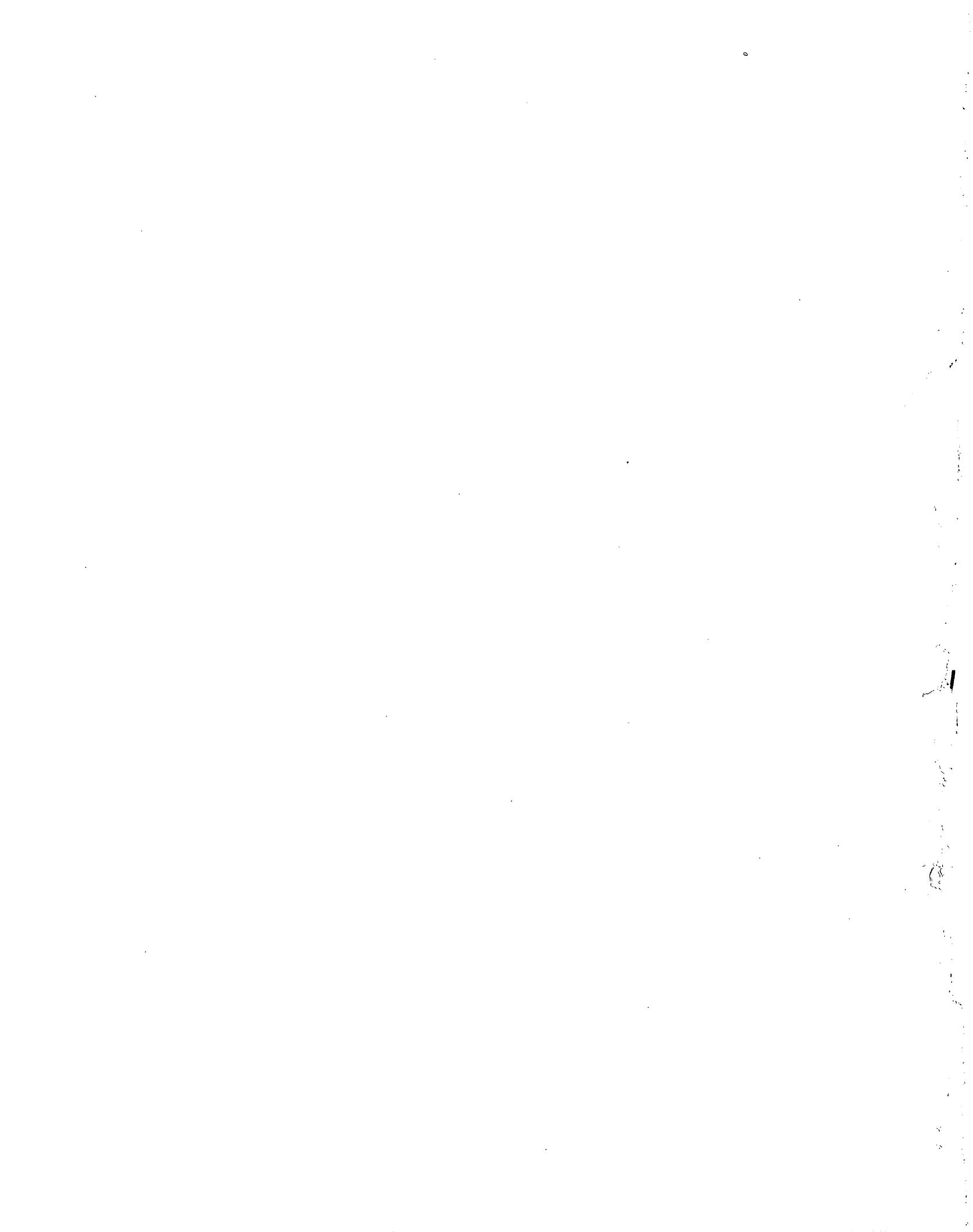CO-0036

ONE-DIMENSIONAL TRANSPORT WITH INFLOW AND STORAGE (OTIS): A SOLUTE TRANSPORT MODEL FOR STREAMS AND RIVERS

U.S. GEOLOGICAL SURVEY

Water-Resources Investigations Report 98–4018

USGS

science for a changing world

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By Robert L. Runkel

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Thomas J. Casadevall, Acting Director

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One-Dimensional Transport with Inflow and Storage (OTIS): A Solute Transport Model for Streams and Rivers

By Robert L. Runkel

Abstract

OTIS is a mathematical simulation model used to characterize the fate and transport of water-borne solutes in streams and rivers. The governing equation underlying the model is the advection-dispersion equation with additional terms to account for transient storage, lateral inflow, first-order decay, and sorption. This equation and the associated equations describing transient storage and sorption are solved using a Crank-Nicolson finite-difference solution.

OTIS may be used in conjunction with data from field-scale tracer experiments to quantify the hydrologic parameters affecting solute transport. This application typically involves a trial-and-error approach wherein parameter estimates are adjusted to obtain an acceptable match between simulated and observed tracer concentrations. Additional applications include analyses of nonconservative solutes that are subject to sorption processes or first-order decay. OTIS-P, a modified version of OTIS, couples the solution of the governing equation with a nonlinear regression package. OTIS-P determines an optimal set of parameter estimates that minimize the squared differences between the simulated and observed concentrations, thereby automating the parameter estimation process.

This report details the development and application of OTIS and OTIS-P. Sections of the report describe model theory, input/output specifications, sample applications, and installation instructions.

1.0 INTRODUCTION

This report describes the development and use of a solute transport model incorporating One-Dimensional Transport with Inflow and Storage (OTIS). The OTIS solute transport model was originally documented by Runkel and Broshears (1991); this document supersedes that earlier work. All of the relevant information contained in Runkel and Broshears (1991) has been updated and included in this report, with the exception of the appendices A-D that are now available at http://webserver.cr.usgs.gov/otis.

1.1 Model Enhancements

Several model features and options have been added to the OTIS solute transport model since the original release described by Runkel and Broshears (1991). A brief summary of these model enhancements is provided below:

- **Sorption Algorithms.** The original model was developed primarily for conservative solutes such as tracers that are not subject to chemical/biological transformation. Nonconservative behavior was modeled through the specification of a first-order decay or production rate. The model now includes a mechanism whereby sorption onto the streambed can be considered. Kinetic sorption algorithms based on the work of Bencala (1983) are described in Section 2.2.

- **Automated Parameter Estimation.** The OTIS model is typically used in conjunction with tracer-dilution data to estimate several parameters that characterize stream hydrodynamics. This parameter estimation process has traditionally been a trial-and-error procedure wherein model parameters are manually adjusted during a series of simulations to obtain an acceptable match between simulated and observed values. OTIS-P is a modified version of OTIS that allows for automated parameter estimation using nonlinear regression techniques (Section 2.7).

- **Steady State Output**. As described in Section 3.7.1, steady-state output is now provided for each segment in the modeled system.

- **Boundary Condition Options.** The model now provides three options for specification of the upstream boundary condition: (a) as a step input concentration, (b) as a step input flux, and (c) as a continuous input concentration. These options are described in Section 3.5.4.

- **Interpolation Option.** Users may request output at any location within the modeled system. In the original model, the concentration at each user-specified "print location" was determined by interpolation. The user now has the option of setting the concentration at a given print location equal to that of the nearest upstream segment (Section 3.5.4).

- **Input File Documentation.** Model users may now insert comments in the OTIS input files to document their work. Any input record with a '#' in column number 1 will be treated as a comment and disregarded by the input subroutines (Section 3.5.2).

- **Miscellaneous Input/Output Changes.** Two changes related to model input/output include a new input format for first-order decay rates (Section 3.5.4), and elimination of the multiple run option (Section 3.5.3).

1.2 Report Organization

The remaining sections of this report are as follows. Section 2.0 provides a description of the theoretical constructs underlying the solute transport model. This section includes descriptions of the simulated processes, the governing differential equations, and the numerical methods used within the model. Section 3.0, a User's Guide, presents the input and output requirements of the Fortran computer program. Model parameters, print options, and simulation control variables are detailed in this section. Section 4.0 presents several applications of the model and includes sample input and output files. The final section, a Software Guide (Section 5.0) describes how to obtain the model, installation procedures, and several programming features.

1.3 Acknowledgments

Many of the concepts and techniques underlying the OTIS solute transport model are based on the pioneering work of Ken Bencala of the U.S. Geological Survey (USGS). The author also acknowledges the guidance and vision of Bob Broshears and Briant Kimball (USGS) and Diane McKnight (University of Colorado, Boulder). Discussions with Jud Harvey and Brian Wagner (USGS), Alan Jackman (University of California, Davis), and Janet Rogers (National Institute of Standards and Technology, U.S. Department of Commerce) led to the development of OTIS-P. Assistance with software development and distribution was provided by Zac Vohs (USGS).

2.0 THEORY

2.1 Background - Transient Storage Models

The model described herein is based on a transient storage model presented by Bencala and Walters (1983). Transient storage refers to the temporary detainment of solutes in small eddies and stagnant pockets of water that are stationary relative to the faster moving waters near the center of the channel (fig. 1a). In addition, significant portions of the flow may move through the coarse gravel of the streambed and the porous areas within the streambank (fig. 1b). The travel time for solutes carried through these porous areas may be significantly longer than that for solutes traveling within the water column. These pockets of water and porous areas of the streambed are the two areas contributing to transient storage, as shown in figure 1.

Transient Storage Mechanisms
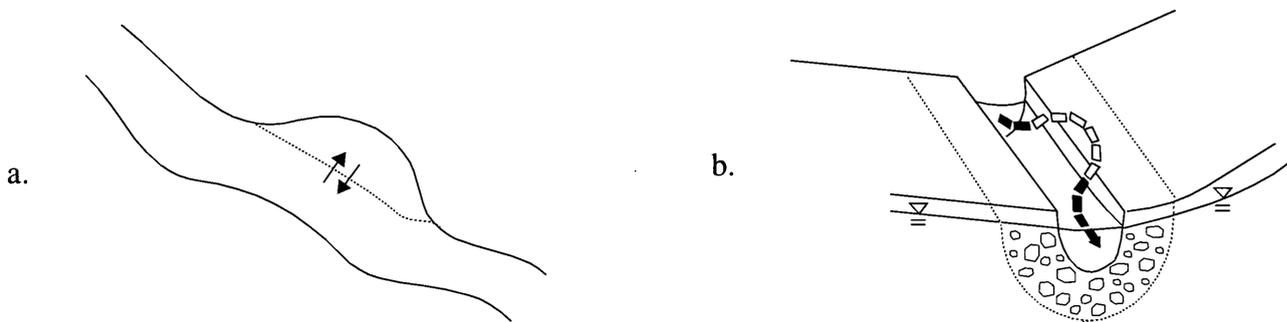
Figure 1. Transient storage mechanisms. Transient storage occurs (a) when solutes enter small pockets of slow-moving water and (b) when solutes leave the main channel and enter the porous media that makes up the bed and banks of the channel. Arrows denote solute movement between the main channel and the transient storage zone (adapted from Runkel and Bencala, 1995).

The model is formed by writing mass balance equations for two conceptual areas: the main channel and the storage zone. The main channel is defined as that portion of the stream in which advection and dispersion are the dominant transport mechanisms. The storage zone is defined as the portion of the stream that contributes to transient storage (pockets of stagnant water and porous areas of the streambed, fig. 1).

Figure 2 depicts the processes that affect solute concentrations in the main channel and the storage zone. Within the main channel, solutes are transported downstream by advection and dispersion. Advection and dispersion are not included in the storage zone, where downstream transport is negligible. Lateral inflow represents additional water entering the main channel as overland flow, interflow, and ground-water discharge. Lateral outflow represents water discharging from the main channel to the surrounding watershed. The main channel and storage zone are linked through the process of transient storage; the exchange of solute mass between the main channel and the storage zone attributable to

transient storage is modeled as a first-order mass transfer process. Chemical reactions occur within the main channel and the storage zone.

Conceptual Model: Main Channel and Storage Zone
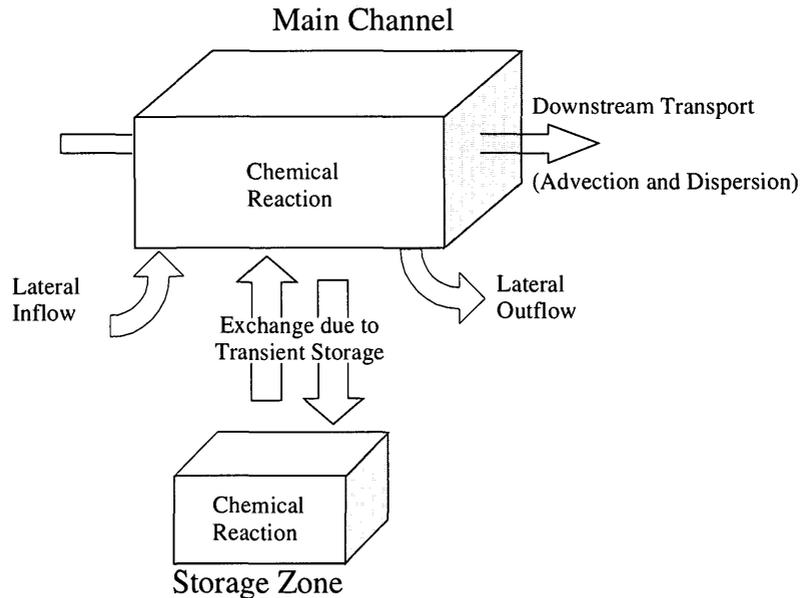
Main Channel

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

Additional descriptions of transient storage are provided by Thackston and Krenkel (1967), Thackston and Schnelle (1970), Valentine and Wood (1977), Nordin and Troutman (1980), Jackman and others (1984), Rutherford (1994), and Harvey and others (1996). A mathematical representation of the transient storage model is presented in the following section.

2.2 Governing Differential Equations

2.2.1 Processes Considered / Model Assumptions

The equations underlying the OTIS solute transport model are presented in the sections that follow. These equations were originally presented by Bencala (1983), Bencala and Walters (1983), and Runkel and Broshears (1991). A detailed derivation is presented in Appendix A of Runkel and Broshears (1991). The primary assumption used within the derivation is that solute concentration varies only in the longitudinal direction (that is, concentration does not vary with depth or width). Given this assumption, equations are developed for a one-dimensional system that consists of a series of stream segments (control volumes). Each segment includes the main channel and the storage zone, two conceptual areas in which mass is conserved. Additional model assumptions are summarized below.

Main Channel - Model Assumptions

- The physical processes affecting solute concentrations include advection, dispersion, lateral inflow, lateral outflow, and transient storage.
- The chemical reactions affecting solute concentrations include sorption to the streambed and first-order decay.
- All model parameters describing physical processes and chemical reactions may be spatially variable.
- Model parameters describing advection and lateral inflow may be temporally variable. These parameters include the volumetric flow rate, main channel cross-sectional area, lateral inflow rate, and the solute concentration associated with lateral inflow. All other model parameters are temporally constant.

Storage Zone - Model Assumptions

- Advection, dispersion, lateral inflow, and lateral outflow do not occur in the storage zone. Transient storage is the only physical process affecting solute concentrations.
- The chemical reactions affecting solute concentrations include sorption and first-order decay.
- All model parameters describing transient storage and chemical reactions may be spatially variable.
- All model parameters describing transient storage and chemical reactions are temporally constant.

2.2.2 Time-Variable Equations

Consideration of the physical processes described in Section 2.2.1 gives rise to a coupled set of differential equations for the main channel and storage-zone (Runkel and Broshears, 1991):

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

$$\frac{dC_s}{dt} = \alpha\frac{A}{A_S}(C - C_S) \tag{2}$$

where[1]

A	- main channel cross-sectional area [L^2]
A_S	- storage zone cross-sectional area [L^2]
C	- main channel solute concentration [M/L^3]
C_L	- lateral inflow solute concentration [M/L^3]
C_S	- storage zone solute concentration [M/L^3]
D	- dispersion coefficient [L^2/T]
Q	- volumetric flow rate [L^3/T]
q_{LIN}	- lateral inflow rate [L^3/T–L]
t	- time [T]
x	- distance [L]
α	- storage zone exchange coefficient [/T]

[1]The fundamental units of Mass [M], Length [L], and Time [T] are used throughout this section. Specific units are introduced in Section 3.0.

These equations describe the physical processes affecting solutes in the aquatic system and are therefore applicable to conservative (non-reactive) solutes such as tracers. Nonconservative (reactive) solutes may be considered by adding terms to equations (1) and (2). Here we consider two types of chemical reactions: kinetic sorption and first-order decay. Sorption may take place directly on the streambed or within the storage zone. Addition of terms representing sorption and decay yields:

$$\frac{\partial C}{\partial t} = \mathcal{L}(C) + \rho\hat{\lambda}(C_{sed} - K_d C) - \lambda C \tag{3}$$

$$\frac{dC_s}{dt} = S(C_s) + \hat{\lambda}_S(\hat{C}_S - C_S) - \lambda_S C_S \tag{4}$$

where

$\hat{C}_S$ - background storage zone solute concentration [M/L^3]

C_{sed} - sorbate concentration on the streambed sediment [M/M]

K_d - distribution coefficient [L^3/M]

λ - main channel first-order decay coefficient [/T]

λ_S - storage zone first-order decay coefficient [/T]

$\hat{\lambda}$ - main channel sorption rate coefficient [/T]

$\hat{\lambda}_S$ - storage zone sorption rate coefficient [/T]

ρ - mass of accessible sediment/volume water [M/L^3]

and $\mathcal{L}(C)$ and $S(C_S)$ represent the physical processes in the main channel and storage zone, respectively [the right-hand sides of equations (1) and (2)]. The sorption parameters introduced here ($\hat{C}_S$, K_d, $\hat{\lambda}$, $\hat{\lambda}_S$ and ρ) are discussed in detail by Bencala (1983). Equation (3) introduces, C_{sed}, a third concentration variable for which a mass balance is required. The streambed sediment concentration (sorbate concentration on the streambed sediment) is governed by:

$$\frac{dC_{sed}}{dt} = \hat{\lambda}(K_d C - C_{sed}) \tag{5}$$

To solve equations (3)-(5) for the general case where the parameters vary in time and space, numerical solution techniques must be employed. Numerical techniques for the solution of the time-variable equations are the topic of Section 2.4.

2.2.3 Steady-State Equations

The governing differential equations and the corresponding numerical solution techniques can be simplified if a steady-state solution is desired. Steady-state conditions arise when model parameters, flow variables, and boundary conditions (Section 2.6) are held constant for an indefinite period of time. Under these conditions, the system reaches an equilibrium state in which concentrations do not change with time.

Setting the change-in-concentration terms ($\partial C/\partial t$, dC_S/dt, and dC_{sed}/dt) to zero, equations (3)-(5) become:

$$0 = \mathcal{L}(C) + \rho\hat{\lambda}(C_{sed} - K_d C) - \lambda C \tag{6}$$

$$0 = S(C_s) + \hat{\lambda}_S(\hat{C}_S - C_S) - \lambda_S C_S \tag{7}$$

$$0 = \hat{\lambda}(K_d C - C_{sed}) \tag{8}$$

Equations (7) and (8) are now solved for the storage zone and streambed sediment concentrations, yielding:

$$C_S = \frac{\alpha A C + \hat{\lambda}_S A_S \hat{C}_S}{\alpha A + \lambda_S A_S + \hat{\lambda}_S A_S} \tag{9}$$

$$C_{sed} = K_d C \tag{10}$$

The governing steady-state equation for the main channel [equation (6)] is solved numerically, as discussed in Section 2.5.

2.3   The Conceptual System

To implement a numerical solution scheme, we first define the physical system. Figure 3 depicts an idealized system in which the stream is subdivided into a number of discrete segments. Each of these segments represents a control volume within which mass is conserved. Equations (3)-(5) therefore apply to each segment in the modeled system.

Figure 4 depicts three arbitrary segments from the conceptual system shown in figure 3. Under this segmentation scheme, the subscripts i, i-1, and i+1 denote concentrations and parameters at the center of each segment, while the subscripts (i-1,i) and (i,i+1) define values at the segment interfaces. The length of each segment, Δx, is also introduced in the figure. These definitions are used in Section 2.4.

