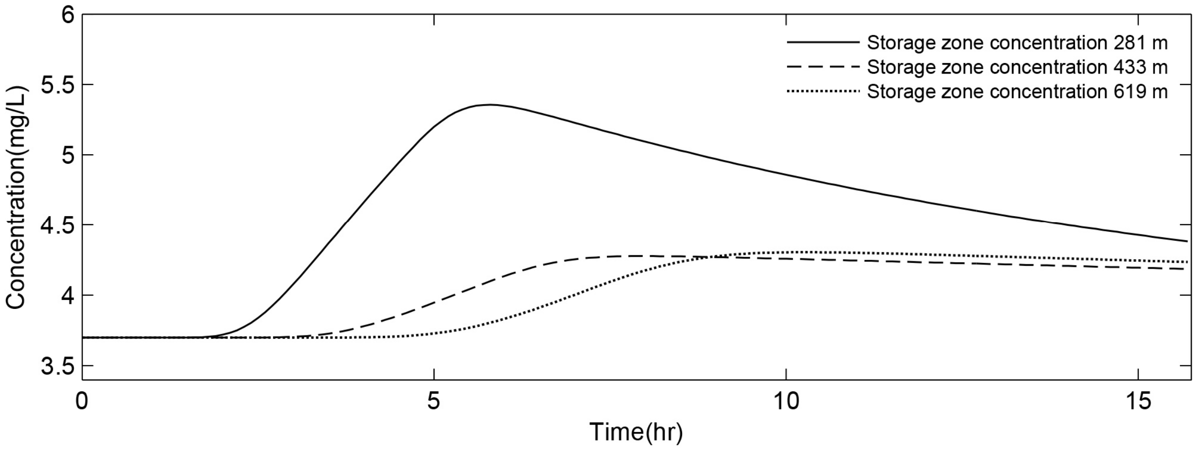


Figure 15. Observes and simulated storage zone concentrations at 281, 433 and 619 m stations.

