Introduction

Solute transport in streams and rivers is governed by a suite of hydrologic and geochemical processes. Knowledge of these processes is needed when assessing the fate of contaminants that are released into surface waters. The study of solute fate and transport often is aided by solute transport models that mathematically describe the underlying processes. This fact sheet describes a model that considers One-Dimensional Transport with Inflow and Storage (OTIS). As shown by several example applications, OTIS may be used in conjunction with field-scale data to quantify hydrologic processes (advection, dispersion, and transient storage) and certain chemical reactions (sorption and first-order decay).

Model Description

OTIS may be used to characterize the fate and transport of water-borne solutes in streams and rivers. Given a description of watershed loading, OTIS determines the solute concentrations that result from hydrologic transport and chemical transformation.

The primary assumption used within the model is that solute concentration varies only in the longitudinal direction; solute concentration does not vary with width or depth. Given this assumption, equations are developed for a one-dimensional system that consists of a series of stream segments. Conservation of mass for each stream segment yields a set of differential equations that are solved using numerical methods. Solution of the differential equations yields a general equation of the form:

$$C(x, t) = \begin{array}{c} \text{Hydrologic} \\ \text{Transport} \end{array} + \begin{array}{c} \text{Chemical} \\ \text{Transformation} \end{array}$$

where
x is the distance,
t is time, and
$C(x,t)$ is the solute concentration at distance x and time t.

This equation describes the spatial and temporal variation in solute concentration as a function of several hydrologic and geochemical parameters. As discussed by Runkel (1998), parameter estimates may be obtained by nonlinear regression using a modified version of OTIS known as OTIS-P.

Hydrologic Transport. Several hydrologic processes that govern the downstream transport of solutes are considered in the model. These processes include advection, dispersion, lateral inflow, and transient storage. Advection, the downstream transport of solute mass at a mean velocity, and dispersion, the spreading of solute mass due to shear stress and molecular diffusion, are considered in most mechanistic models of stream-water quality and solute transport. Consideration of these important mechanisms leads to the familiar advection-dispersion equation.

Within the OTIS model, additional terms are added to the advection-dispersion equation to account for the effects of transient storage and lateral inflow.

Transient storage has been noted in many streams where solutes may be temporarily detained in small eddies and stagnant pools of water that are stationary relative to the faster moving water near the center of the channel (fig. 1A). In addition, significant portions of flow may move through the coarse gravel of the streambed and porous areas within the streambank (fig. 1B). The traveltime for solutes carried through these porous areas may be substantially longer than that for solutes traveling within the water column. These pools of water and porous areas of the streambed are the two areas contributing to transient storage, as shown in figure 1.
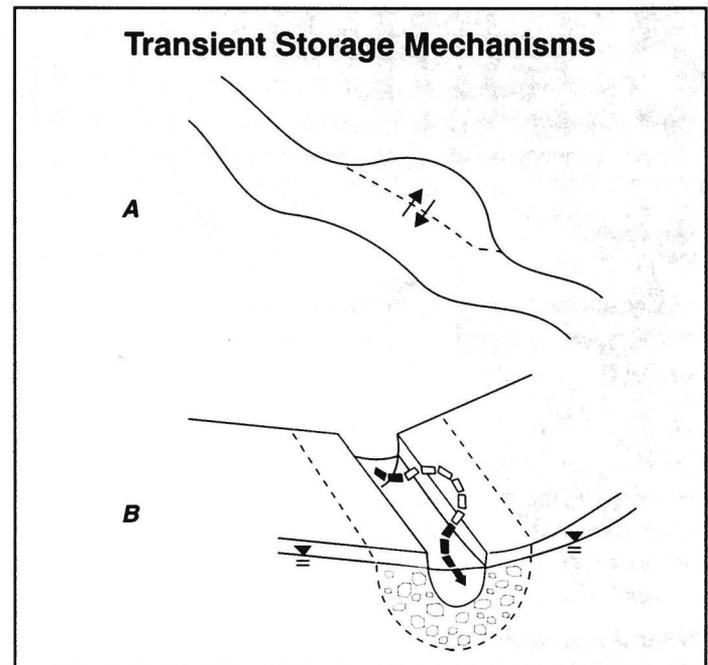

Figure 1. Transient-storage mechanisms. Transient storage occurs (*A*) when solutes enter small pockets of slow-moving water, and (*B*) when solutes leave the main channel and enter the porous media that make up the bed and banks of the channel. Arrows denote solute movement between the main channel and the transient-storage zone.