2.4   Numerical Solution - Time-Variable Equations

2.4.1   Finite Differences

Due to the presence of temporal and spatial derivatives, equation (3) is a partial differential equation (PDE). A common method of solving PDEs is to approximate the spatial derivatives, $\partial/\partial x$, using finite differences. Standard methods (for example, Euler's Method, Runge Kutta, Crank-Nicolson) may then be implemented.

Conceptual System
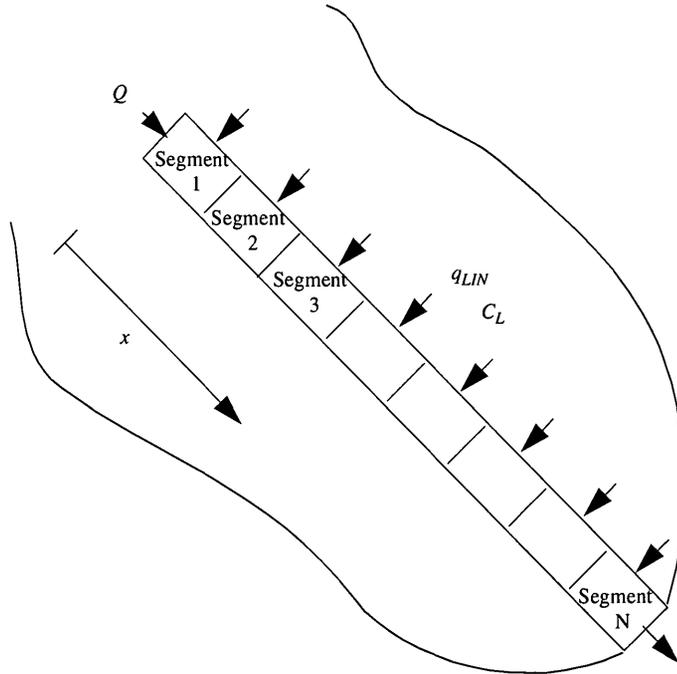
Figure 3.   Conceptual system subdivided into a number of discrete segments (control volumes).

Segmentation Scheme
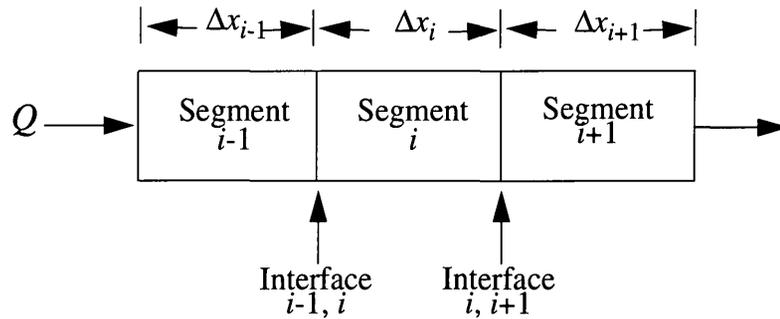
Figure 4.   Segmentation scheme used to implement the numerical solution.

The finite-difference approximations used for the spatial derivatives are developed in appendix B of Runkel and Broshears (1991). Using these approximations, equation (3) becomes:

$$\frac{dC}{dt} = L[C] + \frac{q_{LIN}}{A_i}(C_L - C_i) + \alpha(C_S - C_i) + \rho\hat{\lambda}(C_{sed} - K_d C_i) - \lambda C_i \tag{11}$$

where $L[C]$ is the finite-difference approximation of the advection and dispersion terms given by

$$L[C] = -\left(\frac{Q}{A}\right)_i\left(\frac{C_{i+1} - C_{i-1}}{2\Delta x}\right) + \frac{1}{A_i}\left\{\frac{(AD)_{i,i+1}(C_{i+1} - C_i) - (AD)_{i-1,i}(C_i - C_{i-1})}{\Delta x^2}\right\} \tag{12}$$

Note that Δx and the i subscripts are as defined in Section 2.3 and figure 4. Also note that equation (12) is for the special case of equal segment sizes ($\Delta x_{i-1} = \Delta x_i = \Delta x_{i+1}$). Appendix B of Runkel and Broshears (1991) may be consulted for the general case of variable segment lengths.

2.4.2 The Crank-Nicolson Method

As mentioned in the foregoing paragraphs, ordinary differential equations such as (4), (5) and (11) may be solved using a variety of techniques. These techniques may be loosely grouped into explicit and implicit methods. In short, explicit methods project a solution using values of the dependent variable (for example, solute concentration) from the current time level, whereas implicit methods use values from both current and future time levels. For additional information on implicit and explicit solution techniques, the interested reader is referred to Chapra and Canale (1988).

For reasons of accuracy, efficiency, and stability, the implicit Crank-Nicolson method is used within the solute model. Several advantages of the method led to this choice. First, the Crank-Nicolson method is second-order accurate in both time and space (Chapra and Canale, 1988). Second, the one-dimensional nature of the model results in the formation of a tridiagonal coefficient matrix that can be solved using an efficient LU Decomposition method, the Thomas Algorithm. Finally, the Crank-Nicolson method is unconditionally stable; the solution will not oscillate as the time step is increased.

The following two sections outline the application of the Crank-Nicolson approach to equations (4), (5), and (11). A detailed development of the Crank-Nicolson solution is presented in appendix C of Runkel and Broshears (1991).

2.4.3 Main Channel Solute Concentration

In the Crank-Nicolson algorithm, the right-hand side of equation (11) is evaluated at both the current time (time j) and the future time (time $j+1$). In addition, the time derivative, dC/dt, is estimated using a centered difference approximation:

$$\frac{dC}{dt} = \frac{C_i^{j+1} - C_i^j}{\Delta t} \tag{13}$$

where

Δt - the integration time step [T]
j - denotes the value of a parameter or variable at the current time
$j+1$ - denotes the value of a parameter or variable at the advanced time

Equation (11) thus becomes:

$$\frac{C_i^{j+1} - C_i^j}{\Delta t} = \frac{G[C, C_S, C_{sed}]^{j+1} + G[C, C_S, C_{sed}]^j}{2} \tag{14}$$

where

$$G[C, C_S, C_{sed}] = L[C] + \frac{q_{LIN}}{A_i}(C_L - C_i) + \alpha(C_S - C_i) + \rho\hat{\lambda}(C_{sed} - K_d C_i) - \lambda C_i \tag{15}$$

Because equation (14) involves solute concentrations in the neighboring segments at the advanced time level (C_{i-1}, C_{i+1} at time $j+1$), it is not possible to explicitly solve for C_i^{j+1} (hence we have an implicit method). We can, however, rearrange equation (14) so that all of the known quantities appear on the right-hand side and all of the unknown quantities appear on the left. There are two exceptions to this rearrangement: the storage zone and streambed sediment concentrations at the advanced time level (C_S^{j+1}, C_{sed}^{j+1}) are unknown and remain on the right-hand side. These exceptions are discussed in the Section 2.4.5. For now, rearrangement yields:

$$\left[1 + \frac{\Delta t}{2}\left(\frac{q_{LIN}^{j+1}}{A_i^{j+1}} + \alpha + \rho\hat{\lambda}K_d + \lambda\right)\right]C_i^{j+1} - \frac{\Delta t}{2}L[C]^{j+1} = C_i^j + \frac{\Delta t}{2}\left(G[C, C_S, C_{sed}]^j + \frac{q_{LIN}^{j+1}}{A_i^{j+1}}C_L^{j+1} + \alpha C_S^{j+1} + \rho\hat{\lambda}C_{sed}^{j+1}\right) \tag{16}$$

This, in turn, may be simplified by grouping terms:

$$E_i C_{i-1}^{j+1} + F_i C_i^{j+1} + G_i C_{i+1}^{j+1} = R_i \tag{17}$$

where

$$E_i = -\frac{\Delta t}{2A_i^{j+1}\Delta x}\left(\frac{Q_i^{j+1}}{2} + \frac{(AD)_{i-1,i}^{j+1}}{\Delta x}\right) \tag{18}$$

$$F_i = 1 + \frac{\Delta t}{2}\left(\frac{(AD)_{i-1,i}^{j+1} + (AD)_{i,i+1}^{j+1}}{A_i^{j+1}\Delta x^2} + \frac{q_{LIN}^{j+1}}{A_i^{j+1}} + \alpha + \rho\hat{\lambda}K_d + \lambda\right) \tag{19}$$

$$G_i = \frac{\Delta t}{2A_i^{j+1}\Delta x}\left(\frac{Q_i^{j+1}}{2} - \frac{(AD)_{i,i+1}^{j+1}}{\Delta x}\right) \tag{20}$$

$$R_i = C_i^j + \frac{\Delta t}{2}\left(G[C, C_S, C_{sed}]^j + \frac{q_{LIN}^{j+1}}{A_i^{j+1}}C_L^{j+1} + \alpha C_S^{j+1} + \rho\hat{\lambda}C_{sed}^{j+1}\right) \tag{21}$$

Equations (18)-(21) are for the special case of equal segment sizes. Appendix C of Runkel and Broshears (1991) may be consulted for the general case of variable segment lengths.

After developing equation (17) for all of the segments in the modeled system, we arrive at a set of linear algebraic equations. These equations must be solved simultaneously to obtain the main channel solute concentration, C^{j+1}, in each of the stream segments. A hypothetical set of equations representing a five-segment system is shown below.

$$\begin{bmatrix} F_1 & G_1 & & & \\ E_2 & F_2 & G_2 & & \\ & E_3 & F_3 & G_3 & \\ & & E_4 & F_4 & G_4 \\ & & & E_5 & F_5 \end{bmatrix} \begin{bmatrix} C_1^{j+1} \\ C_2^{j+1} \\ C_3^{j+1} \\ C_4^{j+1} \\ C_5^{j+1} \end{bmatrix} = \begin{bmatrix} R_1 \\ R_2 \\ R_3 \\ R_4 \\ R_5 \end{bmatrix} \tag{22}$$

Systems of equations such as the one shown as equation (22) may be efficiently solved using the Thomas Algorithm. A complete description of the Thomas Algorithm is given by Runkel and Chapra (1993).

2.4.4 Storage Zone and Streambed Sediment Concentrations

The concepts presented in the preceding section can now be applied to the storage zone and streambed sediment equations [equations (4) and (5)]. This results in the following Crank-Nicolson expressions:

$$\frac{C_S^{j+1} - C_S^j}{\Delta t} = \frac{\left(\alpha \frac{A}{A_S}(C - C_S) + \hat{\lambda}_S(\hat{C_S} - C_S) - \lambda_S C_S \right)^{j+1} + \left(\alpha \frac{A}{A_S}(C - C_S) + \hat{\lambda}_S(\hat{C_S} - C_S) - \lambda_S C_S \right)^j}{2} \tag{23}$$

$$\frac{C_{sed}^{j+1} - C_{sed}^j}{\Delta t} = \frac{[\, \hat{\lambda}(K_d C - C_{sed})\,]^{j+1} + [\, \hat{\lambda}(K_d C - C_{sed})\,]^j}{2} \tag{24}$$

In contrast to the main channel equation, Equations (23) and (24) may be solved explicitly for the variables of interest, C_S^{j+1} and C_{sed}^{j+1}. This yields:

$$C_S^{j+1} = \frac{(2 - \gamma^j - \Delta t \hat{\lambda}_S - \Delta t \lambda_S)C_S^j + \gamma^j C^j + \gamma^{j+1} C^{j+1} + 2\Delta t \hat{\lambda}_S \hat{C_S}}{2 + \gamma^{j+1} + \Delta t \hat{\lambda}_S + \Delta t \lambda_S} \tag{25}$$

$$C_{sed}^{j+1} = \frac{(2 - \Delta t \hat{\lambda})C_{sed}^j + \Delta t \hat{\lambda} K_d(C^j + C^{j+1})}{2 + \Delta t \hat{\lambda}} \tag{26}$$

where

$$\gamma = \frac{\alpha \Delta t A}{A_S} \tag{27}$$

These explicit formulations are used in the following section.

2.4.5 Decoupling the Main Channel, Storage Zone, and Streambed Sediment Equations

Runkel and Chapra (1993, 1994) present a technique for decoupling the main channel and storage zone equations. Here we extend the technique to include the streambed sediment equation. Inspection of equation (17) indicates that the main channel concentration is dependent on both the storage zone and streambed sediment concentrations at the advanced time level (C_S^{j+1} and C_{sed}^{j+1}). Because these concentrations are unknown, equation (17) is coupled to equations (25) and (26). This coupling suggests an iterative solution technique whereby equations (17), (25), and (26) are solved in sequence until some desired level of convergence is obtained. This iterative process is inefficient in that (17), (25), and (26) must be solved more than once during each time step.

Fortunately, these equations can be decoupled by noting the explicit forms of equations (25) and (26). Examining (25) we see that the storage concentration is a function of two known quantities, C^j and C_S^j, and one unknown quantity, C^{j+1}. Similarly, the streambed sediment concentration is a function of two known concentrations (C^j and C_{sed}^j) and one unknown (C^{j+1}). Substituting equations (25) and (26) into equation (21), we arrive at a new expression for R:

$$
\begin{aligned}
R_i' = {} & C_i^j + \frac{\Delta t}{2}\left[G[C, C_S, C_{sed}]^j + \frac{q_{LIN}^{j+1}}{A_i^{j+1}} C_L^{j+1} \right. \\
& + \alpha\left(\frac{(2 - \gamma^j - \Delta t\hat{\lambda}_S - \Delta t\lambda_S)C_S^j + \gamma^j C^j + \gamma^{j+1}C^{j+1} + 2\Delta t\hat{\lambda}_S\hat{C}_S}{2 + \gamma^{j+1} + \Delta t\hat{\lambda}_S + \Delta t\lambda_S} \right) \\
& \left. + \rho\hat{\lambda}\left(\frac{(2 - \Delta t\hat{\lambda})C_{sed}^j + \Delta t\hat{\lambda}K_d(C^j + C^{j+1})}{2 + \Delta t\hat{\lambda}} \right) \right]
\end{aligned}
$$

(28)

Although R still contains an unknown quantity, equation (28) is a much more convenient expression. The only unknown quantity is C^{j+1}, a variable that already appears on the left-hand side of equation (17). We can therefore move the terms involving C^{j+1} to the left side of (17), creating new expressions for F and R:

$$
\begin{aligned}
F_i' = {} & 1 + \frac{\Delta t}{2}\left[\frac{(AD)_{i-1,i}^{j+1} + (AD)_{i,i+1}^{j+1}}{A_i^{j+1}\Delta x^2} + \frac{q_{LIN}^{j+1}}{A_i^{j+1}} + \alpha\left(1 - \frac{\gamma^{j+1}}{2 + \gamma^{j+1} + \Delta t\hat{\lambda}_S + \Delta t\lambda_S}\right) \right. \\
& \left. + \rho\hat{\lambda}K_d\left(1 - \frac{\Delta t\hat{\lambda}}{2 + \Delta t\hat{\lambda}}\right) + \lambda \right]
\end{aligned}
$$

(29)

$$R_i'' = C_i^j + \frac{\Delta t}{2}\left[G[C, C_S, C_{sed}]^j + \frac{q_{LIN}^{j+1}}{A_i^{j+1}} C_L^{j+1} \right.$$

$$+ \alpha\left(\frac{(2 - \gamma^j - \Delta t\hat{\lambda}_S - \Delta t\lambda_S)C_S^j + \gamma^j C^j + 2\Delta t\hat{\lambda}_S\hat{C}s}{2 + \gamma^{j+1} + \Delta t\hat{\lambda}_S + \Delta t\lambda_S} \right)$$

$$\left. + \rho\hat{\lambda}\left(\frac{(2 - \Delta t\hat{\lambda})C_{sed}^j + \Delta t\hat{\lambda}K_dC^j}{2 + \Delta t\hat{\lambda}} \right) \right] \tag{30}$$

Because R now involves only known quantities, equation (17) can be solved independently for the main channel solute concentration, C^{j+1}. Having solved (17), the storage zone and streambed sediment equations [equations (25) and (26)] become functions of the known main channel concentration, C^{j+1}. We have thus decoupled the governing Crank-Nicolson expressions.

2.5 Numerical Solution - Steady-State Equations

As with the time-variable equations, we approximate the spatial derivatives in equation (6) using finite differences. These approximations are given in appendix B of Runkel and Broshears (1991). The resultant algebraic equation for the main channel is given by:

$$0 = L[C] + \frac{q_{LIN}}{A_i}(C_L - C_i) + \alpha(C_S - C_i) + \rho\hat{\lambda}(C_{sed} - K_dC_i) - \lambda C_i \tag{31}$$

The main channel equation's dependence on the storage zone and streambed sediment concentrations can be eliminated by substituting equations (9) and (10) into the above. This yields:

$$0 = L[C] + \frac{q_{LIN}}{A_i}(C_L - C_i) + \frac{\alpha A_S(\hat{\lambda}_S\hat{C}s - \lambda_SC_i - \hat{\lambda}_SC_i)}{\alpha A + \lambda_SA_S + \hat{\lambda}_SA_S} - \lambda C_i \tag{32}$$

Since equation (32) includes the solute concentrations in the neighboring segments (C_{i-1}, C_{i+1}), it is not possible to explicitly solve for C_i. We can, however, rearrange equation (32) so that the unknown quantities, C_{i-1}, C_i and C_{i+1}, appear on the left-hand side. This rearrangement yields:

$$E_iC_{i-1} + F_iC_i + G_iC_{i+1} = R_i \tag{33}$$

where

$$E_i = \frac{-1}{A_i\Delta x}\left(\frac{Q_i}{2} + \frac{(AD)_{i-1,i}}{\Delta x} \right) \tag{34}$$

$$F_i = \left(\frac{(AD)_{i-1,i} + (AD)_{i,i+1}}{A_i\Delta x^2} + \frac{q_{LIN}}{A_i} + \alpha A_S\left(\frac{\lambda_S + \hat{\lambda}_S}{\alpha A_i + A_S\lambda_S + A_S\hat{\lambda}_S} \right) + \lambda \right) \tag{35}$$

$$G_i = \frac{1}{A_i \Delta x} \left(\frac{Q_i}{2} - \frac{(AD)_{i,i+1}}{\Delta x} \right) \tag{36}$$

$$R_i = \frac{q_{LIN}}{A_i} C_L + \frac{\alpha A_S \hat{\lambda}_S \hat{C}_S}{\alpha A_i + A_S \lambda_S + A_S \hat{\lambda}_S} \tag{37}$$

Equations (34)-(37) are for the special case of equal segment sizes. Appendix D of Runkel and Broshears (1991) may be consulted for the general case of variable segment lengths. The main channel solute concentrations are determined by solving a system of equations analogous to that shown as equation (22).

2.6 Boundary Conditions

Two boundary conditions must be specified to solve second-order differential equations such as equation (3). For the case of a one-dimensional stream channel, these boundary conditions are applied at the upstream and downstream boundaries.

2.6.1 Upstream Boundary Condition

The upstream boundary condition is defined in terms of a fixed concentration at the upstream boundary (C_{bc}), as shown in figure 5. This boundary condition therefore represents the solute concentration that is entering the upstream end of the modeled system. For solutions of the time-variable equations (Section 2.2.2), the upstream boundary condition may vary over time. User specification of the upstream boundary condition is discussed in Section 3.5.4.

Segment 1 - Upstream Boundary Condition

flow $\longrightarrow$ | C_1 |

C_{bc} $\qquad$ $C_{1,2}$
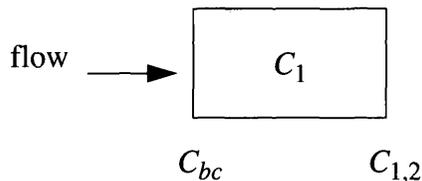
Figure 5. Upstream boundary condition defined in terms of a fixed concentration, C_{bc}.

2.6.2 Downstream Boundary Condition

In contrast to the upstream condition, the downstream boundary condition is not a fixed concentration, but rather a fixed dispersive flux. To implement the downstream boundary condition, a dispersive flux is defined at the interface between segments i and $i+1$. Here the subscript i refers to the

last segment in the modeled system, and $i+1$ refers to a fictitious segment adjacent to the last segment. The dispersive flux is defined as:

$$\left(D\frac{\partial C}{\partial x}\right)\bigg|_{i,\,i+1} = DSBOUND \tag{38}$$

where $DSBOUND$ is a user-supplied value for the dispersive flux. Note that if $DSBOUND$ is set equal to zero, equation (38) is a zero gradient boundary condition. This implies that the concentration in segment i is equal to that in segment $i+1$.