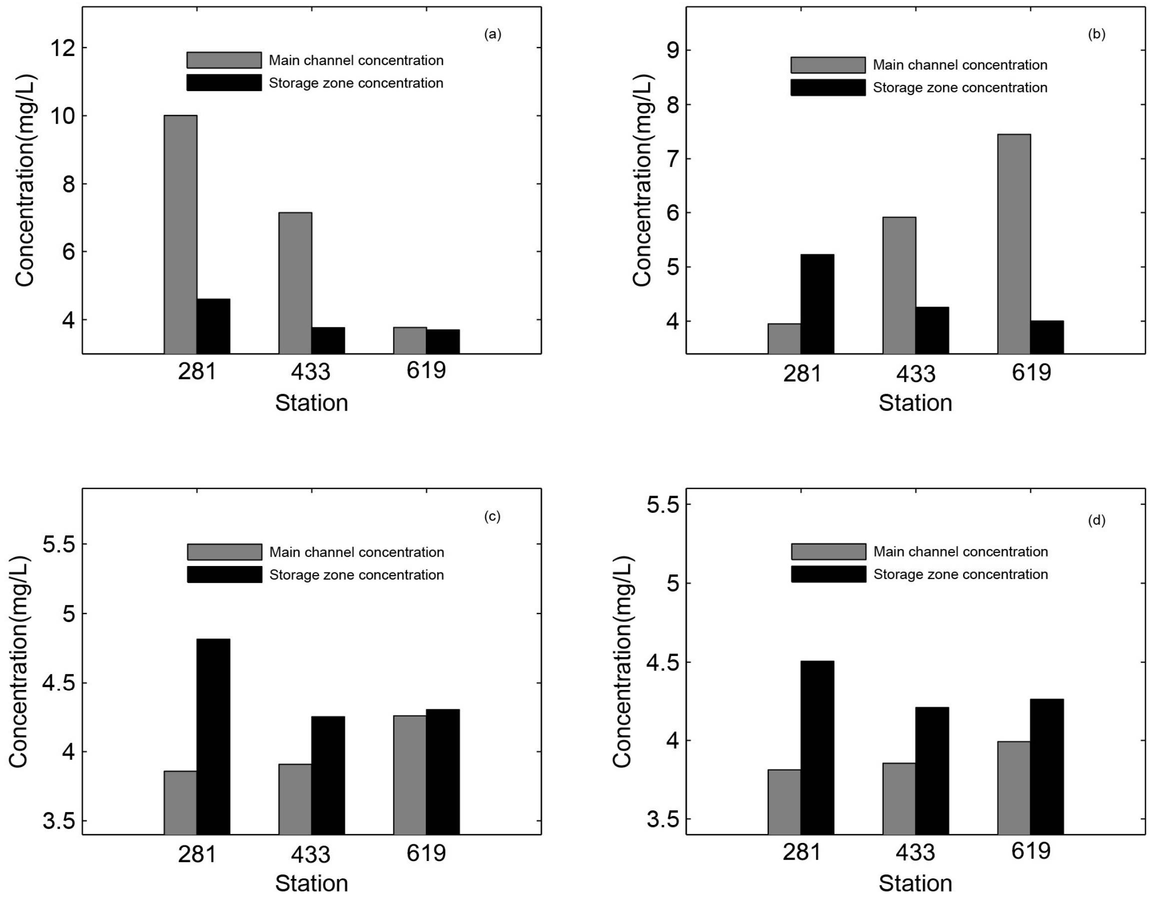


Figure 16. Comparison of main channel concentration (left column) and storage zone (right column) at 281, 433 and 619 m Uvas Creek in various times (a)4.5 (b) 7, (c)5 and (d) 15 hours after simulation start.