Lateral inflow is any water that is added to the stream due to ground-water inflow, overland flow, interflow, or small springs. These flows act to dilute (or concentrate) solutes in the stream channel if they carry solute concentrations that are lower (or higher) than the stream-solute concentration.

Two conceptual areas are defined within the model: the main channel and the storage zone (fig. 2). The main channel is defined as the portion of the stream in which advection and dispersion are the dominant hydrologic transport mechanisms. The

storage zone is defined as the portion of the stream that contributes to transient storage; that is, stagnant pools of water and porous areas of the streambed. Water in the storage zone is considered immobile relative to water in the stream channel. The exchange of solute mass between the main channel and the storage zone is modeled as a first-order mass transfer process.
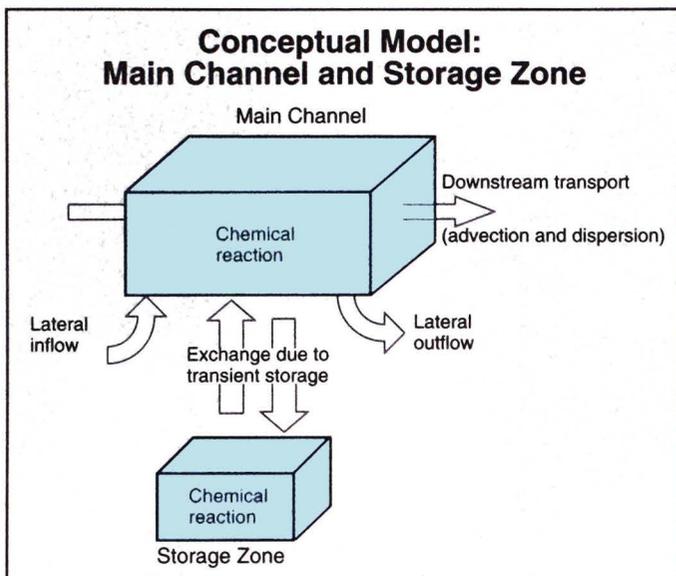

Figure 2. Conceptual model includes the main channel and the storage zone.

Consideration of the hydrologic processes discussed above introduces several model parameters. The main channel cross-sectional area (A) is used with estimates of streamflow to determine the average advective velocity of transported solutes. Spreading of solute mass due to shear stress is described by the dispersion coefficient (D). Solute mixing due to transient storage is governed by the storage-zone cross-sectional area (A_s) and the storage-zone exchange coefficient (α). Lateral inflows are characterized by the lateral inflow rate and the solute concentration associated with the lateral inflow (C_L).

Chemical Transformations. The hydrologic processes described above affect the transport of all water-borne solutes. Additional processes that act to add or remove solute mass are considered for reactive solutes that undergo chemical transformation. OTIS includes two types of chemical transformations: first-order decay and kinetic sorption. Under first-order decay, removal of solute mass is proportional to solute concentration. First-order decay coefficients may be specified for the main channel (λ) and (or) the storage zone (λ_s). Consideration of sorption within OTIS is based on a distribution coefficient approach that allows for sorption onto streambed sediments.

Model Applications

Mixing and Traveltime. Data from tracer-injection studies are frequently used to quantify mixing and traveltime in streams and rivers. These hydrologic characteristics are of importance to water-resource managers who are responsible for protecting

water supplies from contamination. Given data from tracer-injection studies, stream transport models may be used to estimate the timing, magnitude, and duration of a pollutant cloud that enters a stream due to an accidental spill.

In addition to providing management information, hydrologic parameters derived from tracer-injection data provide insight into the physical characteristics of streams. Values of the transient-storage parameters (A_s, α), for example, indicate the degree of mixing due to stagnant pools and flow through porous areas of the streambed. Further, model-derived estimates of traveltime indicate the relevant time scales over which chemical reactions can potentially affect solute concentrations.

In this section, we illustrate the use of OTIS to quantify hydrologic processes using tracer-injection data. Our first example uses data from Uvas Creek, a small pool-and-riffle stream in northern California. Bencala and Walters (1983) describe a continuous, constant-rate injection of chloride into Uvas Creek. Concentrations were monitored at several downstream locations, and streamflow was estimated by tracer dilution.