Application of the downstream boundary condition is shown in figure 6; user specification of $DSBOUND$ is discussed in Section 3.5.4.

Downstream Boundary Condition
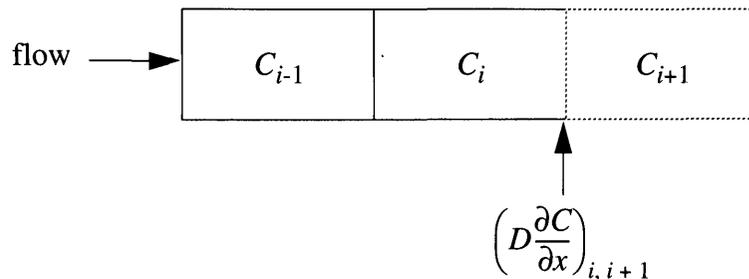
Figure 6. Downstream boundary condition defined in terms of a fixed dispersive flux.

2.7 Parameter Estimation

A goal of many solute transport studies is that of parameter estimation: given a set of observed concentrations, determine a set of parameter values that aptly describes the system under study. Tracer-dilution studies (see Broshears and others, 1993), for example, aim to quantify the hydrologic parameters that characterize physical transport and mixing (Q, A, A_S, α, D).

Parameter estimation often involves a trial-and-error procedure wherein the parameter estimates are manually adjusted during a series of simulations to obtain an acceptable match between simulated and observed concentrations. An alternative to the trial-and-error approach is to use parameter-estimation techniques such as Nonlinear Least Squares (NLS) that automatically determine a set of optimal parameter estimates.

The purpose of this section is to provide a brief overview of how NLS is implemented within the OTIS solute transport model. Readers requiring further information are referred to Draper and Smith (1981), Wagner and Gorelick (1986), and Donaldson and Tryon (1990). Additional details on NLS within OTIS are presented in the User's Guide (Sections 3.2 and 3.5) and two model applications (Sections 4.5 and 4.6).

In general, the observed solute concentration may be expressed as the sum of the simulated concentration and a random error term:

$$c_k = f(\zeta, \overset{\rightarrow}{\theta})_k + \varepsilon_k, \qquad k = 1, N \qquad (39)$$

where

N	- the number of observations
NP	- the number of model parameters
c_k	- the dependent state variable, the observed main channel solute concentration [M/L^3]
$f(\zeta, \overset{\rightarrow}{\theta})_k$	- a nonlinear function that simulates the kth observation, the solution of equations (3)-(5) that provides the simulated main channel concentration, C_k
ζ	- the independent variable. For time-variable problems, $\zeta = t$, whereas for steady-state problems, $\zeta = x$
$\overset{\rightarrow}{\theta}$	- a vector of length NP containing the parameter estimates
ε_k	- random error associated with the kth observation

and the model parameters within $\overset{\rightarrow}{\theta}$ include D, A, A_S, α, λ, λ_S, $\hat{\lambda}$, $\hat{\lambda}_S$, ρ and K_d.

Nonlinear Least Squares may be viewed as an optimization problem with an objective function given by:

$$RSS(\overset{\rightarrow}{\theta}) = \sum_{k=1}^{N} \{ w_k [c_k - f(\zeta, \overset{\rightarrow}{\theta})_k]^2 \} = \sum_{k=1}^{N} (w_k \varepsilon_k^2) \qquad (40)$$

where

$RSS(\overset{\rightarrow}{\theta})$ - weighted residual sum of squares

w_k - weighting factor assigned to the kth observation

The goal of NLS is to determine the vector of parameter estimates, $\overset{\rightarrow}{\theta}$, that minimizes the sum of squared errors [that minimizes $RSS(\overset{\rightarrow}{\theta})$ in equation (40)]. As described by Wagner and Gorelick (1986), this minimization problem may be unweighted, wherein each error is given equal importance ($w_k=1$, $k=1,N$). Alternatively, weights may be assigned based on the magnitude of the solute concentration (Wagner and Gorelick, 1986):

$$w_k = 1 / f(\zeta, \overset{\rightarrow}{\theta})_k^{\ 2} \qquad (41)$$

Here we use an adaptive NLS technique described by Dennis and others (1981) that minimizes $RSS(\overset{\rightarrow}{\theta})$ using an iterative procedure. Within the iterative procedure, parameter estimates are updated in accordance with:

$$\overset{\rightarrow}{\theta}_{m+1} = \overset{\rightarrow}{\theta}_m - (J^T W J + S + Y)_m^{-1} J_m^T W_m \overset{\rightarrow}{\varepsilon}_m^T \qquad (42)$$

subject to

$$\sqrt{\sum_{l=1}^{NP} \left[\frac{(\theta_{m+1,l} - \theta_{m,l})}{SCALE_l} \right]^2} \le d_m \qquad (43)$$

where

S - *NP* by *NP* matrix that approximates a term from the Hessian matrix

SCALE- typical size of a given parameter

W - *N* by *N* diagonal matrix of weighting factors, w_k, $k=1,N$

Y - *NP* by *NP* diagonal matrix chosen such that equation (43) is satisfied

d - diameter of the trust region (Donaldson and Tryon, 1990)

l - denotes quantities corresponding to the *l*th parameter

m - denotes the *m*th iteration

$\vec{\varepsilon}$ - vector of length *N* of residuals, ε_k, $k=1,N$

θ - estimate of the *l*th parameter at iteration *m*

and $\boldsymbol{J}$ is an *N* by *NP* matrix with elements $J_{k,l}$ defined by:

$$J_{k,l} = \frac{\partial f(\zeta, \vec{\theta})_k}{\partial \theta_l} \tag{44}$$

The iterative procedure continues until one of two convergence criteria is met. Convergence may be based on the relative change in the parameters:

$$\frac{max[|\theta_{m+1,l} - \theta_{m,l}|/SCALE_l], \quad l=1, NP}{max[(|\theta_{m+1,l}| + |\theta_{m,l}|)/SCALE_l], \quad l=1, NP} \; < \; STOPP \tag{45}$$

or the change in the residual sum of squares:

$$\frac{fcst[RSS(\vec{\theta})]}{RSS(\vec{\theta}_m)} \; < \; STOPSS \tag{46}$$

where *STOPP* and *STOPSS* are user-specified convergence criteria and $fcst[RSS(\vec{\theta})]$ is the forecasted change in the residual sum of squares.

A flow chart summarizing the iterative parameter-estimation procedure is shown in figure 7. The iterative procedure begins by obtaining the initial parameter estimates, $\vec{\theta}_0$, and the initial diameter of the trust region, d_0. Equations (3)-(5) are then solved to determine the simulated main channel concentrations, $f(\zeta, \vec{\theta})$, corresponding to the *N* observed concentrations. The *NP* parameter estimates, $\vec{\theta}_m$, are revised using equation (42) and a convergence test is conducted. If equation (45) or (46) is satisfied, the solution has converged and the final parameter estimates are given by $\vec{\theta}_m$. If neither equation holds, a new iteration begins.

Parameter Estimation using Nonlinear Least Squares

```
┌─────────────────────────────┐
│ Obtain initial parameter    │
│ estimates, θ̂ₘ₌₀, and the   │
│ initial diameter of the trust│
│ region, dₘ₌₀.               │
└─────────────────────────────┘
```

$$m = 0$$

Begin
Iteration
$$m = m+1$$

```
┌─────────────────────────────┐
│ Solve equations (3)-(5) to  │
│ obtain the main channel     │
│ concentrations, f(ζ, θ̂),   │
│ corresponding to the k=1,N  │
│ observations.               │
└─────────────────────────────┘
```

```
┌─────────────────────────────┐
│ Update the l=1,NP           │
│ parameter estimates, θ̂ₘ,   │
│ using equation (42).        │
└─────────────────────────────┘
```

Does
equation (45)
or equation (46)
hold?

No

Yes

End
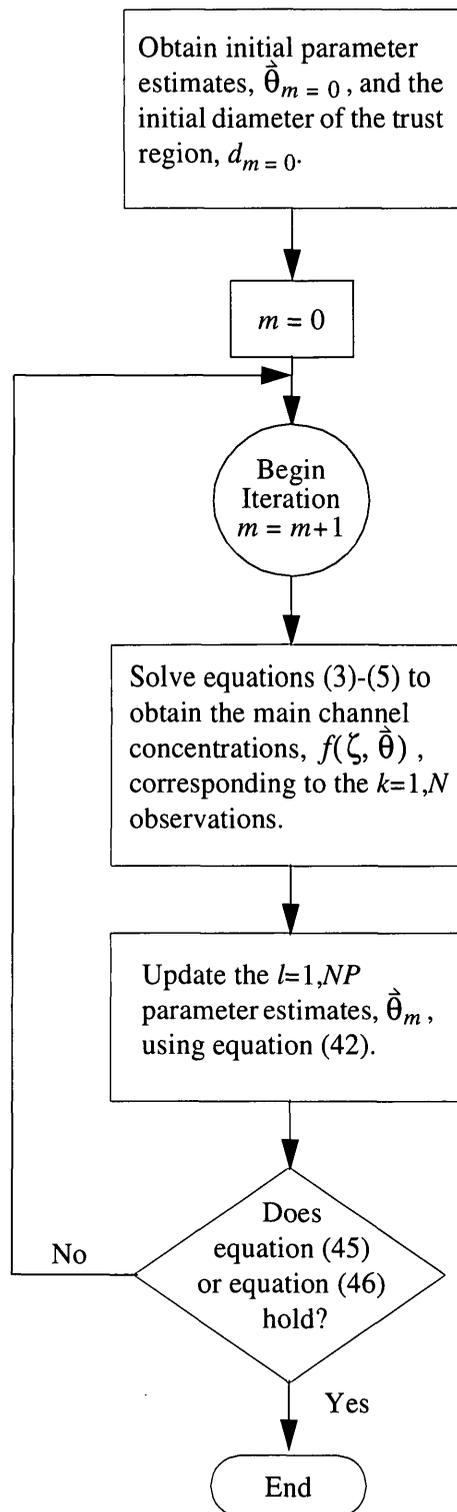
Figure 7.   Iterative parameter-estimation procedure.

3.0 USER'S GUIDE

This section, the OTIS User's Guide, provides information on the use of the OTIS solute transport model. The OTIS solute transport model consists of two operational models. The first model, referred to herein as OTIS, is an updated version of the model originally documented by Runkel and Broshears (1991). OTIS solves the governing equations described in Section 2.2 using the user-specified model parameters, flow information, and system configuration. A second model, OTIS-P, is a modified version of OTIS that is coupled to the Nonlinear Least Squares algorithms described by Donaldson and Tryon (1990). OTIS-P determines an optimal set of parameter estimates corresponding to observed concentration data as described in Section 2.7.

Sections 3.1-3.7 describe input/output specifications for OTIS and OTIS-P. In the discussion that follows, the terms "OTIS solute transport model" and "the model" refer to both OTIS and OTIS-P; unless otherwise noted, the information provided applies to both models. Details specific to a given model are provided as appropriate.

3.1 Applicability

Originally developed for use in small mountain streams, the OTIS solute transport model may be used for any stream or river in which one-dimensional transport can be assumed. The primary assumption of one-dimensional analysis is that solute mass is uniformly distributed over the stream's cross-sectional area. Under this assumption, solute concentration varies only in the longitudinal direction; concentration does not vary with depth or width. Although this uniformity rarely occurs in nature, it is a reasonable assumption for many streams and rivers. Additional details on one-dimensional analysis are provided by Fischer and others (1979).

The model may be used to quantify the physical processes affecting conservative solutes such as tracers. Additional applications include analyses of nonconservative solutes that are subject to sorption and/or first-order decay. A complete overview of the physical and chemical processes included within the model is provided in Section 2.0.

3.2 Model Features

Several simulation options are available within the solute transport model. A general overview of the various options is presented below. More specific details are presented in Section 3.5.

3.2.1 Simulation Modes: Time-Variable and Steady-State

The solute transport model may be used to solve the time-variable (dynamic) equations of Section 2.2.2 or the steady-state equations of Section 2.2.3. The following paragraphs describe these two simulation modes. A full description of the relevant input parameters is presented in Section 3.5.4.

The dynamic simulation option is selected when the user is interested in determining the time-variable nature of the transported solute. This option requires the user to specify a time-variable upstream boundary condition, an integration time step (input variable TSTEP), and a time interval for the printing of results (input variable PSTEP). The dynamic option is invoked for any non-zero TSTEP.

The steady-state option is selected when the long-term response of the system to a constant loading condition is of interest. The steady-state option is invoked by setting the integration time step, TSTEP, to zero.

3.2.2 Conservative and/or Nonconservative Solutes

The model can simulate the fate and transport of conservative or nonconservative solutes. Conservative solutes are subject to the physical processes of advection, dispersion, lateral inflow, and transient storage. Two additional processes, sorption and first-order decay, may be considered when modeling nonconservative solutes.

Conservative solutes are modeled by setting the flags IDECAY and ISORB to 0. Nonconservative solutes subject to sorption are modeled by setting ISORB to 1 and specifying the various sorption parameters (LAMHAT, LAMHAT2, RHO, KD, CSBACK). First-order decay (or production) is modeled by setting IDECAY to 1 and specifying first-order rate coefficients (LAMBDA and LAMBDA2). Positive values for LAMBDA and LAMBDA2 are specified if the solute is subject to first-order decay, whereas negative values are used to specify rates of first-order production. Additional information on the various flags and input parameters is presented in Section 3.5.4.

3.2.3 Flow Regimes

In addition to the foregoing options, the model has the ability to simulate transport under a variety of flow conditions. The model considers spatially (uniform/nonuniform) and temporally (steady/unsteady) varying flows. User specification of the governing hydrologic regime is summarized in table 1. The first two options shown in the table are relatively straightforward, as they involve a steady flow regime. Under a steady flow regime, model parameters such as lateral inflow and cross-sectional area remain constant with respect to time. The third option in table 1, unsteady flow, involves model parameters that vary in time. This option is typically selected when the solute model is used in conjunction with a flow-routing model that provides time-varying lateral inflows, channel flow rates, and cross-sectional areas. Only a small number of unsteady flow model applications have been conducted to date; model users should therefore contact the author in regard to applications involving unsteady flow.

The input format used to specify the flow regime is given in Section 3.5.5. For additional information on the various flow regimes, the reader is referred to Henderson (1966).

Table 1.   User specification of the hydrologic flow regime

Flow regime	User specifications
Steady, uniform flow	Set the lateral flow terms, QLATIN and QLATOUT, to zero. Set the change in flow indicator, QSTEP, to zero.
Steady, nonuniform flow	Set the lateral inflow terms, QLATIN and QLATOUT, to the desired values. Set the change in flow indicator, QSTEP, to zero.
Unsteady, nonuniform flow	Prepare the flow file using flow, lateral inflow, and area data that are generated by a suitable routing model [for example, DR$_3$M, Alley and Smith (1982)]. Set the change in flow indicator, QSTEP, equal to the output time step of the routing model.

3.2.4 Parameter Estimation using OTIS-P

Many modeling studies involve manual procedures wherein model parameters are adjusted during a series of simulations to obtain an acceptable agreement between simulated and observed values. An alternative approach is to use automated parameter-estimation techniques such as the NLS procedures described in Section 2.7. The OTIS-P model couples the mathematical framework of OTIS with the NLS algorithms of STARPAC (Donaldson and Tryon, 1990). OTIS-P thereby provides an automated means of estimating model parameters.

To use the automated parameter-estimation procedure, the user prepares the basic OTIS input files and two additional files required for OTIS-P. These additional files supply the observed concentration data and various STARPAC input parameters. Users may request parameter estimation for any subset of the 10 model parameters (DISP, AREA, AREA2, ALPHA, LAMBDA, LAMBDA2, LAMHAT, LAMHAT2, RHO, and KD).

3.3 Conceptual System, Revisited

Before giving a detailed description of the model's input requirements, it is useful to define some of the program variables in terms of the conceptual system. Figure 8 depicts the modeled system as a series of reaches. For our purposes, a reach is defined as a continuous distance along which model parameters remain constant. A reach, for example, will have a spatially constant dispersion coefficient, decay rate, and lateral inflow rate. The number of reaches defined for a given system reflects both its inherent variability and the availability of data. A spatially uniform stream may be modeled using a single reach, whereas a stream with a well-characterized variation in channel properties may be simulated using several reaches. The number of reaches in the modeled system is specified by the NREACH input parameter.

Conceptual System - Reaches and Segments
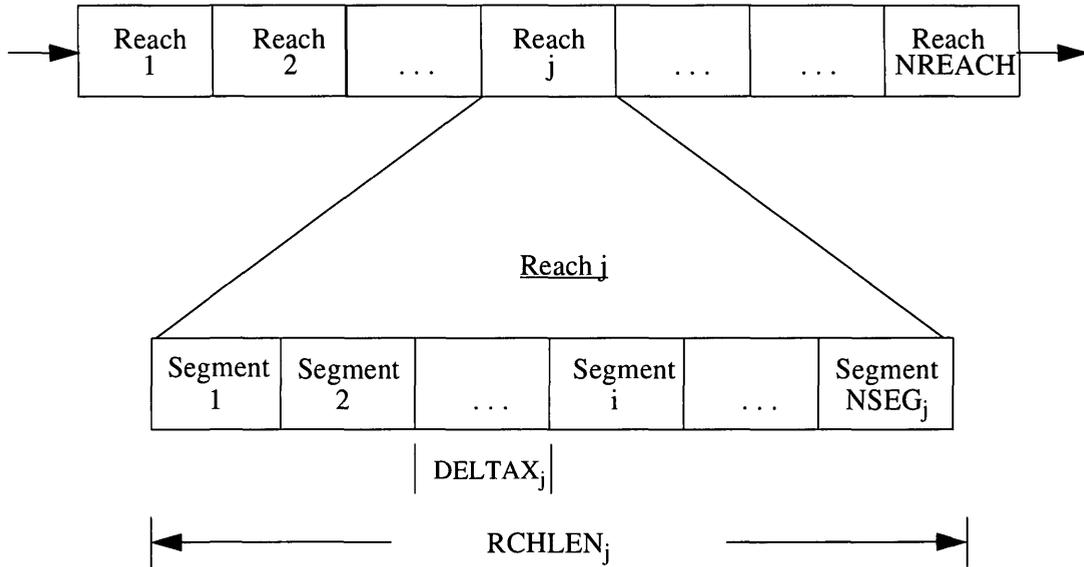
Figure 8. Conceptual system that includes one or more reaches. Each reach is subdivided into a number of computational elements or segments.

Each reach is subdivided into a number of computational elements or segments. Each segment represents a control volume over which the governing mass-balance equations apply. For a given reach, there are NSEG segments of length DELTAX. Note that DELTAX is determined from the reach length, RCHLEN, and the number of segments:

$$DELTAX = \frac{RCHLEN}{NSEG} \tag{47}$$

Additional program variables are shown in figure 9. Here we see the first reach in the stream network and its relationship to some of the required input variables. Because this reach begins at the upstream boundary of the system, we define an incoming flow rate, QSTART, and the solute boundary value, USBC. USBC is the upstream boundary condition, which is discussed in Sections 2.6.1 and 3.5.4 (record type 17, table 11). The program variable denoting the starting stream distance, XSTART, also applies at the upstream end of reach one. Note that these three variables apply only to the first reach of the modeled system.

Conceptual System - Reach 1
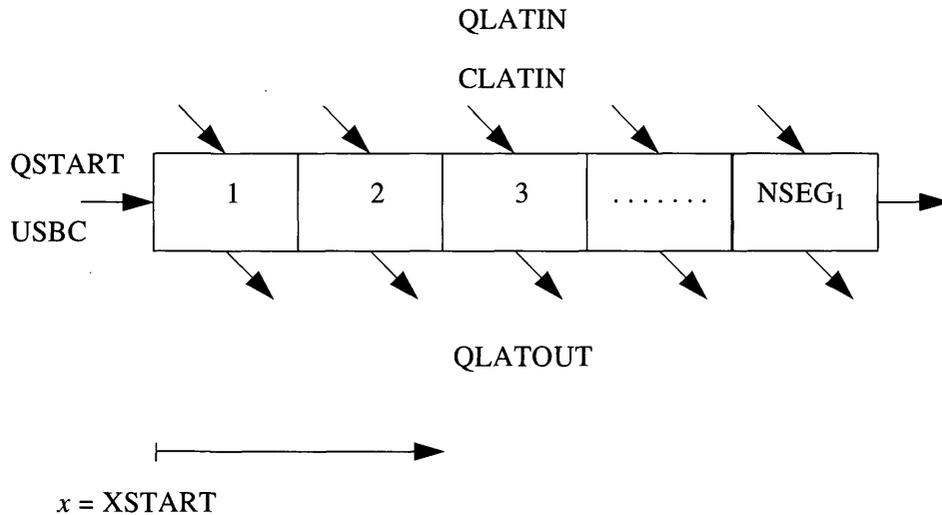
Figure 9. The first reach in the conceptual system and the required input variables.