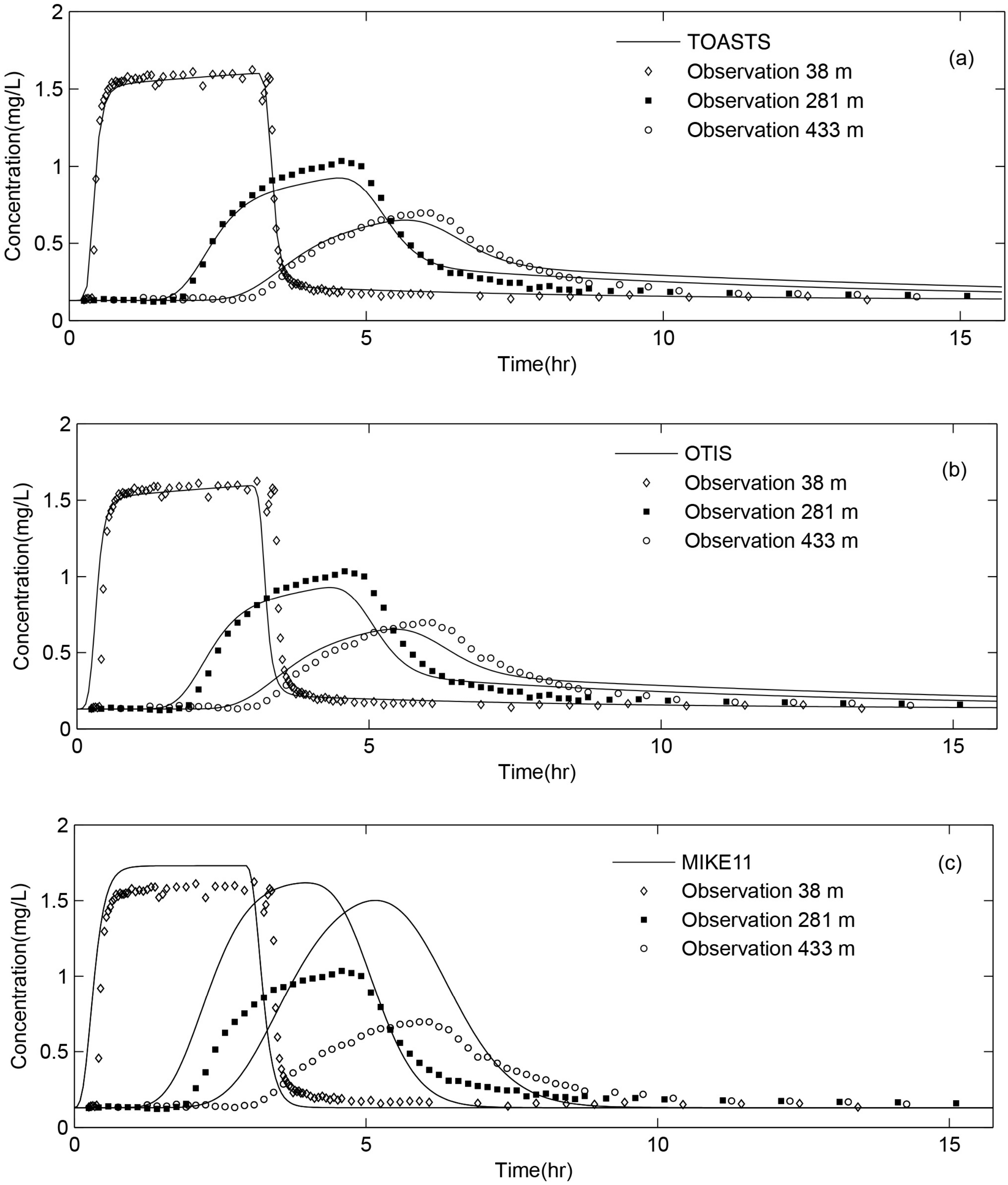


Figure 17. Observed and simulated Strontium concentrations in main channel affected by various physical and chemical processes at 38, 281 and 433m Uvas Creek by (a) TOASTS, (b) OTIS and (c) MIKE11 model.