Application of OTIS to the Uvas Creek chloride injection requires estimates of stream cross-sectional area (A), transient storage (A_s, α), and dispersion (D). Estimates of stream cross-sectional area are related to traveltime as they control the timing of the chloride profile, whereas estimates of the transient-storage parameters represent instream mixing as reflected by the shape of the chloride profile. During a series of simulations, Bencala and Walters (1983) varied A, A_s, α, and D to obtain a match between observed and simulated concentrations. Final simulation results at two sampling locations are shown in figure 3.
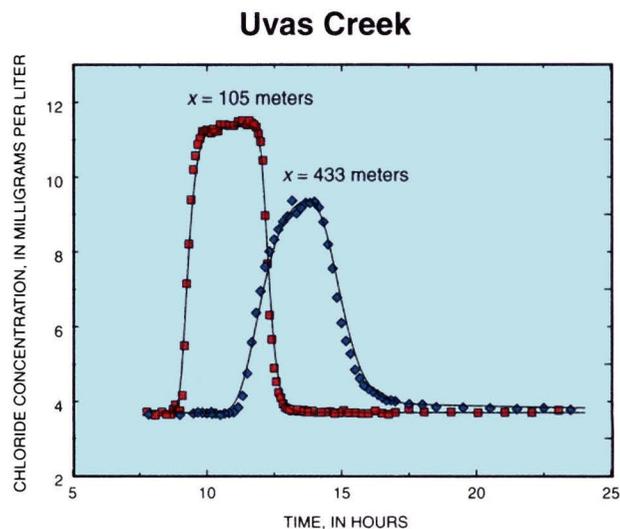

Figure 3. Simulated (solid lines) and observed (symbols) chloride concentrations in Uvas Creek, California.

Estimates of A and A_s developed from the tracer data are consistent with the pool-and-riffle characterization of Uvas Creek reported by Bencala and Walters. The pools act to produce transient storage by temporarily detaining some of the chloride. A dimensionless measure of this storage effect is obtained by calculating the ratio of storage-zone area to

main-channel cross-sectional area (A_s/A). Values of A_s/A for various reaches of Uvas Creek range from 1.0 to 3.0. These values indicate that the pool areas are large relative to the main channel.

Analysis of Uvas Creek data relied on a trial-and-error approach wherein parameter estimates were manually adjusted to produce an acceptable match between simulated and observed tracer concentrations. In the following example, parameter estimates are obtained by nonlinear regression using OTIS-P. Laenen and Risley (1997) describe several studies in Oregon streams where rhodamine WT was used to determine traveltime. In July 1992, a slug of rhodamine was added to the Clackamas River at river mile 13.3 (RM 13.3). Water samples were collected at river miles 11.0, 9.5, and 8.0. Because rhodamine was introduced as a slug (as opposed to a continuous injection), data at the first sampling location (RM 11.0) are used to define the upstream boundary condition (fig. 4). Given the boundary condition, the traveltimes (as given by A) and mixing characteristics (as given by A_s, α, and D) for the two reaches ending at river miles 9.5 and 8.0 may be determined.
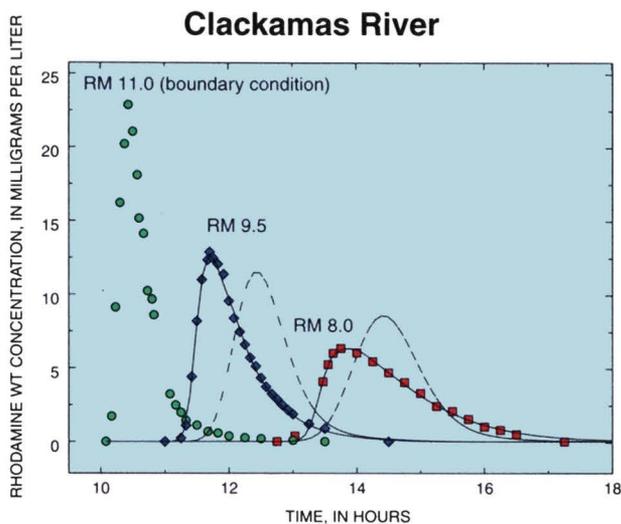

Clackamas River

Figure 4. Upstream boundary condition (RM 11.0), observed concentrations (symbols), simulated concentrations based on initial parameter estimates (dashed lines), and simulated concentrations based on final parameter estimates (solid lines) for the Clackamas River, Oregon.