The remaining program variables shown in the figure, QLATIN, CLATIN and QLATOUT, typically are specified for each reach in the modeled system (an exception is the case of unsteady flow; see Section 3.5.5). The lateral inflow rate, QLATIN, represents the flow entering the channel by overland flow, interflow, and ground-water discharge. This additional flow carries a solute concentration, CLATIN. The final variable, QLATOUT, is a lateral outflow term representing a loss of water from the stream channel. Both QLATIN and QLATOUT are specified on a per unit length basis (in $L^3/T-L$).

3.4 Input/Output Structure

This section describes the input and output files associated with OTIS and OTIS-P. A brief description of each file is presented here; more detailed descriptions are provided in Sections 3.5-3.7.

3.4.1 OTIS

The input/output structure of OTIS is depicted in figure 10. The first input file, the control file, is used to specify the filenames of the remaining input and output files. Unlike the other input files, the filename for the control file is set to control.inp within the software and its name cannot be changed. A second input file, the parameter file, sets simulation options, boundary conditions, and model parameters that remain constant throughout the run. The final input file, the flow file, contains model parameters that can potentially vary during the simulation (for example, volumetric flow rate and main channel cross-sectional area). The filenames of the parameter and flow files are specified by the user in the control file, control.inp.

Input/Output Files: OTIS
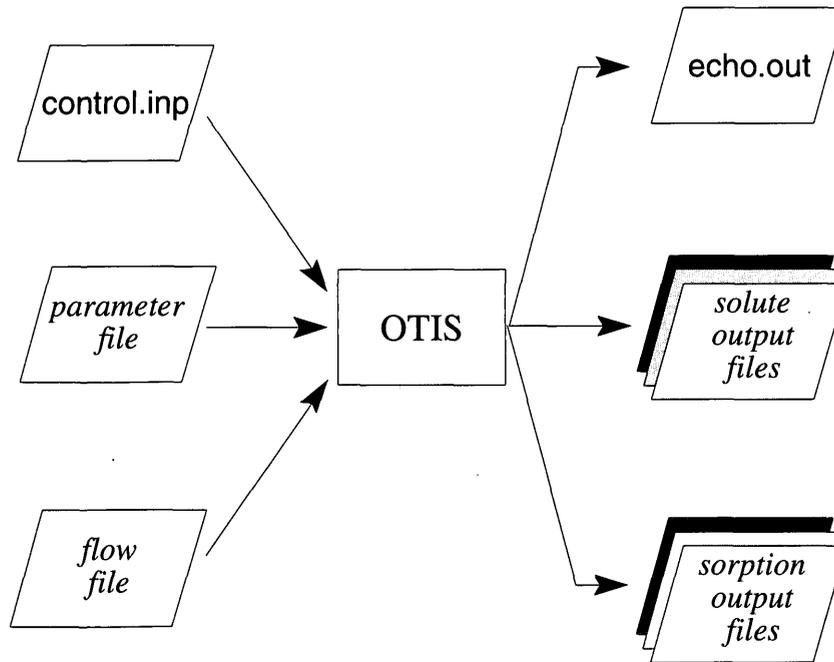
Figure 10. OTIS Input/Output files.

Also shown in figure 10 are the output files created by OTIS. Upon completion of a model run, the file echo.out contains an "echo" of the user-specified simulation options and model parameters. This file also contains any error messages generated during model execution. In addition to the echo file, the model creates one solute output file for each solute. If sorption is being modeled, one sorption output file is also created for each solute. The filenames for the solute and sorption output files are specified by the user in control.inp.

3.4.2 OTIS-P

The input/output structure of OTIS-P is depicted in figure 11. Five input files are required. The first three input files (control, parameter, and flow) are as described in Section 3.4.1 for OTIS. A fourth input file, the data file, provides the observed concentration data that are used within the parameter-estimation procedure. A final input file, the *STARPAC input file*, is used to specify which parameters are to be estimated by OTIS-P as well as other parameter-estimation options. The filenames of the data and STARPAC input files are specified by the user in control.inp.

Also shown in figure 11 are the output files created by OTIS-P. Like the OTIS model, OTIS-P creates echo.out, a solute output file, and if appropriate, a sorption output file. Two additional files are the parameter output file and the STARPAC output file. The parameter file contains the final parameter estimates determined using NLS, while the STARPAC output file contains statistical analyses related to the observed data and the NLS procedure. The filenames for the solute, sorption, parameter and STARPAC output files are specified by the user in control.inp.

Input/Output Files: OTIS-P
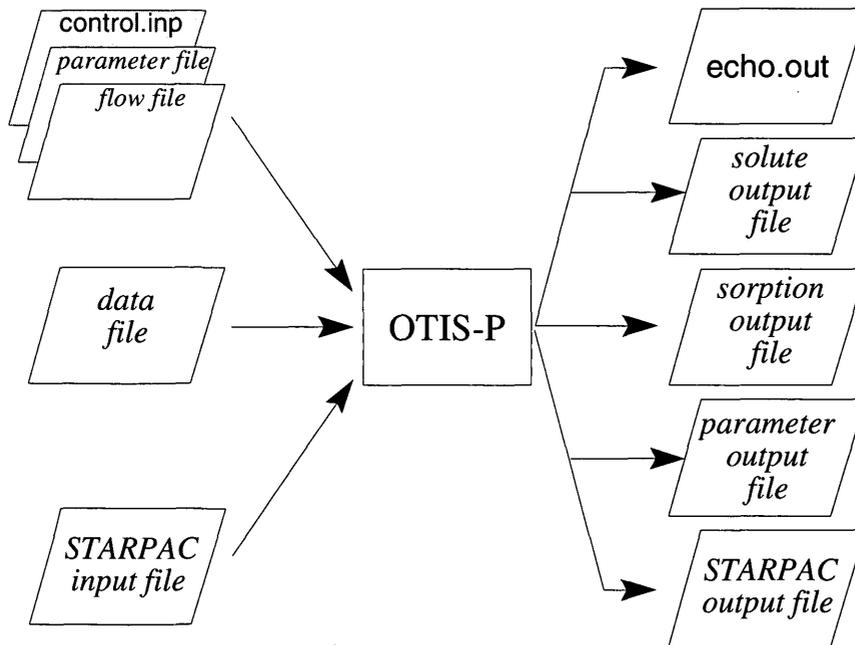
Figure 11. OTIS-P Input/Output files.

3.5 Input Format

As described in Section 3.4, several input files must be assembled prior to model execution. Three of these input files are used by OTIS and OTIS-P (Sections 3.5.3-3.5.5), and the remaining two are used exclusively by OTIS-P (Sections 3.5.6-3.5.7).

In the sections that follow, each input file is described in terms of a set of record types. Within each record type, one or more fields are used to specify various input parameters. In general, record types refer to lines in the input file, and fields correspond to specific columns within each record. Sample input files are presented in Section 4.0.

3.5.1 Units

In Section 2.2 the governing equations and model parameters are described using the fundamental units of Mass [M], Length [L], and Time [T]. Within the OTIS solute transport model, specific units must be assigned to the various input parameters. The model user may select the appropriate units subject to the following:

- **Length Units [L].** Any unit of length may be used when specifying model input variables. The only requirement is that the length unit must be consistent for all model parameters and system configuration variables. The chosen length unit is denoted by an L in the input file descriptions that follow.
- **Concentration Units [CU].** The choice of concentration units is generally independent of the units used for the model parameters and system configuration variables. Consistent concentration units must be used for the specification of the boundary conditions (USBC, DSBOUND), the lateral inflow concentrations (CLATIN), and the sorption variables (RHO, KD, CSBACK). The chosen concentration unit is denoted by a CU in the input file descriptions that follow.
- **Time Units.** All model parameters that require the specification of a time unit (for example, flow rates and rate coefficients) are defined in terms of seconds. Note, however, that simulation control variables such as the simulation start time (TSTART) are specified in terms of hours.

3.5.2 Internal Comments

Model users may document their work by placing comments within any of the input files described below. All lines with a pound sign (#) placed in column number 1 will be treated as comments by the model. This feature is illustrated in the sample input files described in Section 4.0.

3.5.3 The Control File

The control file, control.inp, is used to specify the filenames for the various input and output files. The format of the control file is described below; example control files are given in Section 4.0.

The OTIS Control File

The format of control.inp for OTIS is shown in table 2, where the control file consists of four record types. Record type 1 specifies the filename for the parameter file, record type 2 specifies the name of the flow file, and record type 3 specifies the names of the solute output files. If sorption is modeled, record type 4 specifies the names of the sorption output files. Record type 4 is omitted if sorption is not modeled.

Although table 2 lists four record types, the control file may contain more than four records, as some record types may be repeated. Record types 3 and 4, for example, are repeated for each solute (output files are created for each solute).

Table 2. The OTIS control file

Record type	Input variable	Format	Column	Description
1	FILE	C	1-40	Filename for the *Parameter File*
2	FILE	C	1-40	Filename for the *Flow File*
3*	FILES	C	1-40	Filenames for the *Solute Output Files*
4*	FILES	C	1-40	Filenames for the *Sorption Output Files*

C - Character   *Notes: (1) Omit record type 4 if sorption is not modeled.

(2) Repeat record types 3 and 4 for each solute modeled (NSOLUTE times).

The OTIS-P Control File

The format of control.inp for OTIS-P is given in table 3, where the control file consists of eight record types. Record types 1-8 specify filenames for the parameter, flow, data, STARPAC input, parameter output, STARPAC output, solute output, and sorption output files, respectively. Record type 8 is omitted if sorption is not modeled.

Table 3. The OTIS-P control file

Record type	Input variable	Format	Column	Description
1	FILE	C	1-40	Filename for the *Parameter File*
2	FILE	C	1-40	Filename for the *Flow File*
3	FILE	C	1-40	Filename for the *Data File*
4	FILE	C	1-40	Filename for the *STARPAC Input File*
5	FILE	C	1-40	Filename for the *Parameter Output File*
6	FILE	C	1-40	Filename for the *STARPAC Output File*
7	FILE	C	1-40	Filename for the *Solute Output File*
8*	FILE	C	1-40	Filename for the *Sorption Output File*

C - Character   *Note: Omit record type 8 if sorption is not modeled.

3.5.4 The Parameter File

The parameter file specifies print options, boundary conditions, and the model parameters that remain constant throughout the run. The format of the parameter file is given in tables 4-11. The parameter file is created using the 17 record types discussed below.

Record Type 1 - Simulation Title

The first record in the parameter file is a simulation title of up to 80 characters. This title is printed as part of the echo.out.

Record Types 2 and 3 - Print Parameters

The print option, set in record type 2, determines the format of the solute output files. If the print option is set to 1, solute concentrations are output for the main channel only. Solute concentrations in both the main channel and the storage zone are output if the print option is set to 2.

Record type 3 sets the time interval at which results are printed, the print step. If, for example, results are needed every 15 minutes, a value of 0.25 hour is entered for the print step. The actual print step and the requested print step may differ if the requested step is not an even multiple of the integration time step. In this case, the model sets the print step equal to the nearest multiple of the integration time step.

Record Types 4-6 - Time Parameters

The next step in constructing the parameter file is to enter the appropriate time parameters. Record type 4 is used to set the TSTEP input variable. As discussed in Section 3.2.1, the steady-state solution (Section 2.5) is computed if TSTEP is set to zero. For non-zero values, TSTEP is used as the integration time step (Δt) within the time-variable numerical solution (Section 2.4). Multiple model runs should be performed to determine a time step that yields an accurate solution.

The remaining time parameters, TSTART and TFINAL, are set using record types 5 and 6. The input variable TSTART denotes the simulation start time, and TFINAL specifies the simulation end time. As shown in table 4, values for TSTEP, TSTART, and TFINAL are specified in hours.

Record Type 7 - Distance at the Upstream Boundary

Record type 7 specifies XSTART, the distance at the upstream boundary of the modeled system. During model execution, XSTART is used to determine the distances at various locations downstream. As the upstream boundary is at the beginning of the modeled area, XSTART is commonly set to 0.0.

Record Type 8 - Downstream Boundary Condition

The downstream boundary condition, DSBOUND, is set using record type 8. In many modeling applications, the flux represented by the downstream boundary condition is set to zero. As discussed in Section 2.6, setting DSBOUND to zero implies that the concentration gradient at the downstream boundary is equal to zero. Due to this assumption, the length of the last reach in the modeled system should be specified such that the location of the downstream boundary is sufficiently downstream from the nearest location of interest. Additional details on the downstream boundary condition are provided in Section 2.6 and Section 4.1.

Record Type 9 - The Number of Reaches

As discussed in Section 3.3, the modeled system is divided into a number of reaches, NREACH. This parameter is set by record type 9. For each reach, spatially constant parameters are specified using record type 10.

Table 4. The parameter file - record types 1-9

Record type	Input variable	Format	Column	Units	Description
1	TITLE	C	1-80	---	Simulation title
2	PRTOPT	I	1-5	---	Print option
3	PSTEP	D	1-13	hours	Print step
4	TSTEP	D	1-13	hours	Integration time step
5	TSTART	D	1-13	hour	Simulation starting time
6	TFINAL	D	1-13	hour	Simulation ending time
7	XSTART	D	1-13	L	Distance at the upstream boundary
8	DSBOUND	D	1-13	(L/sec) CU	Downstream boundary condition
9	NREACH	I	1-5	---	Number of reaches

I - Integer
C - Character
D - Double Precision

Record Type 10 - Reach Specific Parameters

Record type 10 sets the parameters for each reach (table 5). Unlike record types 1-9, record type 10 contains more than one input variable. The first field in the record indicates the number of segments located within the reach, NSEG, and a second field specifies the length of the reach, RCHLEN. These two parameters define the length of each segment, DELTAX, as described in Section 3.3. The dispersion coefficient, DISP, storage zone cross-sectional area, AREA2, and the storage zone exchange coefficient, ALPHA, complete record type 10. Because this record type is used for the reach-specific parameters, it is repeated NREACH times, once for each reach in the stream network.

The transient storage mechanism may be turned off by setting ALPHA to 0.0, as shown in Application 3 (Section 4.3). To avoid division by zero, AREA2 must be set to a non-zero value. This value will not affect simulation results, however, provided ALPHA is 0.0.

Table 5. The parameter file - record type 10

Input variable	Format	Column	Units	Description
NSEG	I	1-5	---	Number of segments in reach
RCHLEN	D	6-18	L	Reach length
DISP	D	19-31	L^2/sec	Dispersion coefficient
AREA2	D	32-44	L^2	Storage zone cross-sectional area
ALPHA	D	45-57	/second	Storage zone exchange coefficient

I - Integer
D - Double Precision

Note: Record type 10 is repeated once for each reach (NREACH times).

Record Type 11 - Number of Solutes, Chemistry Options

Record type 11 contains three fields (table 6). The number of solutes, NSOLUTE, is specified in the first field. The second and third fields specify the chemistry options, IDECAY and ISORB. Conservative solutes such as tracers are modeled by setting IDECAY and ISORB to 0 (zero). Nonconservative solutes subject to first-order decay are modeled by setting IDECAY to 1 and specifying first-order rate coefficients in record type 12. Sorption is modeled by setting ISORB to 1 and specifying the sorption parameters in record type 13.

Table 6. The parameter file - record type 11

Input variable	Format	Column	Description
NSOLUTE	I	1-5	Number of solutes
IDECAY	I	6-10	Decay option
ISORB	I	11-15	Sorption option

I - Integer

Record Type 12 - First-Order Decay Coefficients (optional)

Note: Record type 12 is omitted if first-order decay is not modeled (IDECAY=0, record type 11).

First-order decay coefficients are specified using record type 12 (table 7). The first field in record type 12 specifies the first-order decay coefficient for the main channel, LAMBDA; the first-order decay coefficient for the storage zone, LAMBDA2, is specified in the second field [see Equations (3) and (4)].

Because first-order decay coefficients are allowed to vary between reaches and between solutes, record type 12 is used several times within a given parameter file. After specifying the decay coefficients for solute one in reach one, record type 12 is repeated for the remaining reaches (record type 12 is used NREACH times for solute one). In a similar manner, record 12 is repeated NREACH times for the remaining solutes.

Table 7. The parameter file - record type 12

Input variable	Format	Column	Units	Description
LAMBDA	D	1-13	/second	Main channel first-order decay coefficient
LAMBDA2	D	14-26	/second	Storage zone first-order decay coefficient

D - Double Precision   Note: For each solute, record type 12 is repeated once for each reach (NREACH times).

Record Type 13 - Sorption Parameters (optional)

Note: Record type 13 is omitted if sorption is not modeled (ISORB=0, record type 11).

Record type 13 has five fields that specify the sorption parameters for a given solute in each reach (table 8). Fields one and two contain LAMHAT and LAMHAT2, the main channel and storage zone sorption rate coefficients; the remaining fields specify the mass of accessible sediment/volume water (RHO), the distribution coefficient (KD), and the background storage zone solute concentration (CSBACK) [see Equations (3) and (4)].

Because sorption parameters are allowed to vary between reaches and between solutes, record type 13 is used several times within a given parameter file. After specifying the sorption parameters for solute one in reach one, record type 13 is repeated for the remaining reaches (record type 13 is used NREACH times for solute one). In a similar manner, record 13 is repeated NREACH times for the remaining solutes.

Table 8.   The parameter file - record type 13

Input variable	Format	Column	Units	Description
LAMHAT	D	1-13	/second	Main channel sorption rate coefficient
LAMHAT2	D	14-26	/second	Storage zone sorption rate coefficient
RHO	D	27-39	CU	Mass of accessible sediment/volume of water
KD	D	40-52	/CU	Distribution coefficient
CSBACK	D	53-65	CU	Background storage zone solute concentration

D - Double Precision   Note: For each solute, Record Type 13 is repeated once for each reach (NREACH times).

Record Types 14 and 15 - Print Locations

Whereas record types 2 and 3 deal with the timing and type of printed output, record types 14 and 15 control the locations at which results are printed (table 9). The approach described here allows the user to request solute concentrations at a number of locations along the stream. Record type 14 specifies the number of print locations, NPRINT, and the interpolation option, IOPT. Record type 15 specifies the distance of a given print location, PRTLOC, and is repeated NPRINT times.

If the interpolation option (IOPT) is set to 1, the concentration at each print location is determined by linear interpolation using the centers of the two segments closest to the print location. If IOPT is set to 0, the concentration at each print location is set equal to the concentration of the nearest upstream segment. For many applications, specification of IOPT has a negligible effect on simulation results. Selection of the interpolation option (IOPT=1) may be advantageous when long segment lengths (DELTAX) are used. Interpolation is not recommended when the print locations fall near reach endpoints and the downstream reach is characterized by parameters that differ markedly from those of the current reach.

Table 9. The parameter file - record types 14-15

Record type	Input variable	Format	Column	Units	Description
14	NPRINT	I	1-5	---	Number of print locations
14	IOPT	I	6-10	---	Interpolation option
15*	PRTLOC	D	1-13	L	Print location

I - Integer
D - Double Precision

*Note: Record type 15 repeats for each print location (NPRINT times).

Record Types 16 and 17 - Upstream Boundary Conditions

The final record types in the parameter file specify the time-variable upstream boundary condition. As shown in table 10, the number of boundary conditions, NBOUND, and the boundary condition option, IBOUND, are set using record type 16. The NBOUND upstream boundary conditions are characterized by a starting time and a boundary value for each solute. The time at which a boundary condition goes into effect, USTIME, is specified in field one of record type 17 (table 11). Field two, USBC, denotes the boundary values corresponding to USTIME. The USBC field is repeated horizontally for each solute modeled (columns 14-26 contain the boundary value for solute one, columns 27-39 for solute two, and so forth). After specifying the USTIME and USBC, record type 17 is repeated for each change in the boundary concentrations (it is used NBOUND times).