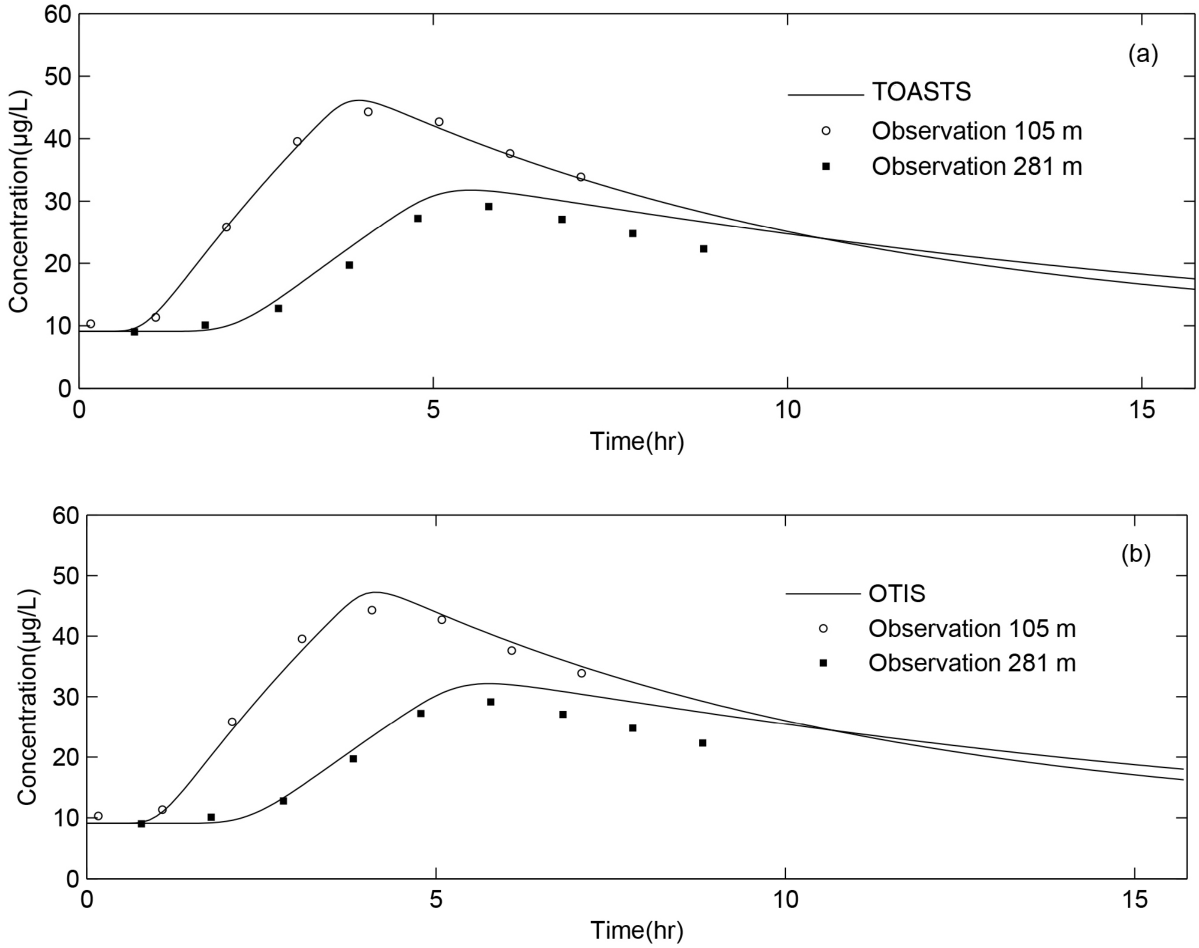


Figure 18. Sorbate and observed Strontium concentrations at 105 and 281 m stations of Uvas Creek by (a) TOASTS and (b) OTIS model

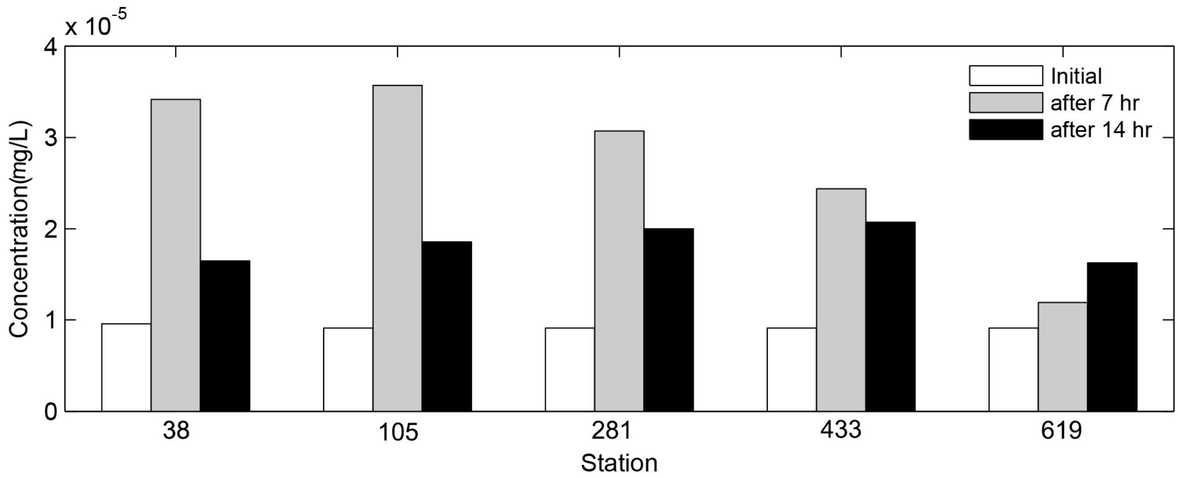


Figure 19. Sorbate concentrations of Strontium at various times at five observation stations of Uvas Creek.