Use of OTIS-P requires a set of initial estimates for the parameters of interest. Here we set A and D for both reaches equal to 50 square meters (m^2) and 10 m^2/s, respectively. The exchange coefficient, α, is initially set to 0.0 such that transient storage is not considered. Preliminary OTIS results based on these initial parameter estimates are shown as dashed lines in figure 4. These preliminary profiles indicate that our initial estimates of stream cross-sectional area are too large; the simulated traveltime is overestimated at both RM 9.5 and RM 8.0. In addition, the symmetric simulation profile at RM 8.0 is in contrast to the asymmetry of the observed data. This observation indicates that transient storage may be an important mixing mechanism. Both of these discrepancies may be addressed by developing

parameter estimates using OTIS-P. As expected, application of OTIS-P results in an improved simulation (solid lines, fig. 4) and a revised set of parameter estimates (A = 30.4, 48.1 m^2; A_s = 7.0, 14.4 m^2; D = 2.0, 0.4 m^2/s; α = 2.0×10^{-4}, 1.7×10^{-4}/s).

Nutrient Uptake. The examples above illustrate the use of OTIS to quantify hydrologic processes. In this example, we show how OTIS may be used to identify chemical reactions. McKnight and Duff (1995) describe an experimental addition of chloride, phosphate, and nitrate into Green Creek, a glacial meltwater stream in Antarctica. The objective of the study was to quantify stream hydrology and to study nutrient uptake by algal mats that cover the bed of Green Creek. As in the previous examples, a conservative tracer (chloride) is used to define the hydrologic system. Hydrologic parameters based on the analysis of chloride transport then are used to evaluate the conservative transport of nitrate and phosphate. A conservative simulation of nitrate is shown as a dashed line in figure 5. As shown in the figure, observed nitrate concentrations are significantly lower than simulated concentrations, based on conservative transport. This discrepancy indicates that nitrate concentrations are attenuated by geochemical processes.

Under the assumption that nutrient uptake is a first-order process, the first-order decay coefficients (λ, λ_s) in OTIS are used to quantify the loss of nitrate. Given the hydrologic characterization, OTIS-P is used to estimate uptake in the main channel (λ) and in the storage zone (λ_s). Reach-specific estimates of λ range from 4×10^{-5} to 4×10^{-4}; estimates of λ_s range from 3×10^{-6} to 2×10^{-3}. Simulation results based on these parameters are shown as a solid line in figure 5. Additional mass-balance calculations based on λ and λ_s indicate that 84 to 93 percent of the nitrate loss occurs in the main channel where algal uptake is the likely mechanism of nitrate loss. The remaining loss occurs in the storage zone where possible mechanisms include microbial uptake and nitrate reduction. In contrast, similar analyses indicate that phosphate loss occurs only in the main channel (λ_s = 0). OTIS thus provides a framework for determining the magnitude and location of processes controlling nutrient concentrations in Green Creek.
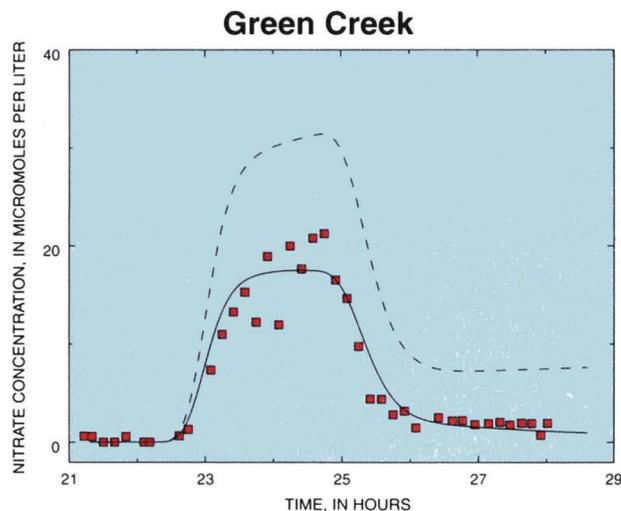

Green Creek

Figure 5. Observed (symbols) and simulated nitrate concentrations in Green Creek, Antarctica, 226 meters from the injection point. Simulation results are shown for conservative transport ($\lambda = \lambda_s = 0$; dashed line) and first-order loss (λ, $\lambda_s > 0$; solid line).