Table 10. The parameter file - record type 16

Input variable	Format	Column	Units	Description
NBOUND	I	1-5	---	Number of boundary conditions
IBOUND	I	6-10	---	Boundary condition option

I - Integer

Table 11. The parameter file - record type 17, upstream boundary conditions

Input variable	Format	Column	Units	Description
USTIME	D	1-13	hour	Time boundary condition begins
USBC	D	14-26[*]	CU; CU-L^3/sec[*]	Upstream boundary value

D - Double Precision

[*]Notes: (1) If there is more than one solute, USBC repeats horizontally (the value for solute one is placed in columns 14-26, the value for solute two is placed in columns 27-39, and so forth).

   (2) Record 17 repeats once for each boundary condition (NBOUND times).

   (3) The units for USBC are dependent on the value of IBOUND in record type 16.

Interpretation of USBC is dependent on the type of upstream boundary condition specified. Three types of boundary conditions may be specified using the boundary condition option, IBOUND, as shown in figure 12. A step concentration profile is imposed at the upstream boundary for IBOUND equal to 1. Under this option, USBC corresponds to the upstream boundary concentration, C_{bc}, described in Section 2.6.1. With a step concentration profile, C_{bc} is initially set to the first boundary value (USBC$_j$) and subsequently updated (to USBC$_{j+1}$, USBC$_{j+2}$, ...) at the appropriate times (USTIME$_{j+1}$, USTIME$_{j+2}$, ...).

A step flux profile is imposed at the upstream boundary for IBOUND equal to 2. Under this option, USBC corresponds to QC_{bc}, where Q is the volumetric flow rate at the upstream boundary (Q=QSTART in figure 9 and table 13). With a step flux profile, the first boundary value (USBC$_j$) is divided by Q to obtain an initial value for C_{bc}. The upstream boundary concentration is subsequently updated at the appropriate times (USTIME$_{j+1}$, USTIME$_{j+2}$, ...). An example of a step flux boundary condition is presented in Section 4.4.

A continuous concentration profile is imposed at the upstream boundary for IBOUND equal to 3. Under this option, C_{bc} is updated at each model timestep. The value assigned to C_{bc} is determined by linear interpolation using specified values of USBC. To allow for interpolation, the time of the last boundary condition (USTIME$_{NBOUND}$) must be greater than or equal to the simulation end time, TFINAL (record type 6). An example of a continuous concentration boundary condition is presented in Section 4.5.

3.5.5 The Flow File

The flow file defines the model parameters that can potentially vary in time. These parameters include the volumetric flow rate (Q, QSTART), lateral flow rates (QLATIN, QLATOUT), main channel cross-sectional area (AREA), and lateral inflow solute concentration (CLATIN). Collectively, these parameters are known as the flow variables.

Upstream Boundary Condition Options

Concentration - Step
IBOUND = 1
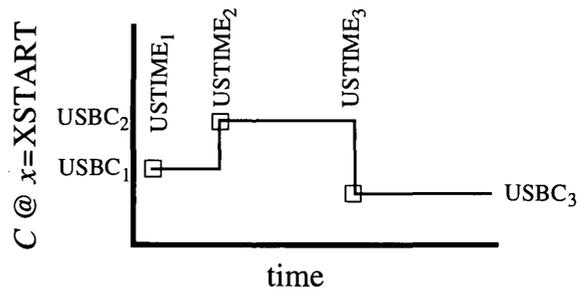
Flux - Step
IBOUND = 2
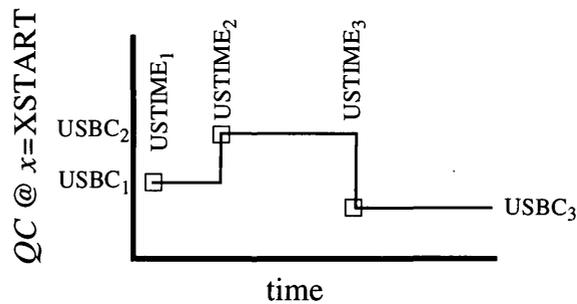
Concentration - Continuous
IBOUND = 3
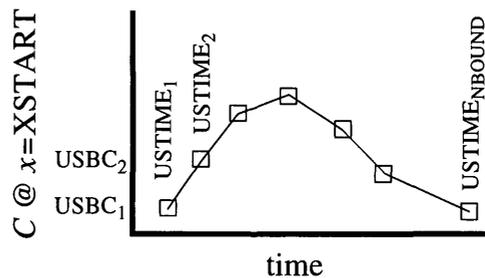
Figure 12. Upstream boundary condition options. The upstream boundary condition may be in terms of a step concentration profile, a step flux profile, or a continuous concentration profile.

The format of the flow file depends on the nature of the parameters contained therein. If all of the flow variables are constant with respect to time, the flow is steady, whereas if any of the flow variables change in time, the flow regime is considered unsteady.

For steady flow conditions, the flow variables are specified on a reach-by-reach basis. When the flow regime is unsteady, the flow variables are specified using flow locations. The formats of the steady and unsteady flow files are given below.

The Flow File - Steady Flow

When the flow variables are constant with respect to time, the steady flow option is invoked. As shown in the following sections, the specification of a steady flow file is fairly straightforward.

Record Type 1 - Change-in-Flow Indicator. The first record type in the flow file is the change-in-flow indicator, QSTEP. This record type is used to define the flow regime. As shown in table 12, QSTEP is the time interval between changes in the flow variables. Here we are concerned with a steady flow regime in which the flow variables are constant. In this case, QSTEP is set to zero.

Table 12.   Steady flow file - record type 1

Input variable	Format	Column	Units	Description
QSTEP	D	1-13	hour	Change-in-flow indicator (set to zero)

D - Double Precision

Record Types 2 and 3 - Flow Variables. The remaining record types for a steady flow file are described in tables 13 and 14. Record type 2 sets the volumetric flow rate at the upstream boundary, QSTART. The remaining flow variables are set using record type 3. As shown in table 14, the first three fields of this record specify the lateral flow rates (QLATIN and QLATOUT) and the cross-sectional area (AREA) for a particular reach. The fourth field, used to indicate the lateral inflow solute concentration (CLATIN), repeats horizontally for each solute modeled. Since the flow variables vary from reach to reach, record type 3 must be repeated for each reach in the network.

Table 13.   Steady flow file - record type 2

Input variable	Format	Column	Units	Description
QSTART	D	1-13	L^3/sec	Flow rate at the upstream boundary

D - Double Precision

Table 14. Steady flow file - record type 3

Input variable	Format	Column	Units	Description
QLATIN	D	1-13	L^3/sec-L	Lateral inflow rate for reach j
QLATOUT	D	14-26	L^3/sec-L	Lateral outflow rate for reach j
AREA	D	27-39	L^2	Main channel area for reach j
CLATIN*	D	40-52*	CU	Lateral inflow solute concentration

D - Double Precision

*Notes: (1) If there is more than one solute, CLATIN repeats horizontally (the lateral inflow concentration for solute one is placed in columns 40-52, the concentration for solute two is placed in columns 53-65, and so forth).

(2) Record type 3 repeats once for each reach in the stream network.

The Flow File - Unsteady Flow

With the allowance for time-variable flow parameters comes an increase in model complexity. As a result, the format of the unsteady flow file differs markedly from that presented for the steady case. In addition, the unsteady flow file is much larger than its steady counterpart, as several record types must be repeated for each change in the flow variables.

The format used here is compatible with standard routing models such as DR$_3$M (Alley and Smith, 1982) and DAFLOW (Jobson, 1989). As discussed below, record types 2-8 allow for the specification of time-varying parameters at various locations along the stream channel. These record types may be created by reformatting output from the selected routing model.

Record Type 1 - Change-in-Flow Indicator. For an unsteady flow regime, the flow variables are read from the flow file when changes in the flow values occur. QSTEP therefore defines the times at which the flow variables are updated (table 15). If the flow variables change every 15 minutes, for example, QSTEP is set to 0.25 hour and the variables are read at the appropriate times.

Table 15. Unsteady flow file - record type 1

Input variable	Format	Column	Units	Description
QSTEP	D	1-13	hour	Time interval between changes in flow

D - Double Precision

Record Types 2 and 3 - Flow Locations. When detailed field measurements are available, it may be appropriate to specify time-varying flow variables at various locations along the stream. These values may be available as output from hydrologic or hydraulic routing models. The format of the flow file allows the user to define a number of flow locations at which the flow variables are specified (table 16). These flow locations often correspond to the reaches that are defined in the parameter file. (This correspondence is not required, however.) Using the data provided at the flow locations, the model linearly interpolates flow and area values (Q, AREA) for each segment in the stream network. Lateral inflow rates and concentrations (QLATIN, CLATIN) are also set using the flow locations.

Record type 2 indicates the number of flow locations, NFLOW. Record type 3 specifies the distance of a given flow location. This record is used NFLOW times, once for each flow location.

Several requirements must be kept in mind when specifying flow locations. The requirements, listed below, are checked internally by the model:

- The flow locations must be entered in ascending (downstream) order; the second location must be downstream from the first, the third must be downstream from the second, and so forth.
- The first flow location must be placed at the upstream end of the stream network. This implies that $FLOWLOC_1$ equals XSTART, where XSTART is the starting location specified in the parameter file. Note that the flow specified at this first location is analogous to the QSTART parameter in the steady flow file.
- The last flow location must be placed at or below the downstream boundary.

Table 16. Unsteady flow file - record types 2 and 3

Record type	Input variable	Format	Column	Units	Description
2	NFLOW	I	1-5	---	Number of flow locations
3[*]	FLOWLOC	D	1-13	L	Flow location

I - Integer

D - Double Precision

[*]Note: Record type 3 repeats for each flow location (NFLOW times).

Record Types 4-7 - Lateral Flows, Flows, and Areas. In contrast to the steady flow file, lateral flows and concentrations (QLATIN, CLATIN) do not necessarily correspond to specific reaches. In the unsteady flow file, these parameters are specified for each flow location. The value specified is used for all segments in between the current flow location and the flow location immediately upstream (from location j-1 to location j). Note that this scheme corresponds to that for the steady flow file if the flow locations are placed at the end of each reach. As stated earlier, the flow and area (Q, AREA) values at the flow locations are used to interpolate values for the segments within the network.

Values for lateral inflow, flow rate, area, and lateral inflow concentration are set for each flow location using record types 4-7, respectively. As shown in table 17, the input fields in these record types (QLATIN, Q, AREA, CLATIN) repeat horizontally for each flow location. The values for flow location one appear in columns 1-13, while those for flow location two appear in columns 14-26, and so on. Record type 7 is used once for each solute (record type 7 is used NSOLUTE times).

Note that record types 4-7 repeat for each change in the flow variables. For example, if the flow variables change every 15 minutes (QSTEP = 0.25 hour), these record types will repeat four times for every hour of simulation time. As a result of this repetition, the unsteady flow file may contain a large number of records.

Table 17. Unsteady flow file - record types 4-7

Record type	Input variable	Format	Column	Units	Description
4[*]	QLATIN	D	1-13[*]	L^3/sec-L	Lateral inflow rate from location j-1 to j
5[*]	Q	D	1-13[*]	L^3/sec	Flow rate at flow location j
6[*]	AREA	D	1-13[*]	L^2	Main channel area at flow location j
7[*]	CLATIN	D	1-13[*]	CU	Lateral inflow conc. from location j-1 to j

D - Double Precision

[*]Notes: (1) QLATIN, Q, AREA, and CLATIN repeat horizontally for each flow location specified (the values for flow location one are set using columns 1-13, for location two using columns 14-26, and so on).
(2) Record type 7 is repeated for each solute (NSOLUTE times).
(3) The block of record types 4-7 repeats for each change in the flow variables.

3.5.6 The Data File (OTIS-P only)

The data file provides the observed concentration data used within OTIS-P for parameter estimation. The data file is composed of two record types. Record type 1 specifies the number of observations associated with each reach, N (table 18). Record type 2 specifies the observed concentration data (tables 19 and 20). Because OTIS-P may be used for steady-state or time-variable simulations, the format of record type 2 is dependent on the simulation mode. For steady-state simulations, field one of record type 2 specifies the distance of each observation, DIST. For time-variable simulations, field one of record type 2 specifies the time associated with each observation, TIME. In both cases, field two of record type 2 specifies the observed concentration, CONC.

Table 18. The data file - record type 1

Input variable	Format	Column	Description
N	I	1-5	Number of observations, reach j

Table 19. The data file - record type 2 (Steady-State Simulations)

Input variable	Format	Column	Units	Description
DIST	D	1-15	L	Distance corresponding to observed data
CONC	D	16-30	CU	Observed concentration

Table 20. The data file - record type 2 (Time-Variable Simulations)

Input variable	Format	Column	Units	Description
TIME	D	1-15	hour	Time corresponding to observed data
CONC	D	16-30	CU	Observed concentration

I - Integer
D - Double Precision

Notes: (1) For each reach, record type 2 is repeated for each observation (N times).

   (2) Repeat the block of record types 1 and 2 for each reach (types 1 and 2 are first specified for reach one, followed by types 1 and 2 for reach two, and so on).

Within the data file, record types 1 and 2 are used several times. For the first reach, record type 1 is used to specify the number of observations, N. Record type 2 is then used N times to specify the observed data points for reach one. This block of N+1 records is repeated for the remaining reaches. Note that for time-variable simulations, the distance associated with each observation is given by the corresponding print location (Section 3.5.4); for example, the distance associated with each observation in reach one is given by print location one. Sample data files are presented in Sections 4.5 and 4.6.

3.5.7 The STARPAC Input File (OTIS-P only)

The STARPAC input file specifies several parameters that control the STARPAC NLS algorithm used within OTIS-P. Many of the STARPAC parameters presented below are discussed in more detail in the STARPAC User's Guide (Donaldson and Tryon, 1990), a document that is part of the OTIS homepage (http://webserver.cr.usgs.gov/otis). Typical parameter values are given in Section 4.5, where a sample STARPAC input file is presented.

Record types 1-7 are shown in table 21. The weight revision option, IWEIGHT (record type 1), determines the weighting factors described in Section 2.7. If IWEIGHT is set to 0, each weighting factor is set to 1.0 such that each error is given equal importance (unweighted NLS). If IWEIGHT is set to 1, weighting factors corresponding to each observation are assigned based on Equation (41) (Section 2.7).

Table 21. The STARPAC input file - record types 1-7

Record type	Input variable	Format	Column	Description
1	IWEIGHT	I	1-5	Weight revision option
2	IVAPRX	I	1-5	Variance-covariance option
3	MIT	I	1-5	Maximum number of iterations
4	NPRT	I	1-5	STARPAC print option
5	DELTA	D	1-13	Maximum scaled change, first iteration
6	STOPP	D	1-13	Stopping value for parameter convergence
7	STOPSS	D	1-13	Stopping value for sum of squares convergence

I - Integer
D - Double Precision

Record type 2 specifies the variance-covariance option, IVAPRX. As described in the STARPAC documentation (Donaldson and Tryon, 1990), three approximations of the variance-covariance matrix are available. The default approximation, based on the assumption of sufficiently small residuals, is selected by setting IVAPRX to 1. Additional values for IVAPRX are described by Donaldson and Tryon (1990).

Record type 3 specifies the maximum number of iterations, MIT, and record type 4 specifies the STARPAC print option, NPRT. NPRT is a five-digit integer that determines the output format of the STARPAC output file. Each digit of NPRT corresponds to one of the five STARPAC output sections. Setting the ith digit of NPRT to 0 suppresses output from the ith section, and values of 1 or 2 result in brief or full output, respectively. A value of 22222, for example, results in full output for all of the sections.

Record type 5 specifies DELTA, the maximum scaled change allowed in the parameters during the first iteration. DELTA is used as the initial diameter of the trust region, d_0 (Section 2.7; figure 7). Although the default value for DELTA is 100, smaller values may be warranted if the parameter estimates leave the region of interest during the first iteration.

Record types 6 and 7 specify the convergence criteria, STOPP and STOPSS. As given by Equations (45) and (46), STOPP and STOPSS are used to determine when the iterative parameter-estimation procedure has converged on the optimal solution. The iterative solution has converged when the parameter values are no longer changing (relative to STOPP) or when the residual sum of squares is no longer changing (relative to STOPSS). STOPP and STOPSS are scale independent; if STOPP equals

10^{-4}, Equation (45) will be satisfied if the first four digits of each parameter are the same on two successive iterations. Similarly, if STOPSS equals 10^{-4}, equation (46) will be satisfied if the first four digits of the residual sum of squares are the same on two successive iterations.

The remaining STARPAC parameters are specified in record type 8 (table 22). Field one of record type 8 specifies IFIXED, an option to denote whether a given parameter is fixed (IFIXED=1) or estimated (IFIXED=0). Fixed parameters are not estimated by the NLS algorithm and remain fixed at their user-specified input values throughout the parameter-estimation procedure. Estimated parameters are adjusted by the NLS algorithm to obtain an optimal solution; user-specified input values for all estimated parameters are used as initial parameter estimates within the parameter-estimation procedure ($\hat{\theta}_0$, fig. 7). Field two specifies SCALE, the typical size of each parameter. SCALE is used to normalize each parameter as in Equation (43). When SCALE is set to 0.0, default values are automatically determined by the NLS algorithm and updated before every iteration.

Table 22. The STARPAC input file - record type 8

Input variable	Format	Column	Description
IFIXED	I	1-5	Fixed parameter option
SCALE	D	6-18	Scale or typical parameter size

I - Integer
D - Double Precision

Note:

Record type 8 is repeated 10 times, once for each of the model parameters that may be estimated. Occurrences of record type 8 apply to the model parameters in the following order: DISP, AREA, AREA2, ALPHA, LAMBDA, LAMBDA2, RHO, KD, LAMHAT, LAMHAT2 (the first occurrence of record type 8 applies to DISP, the second to AREA, and so forth).

Because IFIXED and SCALE are parameter-specific, record type 8 is repeated once for each model parameter. As discussed in Section 3.2.4, there are 10 model parameters that may be estimated. The 10 occurrences of record type 8 therefore apply to DISP, AREA, AREA2, ALPHA, LAMBDA, LAMBDA2, RHO, KD, LAMHAT, and LAMHAT2, respectively.

3.6   Model Execution

This subsection describes how to execute OTIS and OTIS-P under Unix and Windows[2] operating systems.

[2]'Windows' as used herein refers to Microsoft Windows 3.1, Windows 95, and Windows NT.

3.6.1 OTIS

Before running OTIS, the required input files (control, parameter, and flow files) should be placed in the directory from which the model will be executed. To run OTIS, enter the following command at the Unix or MS-DOS prompt:[3]

otis

This command will initiate an OTIS simulation, provided the otis executable is in the current directory or within the user's path (see Section 5.3). OTIS may also be executed within Windows 95/NT by double clicking on the otis executable that is displayed within the Windows Explorer.

As discussed in Section 5.5.3, OTIS error messages are written to the screen and the echo.out output file. Upon completion of the model run, users should inspect echo.out to verify model inputs and to check for execution errors. Solute and sorption output files written during model execution may be analyzed as described in Section 3.7.

3.6.2 OTIS-P

Execution of OTIS-P is very similar to that for OTIS. Several additional steps are required, however, as described in this section.

Before running OTIS-P, the control, parameter, flow, data, and STARPAC input files must be assembled and placed in the directory from which the model will be executed. As discussed in Section 3.5.7, the STARPAC input file allows the user to specify which parameters are to be estimated and which parameters are fixed. Initial estimates for all estimated parameters are taken from the parameter or flow file as appropriate. Fixed parameters remain at their user-specified input values throughout the OTIS-P run.

To run OTIS-P, enter the following command at the Unix or MS-DOS prompt:

otis-p

This command will initiate an OTIS-P simulation, provided the otis-p executable is in the current directory or within the user's path. OTIS-P may also be executed within Windows 95/NT by double clicking on the otis-p executable that is displayed within the Windows Explorer.

As with OTIS, OTIS-P error messages are written to the screen and the echo.out output file. Upon completion of the model run, users should inspect echo.out to verify model inputs and to check for execution errors.

In addition to the solute and sorption output files, OTIS-P creates a parameter output file and a STARPAC output file. The parameter output file contains all of the parameter estimates that were tried during the parameter-estimation procedure and the final parameter estimates. The STARPAC output file contains a summary of the parameter-estimation process for each reach. This summary includes parameter estimates, residual sum of squares, convergence type, and additional statistical information.

---

[3]As with many Unix applications, otis and otis-p may be run in the background by placing an ampersand (&) after the command name.