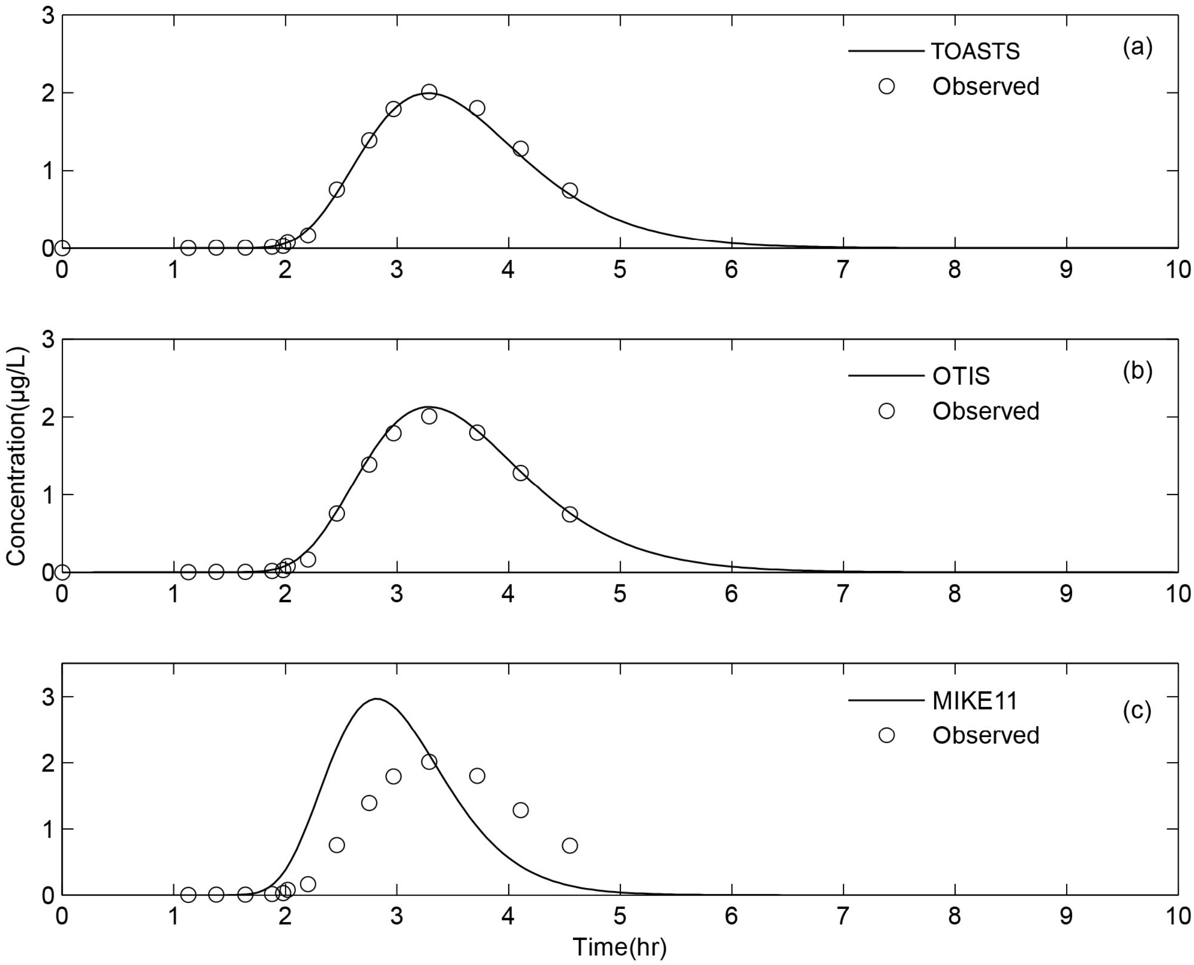


Figure 20. Simulation results for Athabasca River experiment at 11.85 km downstream from injection point by (a) TOASTS, (b) OTIS and (c) MIKE11 model.