Trace Metal Removal. In addition to the time-variable simulations shown in the previous examples, OTIS may be used to determine the steady-state solute concentrations that result from a constant loading scenario. In this application, we consider the spatial concentration profile of dissolved iron in a small stream. The stream is St. Kevin Gulch, a headwater stream in the Rocky Mountains of Colorado. St. Kevin Gulch receives acidic, metal-rich waters from a series of springs that emanate from the toe of a large mine dump. Instream metal concentrations increase and pH levels decrease in the vicinity of the dump. During a synoptic study, water samples were collected at numerous instream locations and the metal-rich springs. Figure 6 depicts the observed profile of dissolved iron concentration. Two features of the spatial profile are of interest. First, there is a large increase in dissolved iron at 400 m; second, there is an abrupt decrease in dissolved iron concentration downstream from 500 m. The purpose of this application is to quantify the processes causing the changes in dissolved iron concentration.
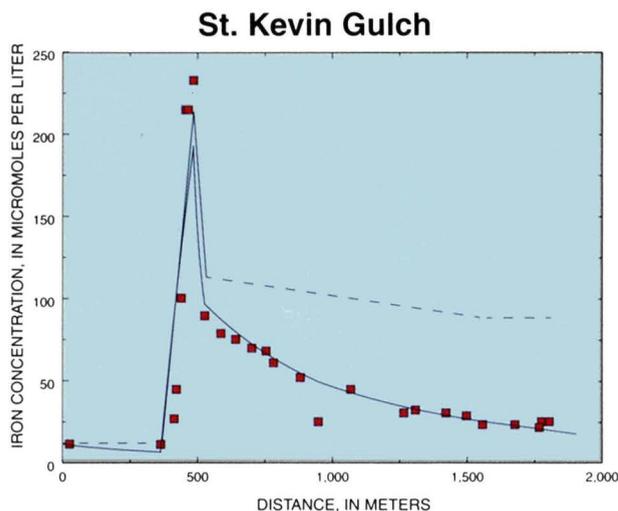
St. Kevin Gulch

Figure 6. Observed (symbols) and simulated iron concentrations in St. Kevin Gulch, Colorado. Simulation results are shown for conservative transport ($\lambda = \lambda_s = 0$; dashed line) and first-order loss ($\lambda = 1 \times 10^{-4}$; solid line).

The first step in the analysis is to define the hydrology of the system. Broshears and others (1993) describe the addition of a conservative tracer that coincided with the synoptic study. Data from the tracer addition are used to determine flow rates and the hydrologic parameters. Observed data from the springs are used to set the lateral inflow concentrations, C_L. OTIS then is used to develop a spatial profile under the assumption that dissolved iron is conservative (nonreactive). Results from this simulation are shown in figure 6 (dashed line). The close correspondence between observed and simulated iron concentrations in the upper portions of St. Kevin Gulch (0–500 m; fig. 6) indicates that the initial increase in iron is due to strictly hydrologic factors; that is, iron loading from the metal-rich springs. Simulated iron concentrations decrease downstream from 500 m due to the addition of water from a relatively dilute tributary but do not match the decrease in the observed data. This discrepancy indicates that chemical reactions affect dissolved iron concentrations downstream from 500 m.

A simple approach to quantifying the chemical reactions is to determine the first-order rate at which iron is lost from the system. This is accomplished by estimating a first-order decay coefficient for the main channel (λ). A first-order decay coefficient of 1×10^{-4}/s results in the simulated profile shown in figure 6 (solid line). Although the decay-rate approach yields an excellent fit to the data, it does not explicitly identify the mechanisms causing the iron loss. Inspection of the spatial pH profile indicates an increase in pH downstream from 500 m that could result in the precipitation of hydrous iron oxides. This observation is confirmed by additional calculations using a chemical equilibrium model.

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References

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Sources of Additional Information

The OTIS solute transport model is available on the World Wide Web (http://webserver.cr.usgs.gov/otis). Funding for OTIS development is provided by the USGS Toxic Substances Hydrology Program (http://toxics.usgs.gov/toxics). For additional information, contact:

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