The success of the parameter estimation process for a given reach is based in part on the type of convergence obtained. Successful simulations result in parameter or residual sum of square convergence. Two other convergence types are possible: false convergence and singular convergence. These types of convergence are discussed in the STARPAC User's Guide (Donaldson and Tryon, 1990):

> Singular convergence means that the model contains too many parameters, at least near the solution, while false convergence can indicate that either STOPSS or STOPP is set too small for the accuracy to which the model and its derivatives are being computed or that there is an error or discontinuity in the derivative.

False and singular convergence may often be eliminated by doing additional OTIS-P simulations. These additional simulations use the final parameter estimates from the previous OTIS-P run as the initial estimates for the current run (parameter estimates are taken from the STARPAC output file and used as initial estimates in revised parameter and/or flow files). Conducting multiple OTIS-P runs in this manner is also advisable in the case of parameter or residual sum of squares convergence; OTIS-P runs are repeated until the final parameter values and residual sum of squares are invariant from one run to the next. An example of this procedure is presented in Section 4.5.

3.7 Output Analysis

This section describes the mechanics of interpreting the solute concentrations that are written to the solute and sorption output files. The discussion includes detailed descriptions of the output file formats (Section 3.7.1), a utility to reformat the output files (Section 3.7.2), and alternatives for plotting the simulation results (Section 3.7.3).

3.7.1 The Solute and Sorption Output Files

As discussed in Section 3.4, the OTIS solute transport model creates a solute output file for each modeled solute. A sorption output file is also created for each solute if sorption is being modeled (ISORB=1, Section 3.5.4). The following paragraphs describe the format of the solute and sorption output files. In the discussion that follows, each line is described in terms of a number of fields; each field is 14 characters long.

The format of the solute and sorption output files depends on the simulation mode. For time-variable simulations, each solute output file contains a time series of solute concentrations at the user-specified print locations. As shown in figure 13, the first field of each line is the simulation time, in hours. The next NPRINT fields give the main channel solute concentration (C) at the NPRINT print locations (PRTLOC, Section 3.5.4). If the print option (PRTOPT, Section 3.5.4) is set to 2, the final NPRINT fields give the storage zone solute concentrations (C_S) at the NPRINT print locations. The format of the sorption output file for time-variable simulations is similar to that of the solute output file; field one specifies the simulation time, and the following NPRINT fields give the streambed sediment-concentration (C_{sed}) at the NPRINT print locations.

Solute Output File - Time-Variable Simulation

Time [hour]	Main Channel Concentration, C			Storage Zone Concentration, C_S		
	@PRTLOC1	@PRTLOC2...	@PRTLOC$_{NPRINT}$	@PRTLOC1	@PRTLOC2...	@PRTLOC$_{NPRINT}$
8.450000E+00	3.700000E+00	3.700000E+00	3.700000E+00	0.000000E+00	1.850000E+00	3.700000E+00
8.550000E+00	3.700230E+00	3.700000E+00	3.700000E+00	0.000000E+00	1.850000E+00	3.700000E+00
8.650000E+00	4.338749E+00	3.700000E+00	3.700000E+00	0.000000E+00	1.850000E+00	3.700000E+00
8.750000E+00	7.305566E+00	3.700021E+00	3.700000E+00	0.000000E+00	1.850000E+00	3.700000E+00
8.850000E+00	9.607778E+00	3.703966E+00	3.700000E+00	0.000000E+00	1.850005E+00	3.700000E+00
8.950000E+00	1.066443E+01	3.773418E+00	3.700000E+00	0.000000E+00	1.850140E+00	3.700000E+00
9.050000E+00	1.109228E+01	4.108784E+00	3.700000E+00	0.000000E+00	1.851210E+00	3.700000E+00
9.150000E+00	1.126551E+01	4.875030E+00	3.700000E+00	0.000000E+00	1.855119E+00	3.700000E+00

Figure 13. Example solute output file for a time-variable simulation.

For steady-state simulations, the solute output file contains one line for each segment in the modeled system. Field one gives the distance associated with a given segment, while field two gives the corresponding main channel solute concentration. If the print option is set to 2, the storage zone solute concentration is given in field three. The sorption output file is arranged in a similar fashion; field one gives the distance and field two gives the streambed-sediment concentration.

3.7.2 The Post-Processor

The solute and sorption output files described in Section 3.7.1 may be reformatted using a simple post-processor that is available with the Unix version of the OTIS solute transport model. For time-variable simulations, the post-processor creates a time-concentration file for each solute at each print location. Distance-concentration files are created for each solute when steady-state simulations are conducted. These post-processor output files may be plotted along with observed data using Unix-based plotting utilities such as Xgraph (Harrison, 1989).

To see a list of available post-processing options, type the following on the command line:

```
postproc -h
```

The post-processor may be used to process output from both OTIS and OTIS-P. Post-processing for OTIS is provided by typing:

```
postproc
```

while OTIS-P post-processing is provided by typing:

```
postproc -p
```

Storage zone solute concentrations are included in the post-processed files by adding the -s flag to the commands shown above (provided PRTOPT=2).

3.7.3 Plotting Alternatives

Model users have several alternatives for plotting results from the OTIS solute transport model. One alternative under the Unix operating system is to use the post-processor described in Section 3.7.2 and the Xgraph plotting utility. An example of this alternative is described here. For the example, assume the name of the solute output file is solute.out and one of the print locations is at a distance of 100. In this case, the post-processor creates an output file named solute.out.100.xgr (additional .xgr files are created for the remaining print locations). Simulation results and observed data from the print location at 100 are plotted as follows:

xgraph -bb -tk -m solute.out.100.xgr obs100.dat

where obs100.dat contains the observed data.

Users running the OTIS solute transport model under Windows may plot simulation results by importing the solute and/or sorption output files into a spreadsheet. The columns in the spreadsheet correspond to the format of the output files described in Section 3.7.1.

4.0 MODEL APPLICATIONS

In this section, several applications of the OTIS solute transport model are presented. Each application is designed to illustrate one or more unique features of the model. The reader is encouraged to review all of the applications provided to obtain a complete overview of the model's capabilities. Additional applications of the model are presented by Broshears and others (1993), Valett and others (1996), and Morrice and others (1997).

Each application has four basic components: (a) a description of the model features that are illustrated in the application, (b) a brief problem statement, (c) sample input files, and (d) simulation results. The sample input files supplement the description of the input requirements presented in Section 3.5. These sample input files are annotated to illustrate how the record types are used within the various files. Due to space limitations, not all of the input files are shown for each application. A complete set of input files is available as part of the software distribution (Section 5.2).

4.1 Application 1: Conservative Transport (OTIS)

This application illustrates the format of the input files used within OTIS. The application involves a time-variable simulation of a conservative tracer, perhaps the most common use of the OTIS solute transport model.

Bencala and Walters (1983) describe an instream experiment in which chloride is used as a conservative tracer. The experiment was conducted in Uvas Creek, a small pool-and-riffle stream in northern California. During the experiment, chloride was injected at a constant rate for 3 hours and concentrations were monitored at five downstream locations (38, 105, 281, 433, and 619 meters). Simulations were combined with experimental data to quantify the hydrodynamic characteristics of Uvas Creek (Bencala and Walters, 1983).

Sample input files corresponding to the Uvas Creek chloride simulation are shown below. In the input files, the user-determined units for concentration (CU) and length (L) are milligrams per liter and meters, respectively. Figure 14 depicts the control file, where the names of the parameter, flow, and solute output files are specified. Time-invariant model parameters are read from params.inp, and flow information is read from q.inp (record types 1 and 2). Simulated chloride concentrations are written to cl.out (record type 3).

Control File for Application 1

```
###################################################################
#
#                        OTIS control file
#
#
# line                          name of the:
# ----                          --------------
# 1                             parameter file
# 2                             flow file
# 3 to 2+NSOLUTE                solute output files
# 3+NSOLUTE to 2+(NSOLUTE*2)    sorption output files (ISORB=1 only)
#
###################################################################
1   params.inp
2   q.inp
3   cl.out
```

Record Type
1 params.inp
2 q.inp
3 cl.out

Figure 14. Control file for Application 1.

Figure 15 depicts the parameter file for the chloride simulation. For this simulation, main channel and storage zone concentrations are printed every 0.1 hour (record types 2 and 3). The integration time step is 0.05 hour, with the simulation beginning at 8.25 hours and ending at 24.0 hours (record types 4, 5, and 6). The upstream boundary of the network is located at 0.0 meters and there is a no-flux downstream boundary condition (record types 7 and 8).

The stream is divided into five reaches (record type 9). Record type 10 is used repeatedly to specify reach geometry and reach-specific parameters (dispersion coefficient, storage zone area, exchange coefficient). The length of reaches one through four is specified such that the reaches end at the sampling locations. The last reach extends an additional 50 meters downstream to reduce any error introduced by the downstream boundary condition (see Section 2.6.2 and Section 3.5.4).

A single solute is modeled and no chemical reactions are included (record type 11). Because chloride is modeled as a conservative solute (ISORB=IDECAY=0), record types 12 and 13 are omitted. Simulation results are printed at five print locations corresponding to the sampling locations, and interpolation is not requested (record types 14 and 15).

As with many simulations of tracer experiments, the upstream boundary concentration is in terms of a step-input function representing three time periods (record type 16). The first and third boundary conditions specify the background chloride concentrations corresponding to the pre- and post-injection periods; the second boundary condition is in effect for 3 hours to represent the injection period (record type 17).

The flow file for Uvas Creek is shown in figure 16. Steady-flow conditions are specified, and flow at the upstream boundary is 0.0125 cubic meter per second (record types 1 and 2). Record type 3 is used repeatedly to specify the flow variables for each reach. Flow increases in the downstream direction due to lateral inflow (QLATIN > 0). Main channel cross-sectional areas vary from reach to reach, while the chloride inflow concentration is spatially constant.

Simulation results from the solute output file (cl.out) are shown in figure 17. Simulated chloride concentrations at the second and fourth print locations (105 and 433 meters) compare favorably with observed concentrations.

Parameter File for Application 1

```
################################################################
#
#                       OTIS parameter file
#
#     1972 Uvas Creek Tracer Injection, Conservative Transport of Chloride
#
#     Parameter Values from:
#
#     Bencala, K.E. and R.A. Walters, 1983, Water Resour.Res.,19(3),718-724.
#
################################################################
```

```
##########################################################
#
#   Physical Parameters for each reach
#
#NSEG  RCHLEN       DISP        AREA2        ALPHA
#      |            |           |            |
##########################################################
```

Record Type	NSEG	RCHLEN	DISP	AREA2	ALPHA
10	38	38.0	0.12	0.05	0.0
10	67	67.0	0.15	0.05	0.0
10	176	176.0	0.24	0.36	3.0e-5
10	152	152.0	0.31	0.41	1.0e-5
10	236	236.0	0.40	1.56	4.5e-5

```
##########################################################
#
# Number of Solutes and flags for decay and sorption
#
# NSOLUTE (col.1-5) IDECAY(col.6-10) ISORB(col.11-15)
#      |       |
##########################################################
```

11	1	0	0

```
##########################################################
#   Print Information
##########################################################
```

Record Type		
14	5 0	NPRINT (col.1-5) IOPT (col.6-10)
15	38.0	(PRTLOC for I = 1, NPRINT)
15	105.0	
15	281.0	
15	433.0	
15	619.0	

```
##########################################################
#  Boundary Conditions
##########################################################
```

16	3 1	NBOUND (col.1-5) IBOUND (col.6-10)

```
##########################################################
#               for I = 1,NBOUND
#
#USTIME        USBC (for i=1,NSOLUTE)
#      |           |                |
##########################################################
```

Record Type		
17	8.25	3.7
17	8.4	11.4
17	11.4	3.7

Figure 15. Parameter file for Application 1.

Steady Flow File for Application 1

Record Type

```
####################################################################
#
#                       OTIS steady flow file
#
#    1972 Uvas Creek Tracer Injection, Conservative Transport of Chloride
#
#    Parameter Values from:
#
#    Bencala, K.E. and R.A. Walters, 1983, Water Resour.Res.,19(3),718-724
#
####################################################################
```
1 `0.00                    QSTEP [hour]`
2 `0.0125                  QSTART [L^3/second]`
```
###############################################################
#               for I = 1, NREACH
#
#QLATIN         QLATOUT      AREA         (CLATIN J=1,NSOLUTE)
#                  |           |            |             |
###############################################################
```
3 `0.00           0.00         0.30         3.7`
3 `0.00           0.00         0.42         3.7`
3 `4.545E-6       0.00         0.36         3.7`
3 `1.974E-6       0.00         0.41         3.7`
3 `2.151E-6       0.00         0.52         3.7`

Figure 16.   Steady flow file for Application 1.

Uvas Creek Chloride

Figure 17.   Simulated and observed chloride concentrations at 105 and 433 meters.

4.2 Application 2: Transport with Kd Sorption (OTIS)

The purpose of this application is to illustrate the use of OTIS for nonconservative solutes. Bencala (1983) describes a three-hour injection of strontium that coincided with the chloride injection described above (Application one, Section 4.1). Because strontium sorbs to streambed sediments, it cannot be modeled as a conservative solute. The sorption algorithms within OTIS are used to model the fate and transport of strontium in Uvas Creek.

Sample input files for the Uvas Creek strontium simulation are very similar to those for application one. The control file includes an additional line to specify the name of the sorption output file (record type 4), and the format of the flow file is identical to that for application one.

Figure 18 is a partial listing of the parameter file for the strontium simulation. Record types 1-10 are not shown because they are identical to those in figure 15. Record type 11 is used to specify the number of solutes and the chemistry options. Sorption is modeled by setting ISORB to 1 and using record type 13 repeatedly to specify the reach-specific sorption parameters. Record type 13 is followed by record types 14-17 in a manner similar to that shown in figure 15.

Record Types 11 and 13 from Application 2 Parameter File

```
Record Type

         ################################################################
         #
         # Number of Solutes and flags for decay and sorption
         #
         # NSOLUTE (col.1-5)  IDECAY(col.6-10)  ISORB(col.11-15)
         #
         #      |       |
         ################################################################
11       1       0       1
         ################################################################
         #
         #   Sorption Parameters (ISORB=1, only)
         #
         #                   for I = 1, NREACH
         #
         #LAMHAT     LAMHAT2     RHO         KD          CSBACK
         #      |           |           |           |           |
         ################################################################
13       5.6e-5     1.0         4.0e+4      70.0e-6     0.13
13       5.6e-5     1.0         2.0e+4      70.0e-6     0.13
13       5.6e-5     1.0         2.0e+4      70.0e-6     0.13
13       5.6e-5     1.0         2.0e+4      70.0e-6     0.13
13       5.6e-5     1.0         4.0e+4      70.0e-6     0.13
```

Figure 18. Partial listing of the parameter file for Application 2.

Simulation results from the solute and sorption output files are shown in figures 19 and 20. Simulated and observed strontium concentrations in the main channel are plotted for the first and third print locations (38 and 281 meters) in figure 19. Streambed-sediment concentrations (C_{sed}) at all five print locations are plotted in figure 20.

Uvas Creek Strontium
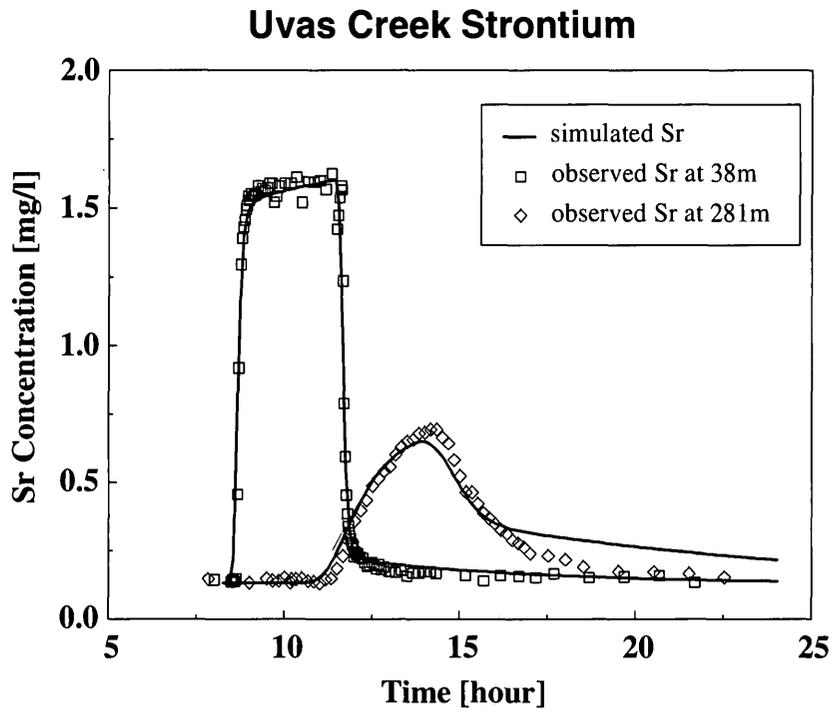
Figure 19. Simulated and observed strontium concentrations at 38 and 281 meters.

Uvas Creek - Sorbed Strontium
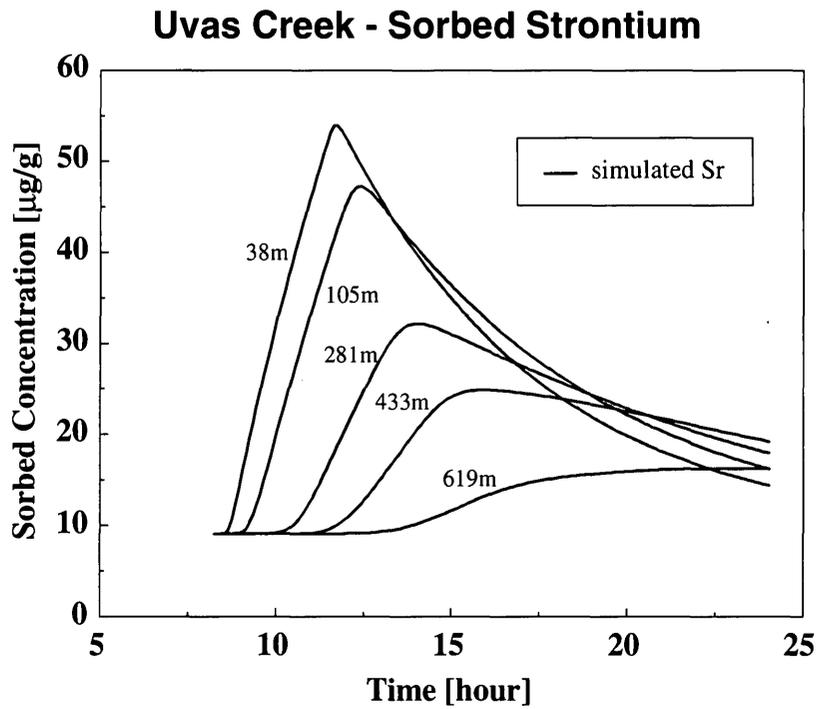
Figure 20. Simulated sorbed strontium at the five print locations.

4.3 Application 3: Transport with First-Order Decay (OTIS)

This application illustrates the use of OTIS for a solute undergoing first-order decay. Runkel (1996) presents a hypothetical problem in which a decaying substance enters a stream during a 2-hour period. The solute concentration at the upstream boundary is 100 concentration units, and steady, uniform flow is assumed. Advection and dispersion are the only physical transport mechanisms modeled (transient storage is not considered; ALPHA=0.0).

Control and flow files for this application are similar to those presented previously and are not presented here. Figure 21 is a partial listing of the parameter file for the hypothetical problem. Record type 11 is used to specify the number of solutes and to indicate that first-order decay is considered (IDECAY=1). First-order decay rates for the first and only reach are specified using record type 12. (Note that for applications with multiple reaches, record type 12 repeats NREACH times.)

Record Types 11 and 12 from Application 3 Parameter File

```
Record Type

        #####################################################################
        #
        # Number of Solutes and flags for decay and sorption
        #
        # NSOLUTE (col.1-5)  IDECAY(col.6-10)  ISORB(col.11-15)
        #
        #        |        |
        #####################################################################
11      1      1        0
        #####################################################################
        #
        #   Decay Coefficients (IDECAY=1, only)
        #
        #LAMBDA           LAMBDA2
        #                 |
        #####################################################################
12      1.E-4            0.0
```

Figure 21. Partial listing of the parameter file for Application 3.