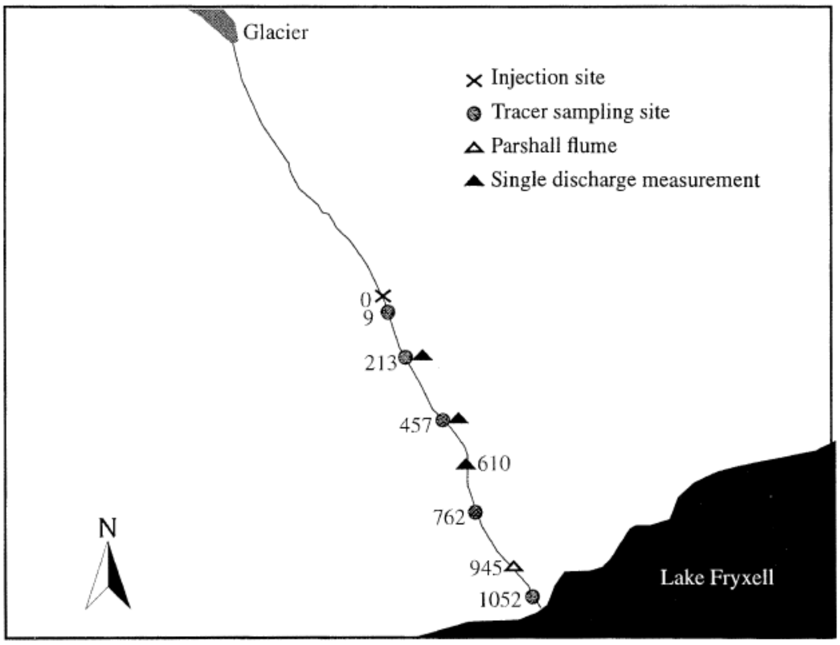
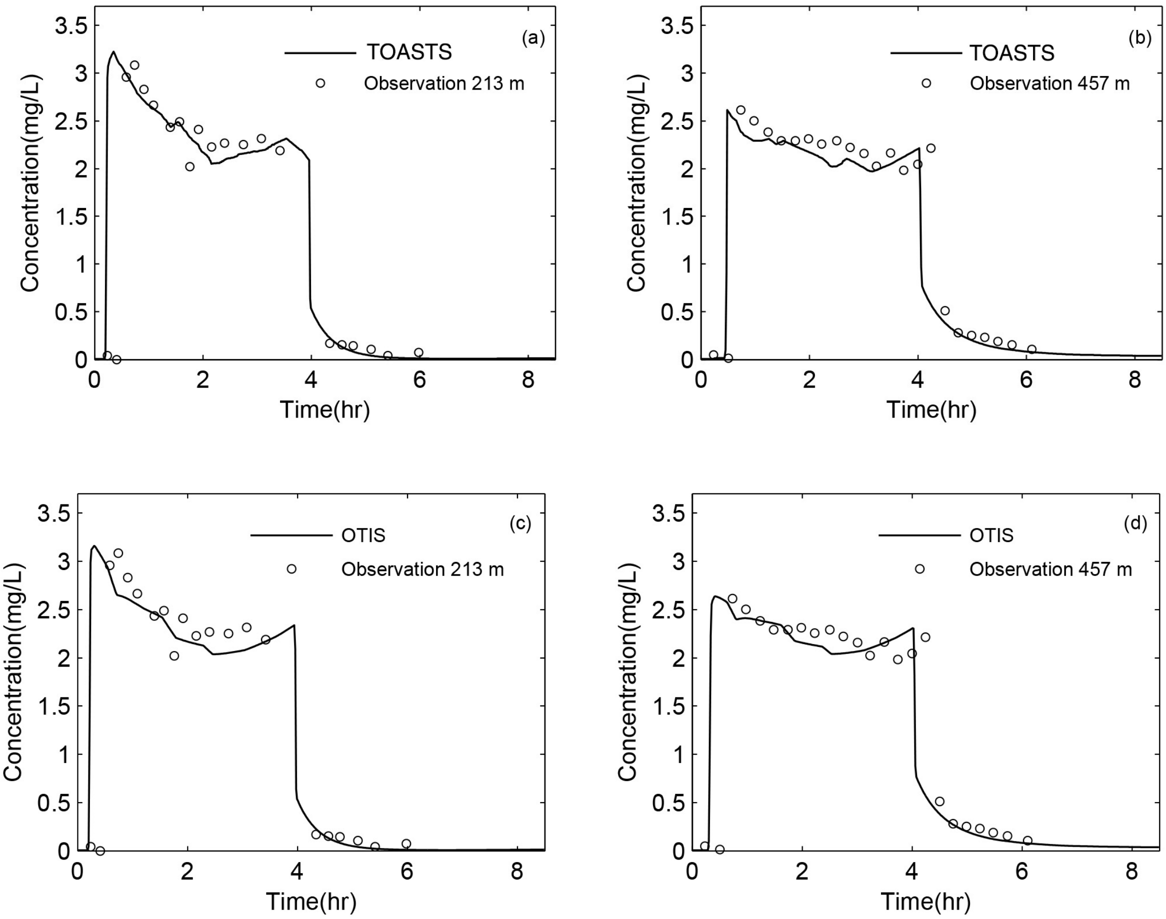


Figure 21 – Map of Huey creek, showing tracer sampling and stream-flow measurement stations. Site numbers refer to distance (m) from the tracer injection (Runkel et al. 1998).