Simulation results are compared with an analytical solution (Runkel, 1996) in figure 22. Close correspondence between OTIS results and the analytical solution indicate that the numerical solution (Section 2.4) is accurate for the problem at hand. The effect of first-order decay can be seen at 2,000 meters, where the peak concentration (10) is much less than the concentration at the upstream boundary (100).

x = 100 meters   x = 2,000 meters

Concentration

Time [hours]

OTIS Simulation
□ Analytical Solution
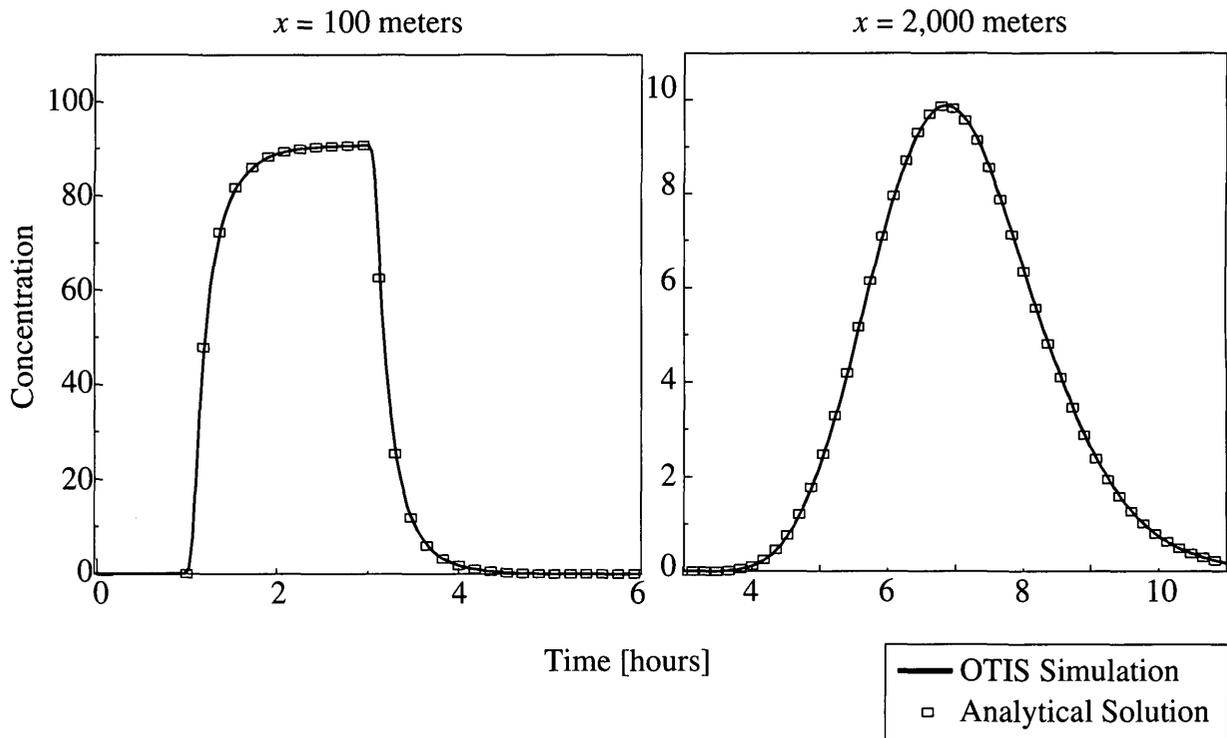
Figure 22. OTIS results compared to analytical solution.

4.4 Application 4: Conservative Transport with Unsteady Flow (OTIS)

This application illustrates the use of OTIS to simulate solute transport under an unsteady flow regime. McKnight and Andrews (1993) describe a solute transport experiment conducted on Huey Creek, a glacial meltwater stream in the McMurdo Dry Valleys of Antarctica. In January 1992, a lithium tracer was injected into Huey Creek over a 3.75-hour period. Samples were collected at several downstream locations, and streamflow was monitored continuously. During the experiment, streamflow varied from less than 1 cubic foot per second to approximately 4 cubic feet per second.

Analysis of the Huey Creek experiment requires consideration of the large flow variations described above. Flow variability is considered by preparing an unsteady flow file as described in Section 3.5.5. An unsteady flow file for Huey Creek was created by reformatting output from a kinematic-wave routing module within the Modular Modeling System (MMS, Leavesley and others, 1996). Input data used by the routing module included an inflow hydrograph, estimates of channel roughness, slope, and channel width (Runkel and others, 1995).

A partial listing of the unsteady flow file for Huey Creek is shown in figure 23. Record type 1 specifies QSTEP, the time interval at which the flow variables change. In this example, QSTEP is equivalent to the output interval of the routing module. Six flow locations are defined using record types 2 and 3. The flow locations are entered in ascending (downstream) order, with the first location at the upstream end of the stream network. After defining the flow locations, record types 4-7 are used to set the lateral inflow rate, volumetric flow rate, main channel cross-sectional area, and lateral inflow concentration for each flow location. Record types 4-7 are repeated for every QSTEP hours of simulation time.

Unsteady Flow File for Application 4

Record Type

```
###########################################################################
#
#                          OTIS unsteady flow file
#
#    1/7/1992 Huey Creek, Antartica
#    Conservative Transport of Lithium
#
#
###########################################################################
1    1.66666667e-2          QSTEP [hour]
     #####################################################################
     #     Flow Locations
     #####################################################################
2         6                 NFLOW
3             0.00          (FLOWLOC   for I = 1, NFLOW)
3             9.00
3           213.00
3           457.00
3           610.00
3           762.00
     #####################################################################
     #     Flow Data from DR3M/MMS
     #####################################################################
     #
     # starting time, 11.30
     #
4         0.00          0.00          0.00          0.00          0.00          0.00
5     0.061573      0.061472      0.059380      0.056964      0.055279      0.053600
6     0.109640      0.109532      0.098029      0.089586      0.095372      0.092534
7         0.00          0.00          0.00          0.00          0.00          0.00
     #
     # time = 11.3 + QSTEP
     #
4         0.00          0.00          0.00          0.00          0.00          0.00
5     0.062194      0.062093      0.060010      0.057605      0.055927      0.054242
6     0.110300      0.110193      0.098650      0.090189      0.096041      0.093197
7         0.00          0.00          0.00          0.00          0.00          0.00
     #
     # time = 11.3 + 2 QSTEP
     #
4         0.00          0.00          0.00          0.00          0.00          0.00
5     0.062814      0.062714      0.060639      0.058246      0.056576      0.054891
6     0.110958      0.110852      0.099269      0.090788      0.096707      0.093863
7         0.00          0.00          0.00          0.00          0.00          0.00
     #
     # time = 11.3 + 3 QSTEP
     #
4         0.00          0.00          0.00          0.00          0.00          0.00
5     0.063435      0.063335      0.061269      0.058887      0.057225      0.055545
6     0.111613      0.111508      0.099885      0.091385      0.097370      0.094531
7         0.00          0.00          0.00          0.00          0.00          0.00
     #
     # continued......
     #
```

(Record types 4-7 repeat for each change in flow.)

Figure 23. Unsteady flow file for Application 4.

Although the parameter file for the Huey Creek lithium simulation is not shown here, two comments are in order. First, the integration time step is selected such that it divides evenly into the routing timestep (QSTEP/TSTEP is an integer value). Second, specification of the upstream boundary condition is greatly simplified by imposing a flux boundary condition (IBOUND=2, Section 3.5.4). Whereas the upstream boundary concentration changes with streamflow, the injectate flux is constant. Specification of a constant flux allows for a simple step boundary condition wherein the three specified values correspond to the pre-injection, injection, and post-injection periods.

Simulation results for the Huey Creek experiment are depicted in figure 24. As shown in the figure, lithium concentrations vary during the injection period (12 to 15 hours) due to changes in streamflow. Failure to consider this streamflow variability would produce a flat simulation profile during the injection period.

Huey Creek Lithium
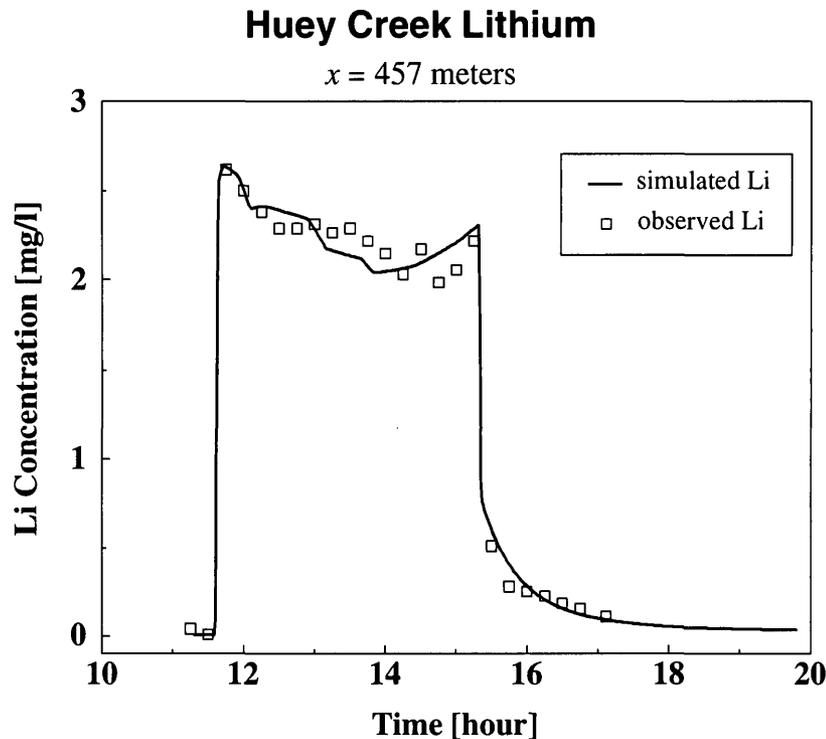
$x = 457$ meters

Figure 24. Simulated and observed lithium concentrations at 457 meters.

4.5   Application 5:   Continuous Boundary Condition and Parameter Estimation (OTIS-P)

The primary purpose of this application is to show how OTIS-P may be used to estimate model parameters using nonlinear least squares. A secondary purpose is to present an example of the continuous boundary condition option.

Laenen and Risley (1997) describe several studies where rhodamine dye is used to characterize streams and rivers in Oregon. In July 1992, a slug of rhodamine was added to the Clackamas River. Water samples were collected at three downstream locations: river miles 11.0, 9.5, and 8.0. These data were used to estimate travel times and mixing characteristics for the two reaches ending at river miles 9.5 and 8.0.

Control File for Application 5

```
################################################################################
#
#                        OTIS-P control file
#
#
#
#       line                  name of the:
#       ----                  --------------
#       1                     parameter file
#       2                     flow file
#       3                     data file
#       4                     STARPAC input file
#       5                     parameter output file
#       6                     STARPAC output file
#       7                     solute output file
#       8                     sorption output file (ISORB=1 only)
#
################################################################################
1   params.inp
2   q.inp
3   data.inp
4   star.inp
5   params.out
6   star.out
7   solute.out
```

Figure 25. Control file for Application 5.

Figure 25 depicts the OTIS-P control file for the Clackamas River rhodamine study. Like the OTIS control file, the OTIS-P control file specifies the names of the various input and output files as described in Section 3.5.3.

The parameter and steady flow files for the Clackamas River application are very similar to those presented for the other applications (Sections 4.1-4.4) and are not shown here. It should be noted, however, that this application makes use of the continuous boundary condition option (IBOUND=3, Section 3.5.4). Because the rhodamine is introduced as a slug (as opposed to a continuous injection), data at the first sampling location (river mile 11.0) are used to define the upstream boundary condition. This is accomplished by setting NBOUND equal to the number of observed data points, setting IBOUND equal to 3, and using the observed time-concentration data to specify USTIME and USBC (record types 16 and 17 of the parameter file). The observed data used as the boundary condition are plotted with simulation results at the end of this application (fig. 28).

Two additional input files are required for OTIS-P. Figure 26 is a partial listing of the data file for the Clackamas River simulation. The data file contains the observed time-concentration data that are used to estimate the model parameters. In this example, two reaches terminate at the second and third sampling locations (river miles 9.5 and 8.0). Record type 1 is used to specify N, the number of observed data points for the first reach. Record type 2 is then used N times to specify the time-concentration data from river mile 9.5. Record types 1 and 2 are then repeated for the second reach, using data from river mile 8.0.

A final input file, the STARPAC input file, is depicted in figure 27. Record types 1-7 are used to specify several STARPAC options as described in Section 3.5.7. Record type 8 is then used to indicate which model parameters are to be estimated using observed concentration data from the data file. The estimated parameters (IFIXED=0) in this example include the dispersion coefficient (D), main channel and storage zone cross-sectional areas (A, A_S), and the storage zone exchange coefficient (α). The remaining model parameters are fixed (IFIXED=1) at their user-specified input values.

Data File for Application 5

```
############################################################
#
#                        OTIS-P data file
#
#
#       line        for J = 1, NREACH
#       ----
#       1           N - Number of observations for reach J.
#       2-N+1       TIME (time-variable) or DIST (steady-state) associated
#                   with each observation (col. 1-15).
#
#
#       Clackamas River Rhodamine - July 1992
#       Data from Laenen and Risley (1997)
#
############################################################
#
#   Site 1, 2414 m (River Mile 9.5)
#
```

Record Type		
1	27	
2	11.00	0.00
2	11.25	0.23
2	11.33	1.10
2	11.42	4.41
2	11.50	8.19
2	11.58	11.00
2	11.67	12.35
2	11.70	12.88
2	11.75	12.49
2	11.83	12.06
2	11.92	11.38
2	12.00	9.56
2	12.08	8.38
2	12.17	7.45
2	12.25	6.59
2	12.33	5.70
2	12.42	5.11
2	12.50	4.32
2	12.58	3.72
2	12.67	3.23
2	12.75	2.88
2	12.83	2.50
2	12.92	2.15
2	13.00	1.86
2	13.25	1.20
2	13.50	0.89
2	14.50	0.00

```
#
#   Site 2, 4828 m (River Mile 8.0)
#
```

Record Type		
1	18	
2	12.75	0.00
2	13.03	0.37
2	13.47	4.07
	Continued........	

Figure 26. Partial listing of the data file for Application 5.

STARPAC Input File for Application 5

```
################################################################################
#
#
#                           STARPAC Parameter Input File
#                                                           Rob Runkel 3/11/95
#
################################################################################
#
#   Record Types 1-4, Integer values in Columns 1-5
#   ------------------------------------------------
#   IWEIGHT    Weight Revision Option
#   IVAPRX     Variance/Covariance Option
#   MIT        Maximum Number of Iterations
#   NPRT       STARPAC Print Option
#
```

Record Type (left margin label)

```
1   0
2   1
3   100
4   22222
#
#   Record Types 5-7, Double precision values in Columns 1-13
#   ---------------------------------------------------------
#   DELTA      Maximum Scaled Change, First Iteration
#   STOPP      Stopping Value for Parameter Convergence
#   STOPSS     Stopping Value for Sum of Square Convergence
#
5   1.0
6   1.D-5
7   1.D-5
#
# For each of the ten model parameters, enter IFIXED (Integer, Col. 1-5)
# and SCALE (Floating Point, Col 6-18).
#
#IFXD SCALE
#    |                          | IFIXED and SCALE for:
#---------------------------------------------------
8   0    0.0D0                  | Dispersion Coefficient, DISP
8   0    0.0D0                  | Main Channel Cross-Sectional Area, AREA
8   0    0.0D0                  | Storage Zone Cross-Sectional Area, AREA2
8   0    0.0D0                  | Storage Zone Exchange Coeffiecient, ALPHA
8   1    0.0D0                  | Main Channel First-Order Decay Coefficient, LAMBDA
8   1    0.0D0                  | Storage Zone First-Order Decay Coefficient, LAMBDA2
8   1    0.0D0                  | Mass of Accessbile Sediment/Volume Water, RHO
8   1    0.0D0                  | Distribution Coefficient, KD
8   1    0.0D0                  | Main Channel Sorption Rate Coefficient, LAMHAT
8   1    0.0D0                  | Storage Zone Sorption Rate Coefficient, LAMHAT2
```

Figure 27.   STARPAC input file for Application 5.

As described in Section 3.6.2, OTIS-P should be executed several times to determine the optimal set of parameter values for each reach. In this example, three OTIS-P runs are conducted to obtain the final parameter set. This process is summarized in table 23, where parameter values for reach 2 are shown (similar comments are relevant for reach 1). For the first run, initial parameter estimates for D, A, A_S, and α are specified by the model user. These initial estimates are taken directly from the parameter (D, A_S, α) and flow (A) files. At the end of the first run, parameter estimates for each reach are taken from the STARPAC output file and used as the initial parameter estimates for the second run. This process is repeated for the third and final run. As shown in table 23, parameter estimates and the residual sum of squares (RSS) from the second and third runs are almost identical. This observation and the fact that RSS

and/or parameter convergence (no false or singular convergence) is obtained for both reaches indicate that a fourth OTIS-P run is not required. Final parameter estimates for reach 2 and the associated ratios are given in the last row of the table. The low ratio for D indicates that the parameter estimate is highly uncertain.[4]

Table 23. Parameter estimates for reach 2

Parameter estimates from....	D [m²/sec]		A [m²]		A_S [m²]		α [/sec]		RSS
	Value	Ratio	Value	Ratio	Value	Ratio	Value	Ratio	
Initial estimates	0.20		50.0		25.0		5.00×10^{-5}		
Run 1	1.74	SC	50.2	SC	13.1	SC	9.59×10^{-5}	SC	1.658
Run 2	0.40	0.44	48.2	110.0	14.4	20.0	1.67×10^{-4}	11.6	0.3415
Run 3	0.41	0.44	48.1	111.0	14.4	20.0	1.67×10^{-4}	11.6	0.3412

SC - Singular Convergence, Ratio Unavailable

The parameter-estimation process described above results in a set of parameters for reaches 1 and 2 that provide a close correspondence between observed and simulated rhodamine concentrations. This correspondence is depicted in figure 28, where simulation results at river mile 9.5 (2414 meters) and river mile 8.0 (4828 meters) are shown.

4.6   Application 6: Steady-State Simulation and Parameter Estimation (OTIS-P)

As noted in Section 3.2.1, the OTIS solute transport model may be used to determine the steady-state solute concentrations that result from a constant loading scenario. In this application, OTIS-P is used in steady-state mode to model the spatial concentration profile of dissolved iron in a small stream. The stream is St. Kevin Gulch, a first-order stream in the Colorado Rocky Mountains that is affected by acid mine drainage.

Kimball and others (1991) describe a synoptic study conducted in August 1986. During the study, water samples were collected at numerous instream locations and analyzed to determine dissolved metal concentrations. Additional samples were collected from a series of springs that enter the stream along the study reach. Figure 29 depicts the observed profile of dissolved iron concentration. Two features of the spatial profile are of interest. First, a large increase in dissolved iron occurs at about 400 meters; a second feature is the abrupt decrease in dissolved iron concentration at about 525 meters. The purpose of this application is to quantify the processes responsible for the changes in dissolved iron concentration.

---

[4]The ratio is equal to the parameter estimate divided by its standard deviation.
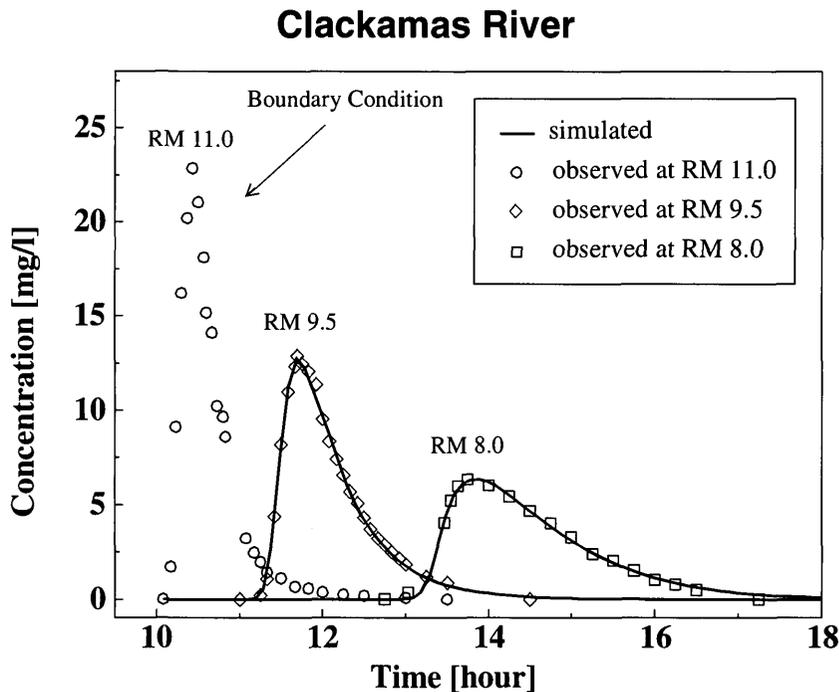
Clackamas River

Figure 28. Upstream boundary condition (river mile 11.0) and simulated and observed concentrations at river miles 9.5 and 8.0.