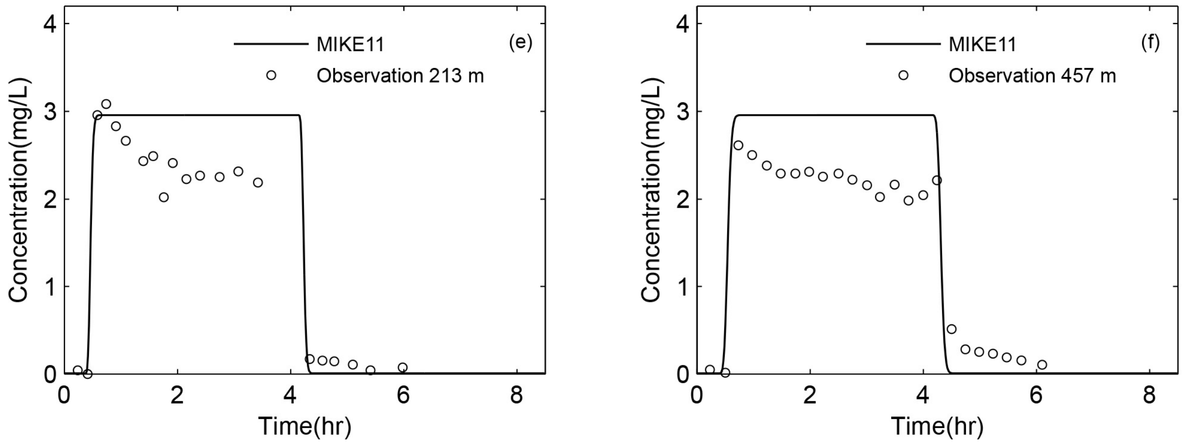


Figure 22. Observed and simulated main channel Li concentrations at 213 and 457 m stations of Huey Creek by (a), (b) TOASTS, (c), (d)OTIS and (f),(e) MIKE11 model.

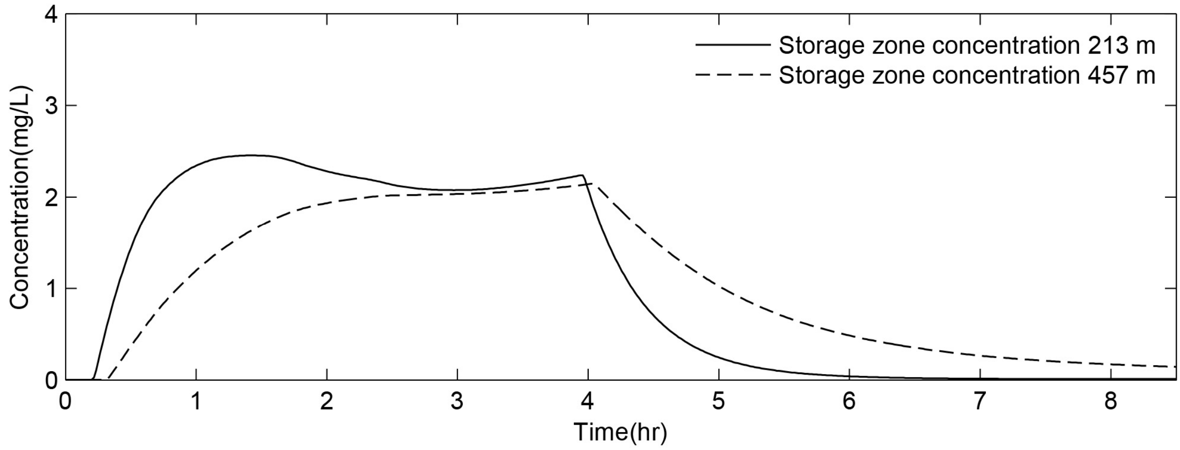


Figure 23. Storage zone concentration at 213 and 457 m station of Huey Creek