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 is used to determine the flow rates and the physical parameters (D, A, A_S, α). This information is then combined with observed lateral inflow concentrations to develop a spatial profile under the assumption that dissolved iron is conservative (nonreactive). The results from this conservative steady-state OTIS simulation are shown in figure 29. The close correspondence between observed and simulated iron concentrations in the upper portions of St. Kevin Gulch (0-500 meters) indicates that the initial increase in iron is due to strictly hydrologic factors, that is, the iron loading from the iron-rich springs that emanate from a nearby mine dump. Simulated iron concentrations decrease downstream after 500 meters 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 and/or biological reactions affect dissolved iron concentrations below 500 meters.

A simple approach to quantifying the chemical/biological reactions is to determine the first-order rate at which iron is lost from the system. This is accomplished by fixing the physical parameters and estimating a first-order decay rate for each reach using OTIS-P. Input files and the parameter-estimation procedures are generally the same as those presented in Application 5. Observed data from the springs are used to set the lateral inflow concentrations in the flow file. Within the parameter file, the time step is set to 0.0 to invoke the steady-state option, and initial estimates for the main channel first-order decay rate are specified. The data file is depicted in figure 30, where the observed distance-concentration data are specified for each reach. As in Application 5, three OTIS-P runs are required to obtain the final parameter estimates. First-order decay rates in the main channel ranged from 8.0×10^{-6} to 5.8×10^{-4} per second, resulting in the simulated profile shown in figure 29.
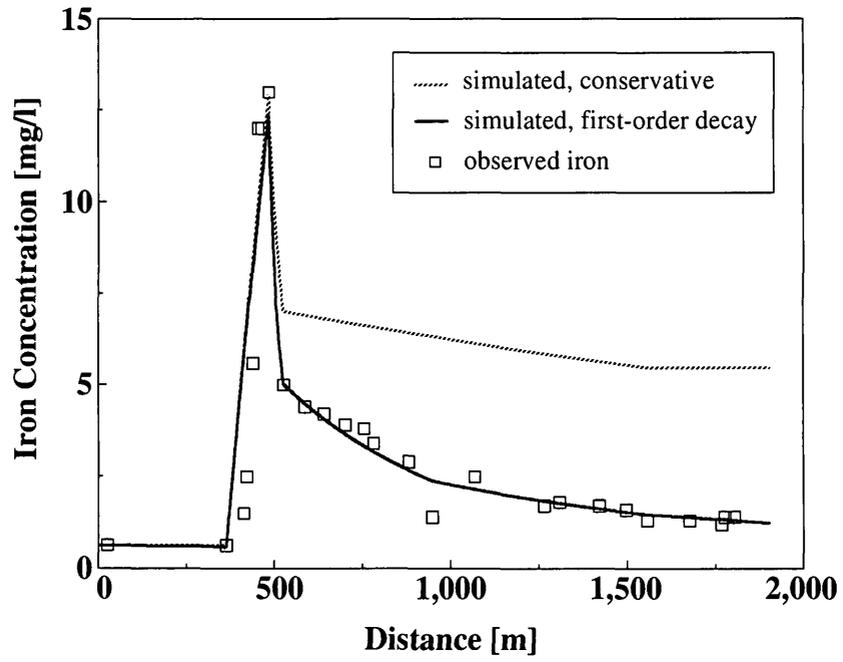
St. Kevin Gulch - Steady-State Iron

Figure 29. Spatial profile of dissolved iron concentration in St. Kevin Gulch.

Data File for Application 6

```
###################################################################
#
#                       OTIS-P data file
#
#
#      line         for J = 1, NREACH
#      ----
#      1            N - Number of observations for reach J.
#      2-N+1        TIME (time-variable) or DIST (steady-state) associated
#                   with each observation (col. 1-15) and CONC (col. 16-30)
#
#
#      1986 St. Kevin Steady-State Iron.  Data from Kimball et al.(1991)
#
###################################################################
#
#   Reach 1  0-26m
#
0
#
#   Reach 2  26-363m
#
2
26.0              0.64
363.0             0.63
#
#   Reach 3  363-484m
#
7
363.0             0.63
413.0             1.5
421.0             2.5
439.0             5.6
455.0             12.0
464.0             12.0
484.0             13.0
#
#   Reach 4  484-526m
#
2
484.0             13.0
526.0             5.0
#
#   continued.....(data for Reaches 5-7)
#
```

Record Type (left margin labels): 1, 1, 2, 2, 1, 2, 2, 2, 2, 2, 2, 2, 1, 2, 2

Figure 30. Partial listing of the data file for Application 6.

5.0 SOFTWARE GUIDE

This section provides information on how to obtain and install the OTIS solute transport model (Sections 5.1-5.4). Additional aspects of the software are described in Section 5.5.

5.1 Supported Platforms

Executable binary files are available for both personal computers and workstations running Windows[5] and Unix operating systems. A summary of supported operating systems and hardware platforms is provided in table 24. Users with other computer systems will need to compile the source code as described in Section 5.4.

Table 24. Supported systems

Hardware	Operating System	ARC
Personal computer (Intel x86)	Windows 3.x / DOS	31
Personal computer (Intel x86)	Windows 95 / NT	95
Personal computer (Intel x86)	Linux	LIN
Unix workstation (DEC)	Digital Unix 3.x	DEC
Unix workstation (DG)	DG-UX 5.x	DG
Unix workstation (IBM)	IBM AIX 3.x	AIX
Unix workstation (SUN)	Solaris 2.x	SOL
Unix workstation (SUN)	SunOS 4.x	SUN

Column 3 of table 24 contains ARC, the notation used throughout the remainder of this section to generically denote system architecture. Personal computer users running Windows 95, for example, should replace the letters "ARC" with "95" when following the specific instructions given in Sections 5.2-5.4.

5.2 Software Distribution

The OTIS solute transport model may be obtained over the World Wide Web (www) or by File Transfer Protocol (ftp). Both methods allow potential model users to download source code, hardware-specific executables, and sample input files. Most users will want to download a binary executable and

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[5]'Windows' as used herein refers to Microsoft Windows 3.1, Windows 95, and Windows NT.

the set of sample input files. These files are stored at the www and ftp sites as compressed tar files (Unix) and self-extracting zip files (Windows). A summary of the downloadable files is presented in table 25.

Table 25.   Files to download for Unix and Windows systems

File contents	UNIX (Compressed tar file)	Windows (Self-extracting zip file)
OTIS/OTIS-P Executables	otis.ARC.tar.Z	otisARC.exe
OTIS/OTIS-P Source Code	otis.source.tar.Z	otissrc.exe
Sample input files	otis.examples.tar.Z	otisexam.exe
Installation batch file	not applicable	instalARC.bat

World Wide Web (www)

The OTIS home page (http://webserver.cr.usgs.gov/otis) includes a Software Distribution page that allows Internet users to download the files listed in table 25. Model users may obtain the model over the World Wide Web by accessing the home page and following the instructions provided.

File Transfer Protocol (ftp)

The files shown in table 25 may also be accessed using standard file transfer protocol. The ftp procedure is as follows:

(1) Log into the ftp depot as anonymous:
   ftp ftpdcolka.cr.usgs.gov   (ftp to depot)
   anonymous   (enter anonymous at the login prompt)
   anypassword   (enter any password)

(2) Prepare to download the files:
   cd pub/otis   (get into appropriate directory)
   hash   (request hash marks)
   type binary   (request binary file transfer)

(3) Download the sample input files:
   get otis.examples.tar.Z   (UNIX only)
   get otisexam.exe   (Windows only)

(4) Download a binary executable, if appropriate:
   get otis.ARC.tar.Z   (UNIX only)
   get otisARC.exe   (Windows only)

(5) Download the source code, if appropriate:
   get otis.source.tar.Z   (UNIX only)
   get otissrc.exe   (Windows only)

(6) Download the installation batch file, if appropriate:
   get instalARC.bat   (Windows only)

5.3 Installation

The files described in Section 5.2 may be used to install the OTIS solute transport model as described here. The installation procedure is designed to create the directory structure shown in figure 31. To begin the installation process, move the downloaded files (Section 5.2) into the *base-directory*. The *base-directory* is a user-selected directory under which the OTIS directory tree will be placed (fig. 31). After moving the files, follow the instructions for Unix or Windows systems given below.
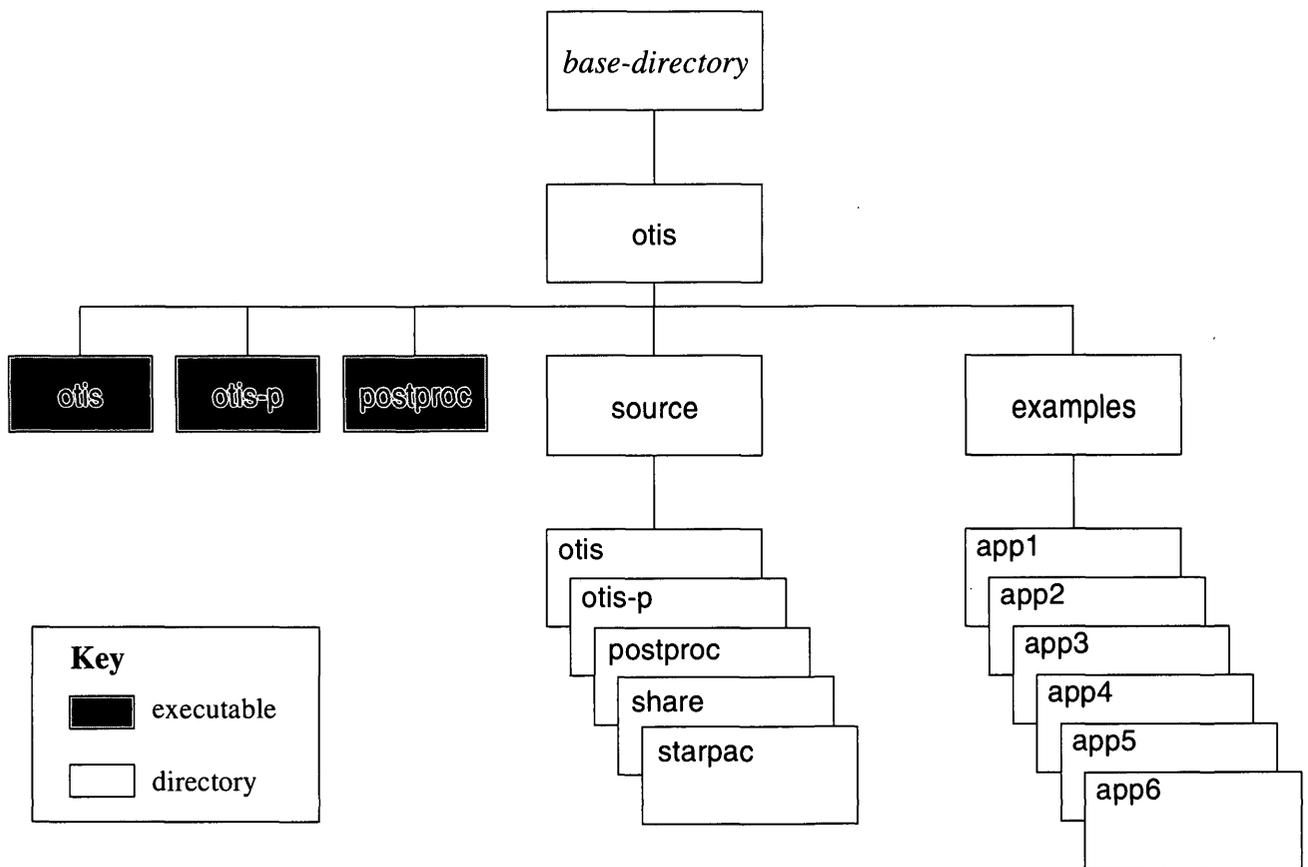
OTIS/OTIS-P Directory Structure

Figure 31. OTIS/OTIS-P directory structure.

Unix Installation Instructions

Installation on Unix systems consists of uncompressing the tar files and extracting the directory structure. This is done by issuing the following commands:

(1) Uncompress the tar files:
     uncompress otis.examples.tar.Z
     uncompress otis.source.tar.Z   (if appropriate)
     uncompress otis.ARC.tar.Z   (if appropriate)

(2) Extract the directory structure:

    tar -xovf otis.examples.tar
    tar -xovf otis.source.tar   (if appropriate)
    tar -xovf otis.ARC.tar   (if appropriate)

Windows Installation Instructions

Installation on Windows systems is accomplished by issuing the following command at the MS-DOS prompt:

    instalARC

Update the user's path (optional)

After completing the installation procedure, the otis, otis-p, and postproc executables will reside in *base-directory*/otis/. Under this arrangement, all model runs must be initiated from *base-directory*/otis/. To initiate model runs from any directory, *base-directory*/otis/ may be added to the user's path.

5.4 Compilation

As discussed in Section 5.1, executable binary files for the OTIS solute transport model are available for a number of hardware platforms and operating systems. As a result, compilation of the source code may not be required. Compilation is required in the following situations:

- Executable binaries are not available for your specific hardware platform/operating system.

- The dimensions of the modeled system exceed the maximum dimensions specified in the include files (Section 5.5.2).

- Modifications have been made to the underlying computer code.

The compilation procedure for Windows systems is not discussed here because it is dependent on the type of compiler used. Under UNIX, the model is compiled using the make utility, as described below.

Unix Compilation Instructions

(1) Edit the makefiles (optional). The makefiles used to compile OTIS and OTIS-P are configured to invoke the f77 Fortran-77 compiler with the -O option (default optimization). Users requiring other compilers and optimization flags will need to edit the makefiles as appropriate.

(2) Modify the include files (optional). Changes to the maximum dimensions or logical device assignments may be made by editing the include files described in Section 5.5.2.

(3) From the *base-directory*/otis/ directory, enter:

    make

When compilation is complete, otis, otis-p, and postproc executables will reside in *base-directory*/otis/.

5.5 Software Overview

5.5.1 Model Development

The OTIS solute transport model is written in ANSI standard Fortran-77. The model has been compiled and tested on a variety of hardware platforms and operating systems (Section 5.1). Specific development environments used to compile the source code are presented in table 26.

Table 26. Development environments

Processor	Operating system	Compiler	Compiler options	ARC
Pentium 75	Windows 3.1	Microsoft Fortran PowerStation, Version 1.0a	optimize for time, improve floating point consistency.	31
Pentium 133	Windows 95	Microsoft Fortran Powerstation, Version 4.0	full optimization, automatic inlining, improved floating point consistency	95
Pentium II	Red Hat Linux 2.0.3	GNU Fortran 0.5.18	-O	LIN
DEC Alpha	Digital Unix V3.2C	Digital Fortran 77	-O4	DEC
DG AViiON	DG/UX 5.4R3.10	Green Hills Ftn-88000 1.8.6.1	-OLM	DG
IBM RS/6000	AIX 3.2	XL Fortran Compiler 6000	-O3	AIX
SUN SPARC 10	Solaris 2.4	SPARCompiler Fortran 3.0	-fast -O3	SOL
SUN4	SunOS 4.3.1	SPARCompiler Fortran 2.0.1	-fast -O3	SUN

5.5.2 Include Files

The source code used to develop OTIS and OTIS-P consists of many small subroutines. To facilitate program modification, three include files are used. Use of include files allows program information to be shared between subroutines. This information may be modified by editing the include files rather than each individual routine.

Maximum Dimensions - fmodules.inc, fmodules2.inc

Under Fortran-77, the dimension of each vector and array must be fixed prior to program execution. This requires some knowledge of the maximum dimension for each model parameter. Selection of an appropriate size for each parameter is an important task because excessively small values limit program applicability and excessively large values waste program memory.

To address this problem, the maximum dimensions for the entire model are defined using two include files: fmodules.inc and fmodules2.inc. Increases or decreases in the maximum dimensions are made by editing the include files and compiling the model as described in Section 5.4.

The default values for the maximum dimensions are given in tables 27 and 28. In general, each of the dimensions corresponds to a user-supplied input variable. This correspondence is shown parenthetically in the third column of the table.

When running the model, the input variables may not exceed the maximum values. The number of print locations (see Section 3.5.4 - Record type 14), for example, may not exceed the maximum value given by MAXPRINT. When an input value exceeds its given maximum, program execution is terminated and an error message is issued. At this point the user must increase the appropriate maximum value (by editing fmodules.inc or fmodules2.inc) and recompile the program.

Table 27.   Maximum dimensions and default values from fmodules.inc

Dimension	Default maximum	Maximum number of .....
MAXREACH	30	Stream reaches (NREACH)
MAXPRINT	30	Print locations (NPRINT)
MAXBOUND	200	Upstream boundary conditions (NBOUND)
MAXSEG	5,000	Stream segments (Σ NSEG$_j$, j=1 to NREACH)
MAXSOLUTE*	3, 1	Solutes modeled (NSOLUTE)
MAXFLOWLOC	30	Flow locations (NFLOW)

*Note: MAXSOLUTE=3 for OTIS; MAXSOLUTE=1 for OTIS-P.

Table 28.   Maximum dimensions and default values from fmodules2.inc (OTIS-P only)

Dimension	Default maximum	Maximum number of .....
MAXOBS	200	Observations for a reach (N)
MAXPAR	10	Model parameters

Logical Devices - lda.inc

In Fortran-77, a unit number is assigned to each file used for input and/or output. These unit numbers, also known as logical device assignments (*ldas*), must be specified for each read and write operation. Program variables used to store the unit numbers are shared between the input and output subroutines using a Fortran common block. This common block is defined in the include file lda.inc.

5.5.3 Error Checking

The model's input subroutines perform several tests to validate the input data. If fatal errors are detected, an error message is written to echo.out and program execution is terminated. The error-checking capabilities of the model are summarized below.

Fatal Errors, OTIS and OTIS-P

- The number of reaches, NREACH, must not exceed the maximum, MAXREACH.
- The number of segments, IMAX, must not exceed the maximum, MAXSEG.
- The number of print locations, NPRINT, must not exceed the maximum, MAXPRINT.
- The number of solutes, NSOLUTE, must not exceed the maximum, MAXSOLUTE.
- The number of upstream boundary conditions, NBOUND, must not exceed the maximum, MAXBOUND.
- The number of flow locations, NFLOW, must not exceed the maximum, MAXFLOWLOC.
- The storage zone cross-sectional area, AREA2, must be greater than zero.
- A given print location, $PRTLOC_i$, must lie within the modeled network.
- The flow locations, FLOWLOC, must be entered in ascending (downstream) order.
- The first flow location, $FLOWLOC_1$, must be placed at the upstream boundary. The last flow location must be at or below the downstream boundary.
- For a continuous concentration boundary condition (IBOUND equal to 3), the time of the last boundary condition ($USTIME_{NBOUND}$) must be greater than or equal to the simulation end time, TFINAL
- The print option, PRTOPT, must equal 1 or 2.
- The interpolation option, IOPT, must equal 0 or 1.
- The boundary condition option, IBOUND, must equal 1, 2, or 3.
- The decay option, IDECAY, must equal 0 or 1.
- The sorption option, ISORB, must equal 0 or 1.

Fatal Errors, OTIS-P

- The number of observations for a reach, N, must not exceed the maximum, MAXOBS.
- The time of the first observation must be greater than the simulation start time plus the integration time step ($TIME_1 > TSTART + TSTEP$).
- Observations must be entered in order of ascending time ($TIME_{j+1} > TIME_j, j=1,N$).
- The time between successive observations must be greater than the time step ($TIME_{j+1} - TIME_j > TSTEP, j=1,N$).
- The distance specified, DIST, must lie within the modeled network.
- The weight revision option, IWEIGHT, must equal 0 or 1.

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