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Documentation for the MODFLOW 6 Groundwater Transport Model

Chapter 61 of
Section A, Groundwater
Book 6, Modeling Techniques

Techniques and Methods 6–A61

U.S. Department of the Interior
U.S. Geological Survey

Cover. Binary computer code illustration.

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Preface

The report describes the Groundwater Transport (GWT) Model for the U.S. Geological Survey (USGS) modular hydrologic simulation program called MODFLOW 6. The program can be be downloaded from the USGS for free. The performance and accuracy of the GWT Model has been tested in a variety of applications. Future applications, however, might reveal errors that were not detected in the test simulations. Users are requested to send notification of any errors found in this model documentation report or in the model program to the MODFLOW contact listed on the Web page. Updates might be made to both the report and to the model program. Users can check for updates on the MODFLOW Web page (https://doi.org/10.5066/F76Q1VQV).

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Documentation for the MODFLOW 6 Groundwater Transport Model

By Christian D. Langevin,[1] Alden M. Provost,[1] Sorab Panday,[2] and Joseph D. Hughes[1]

Abstract

This report documents a new Groundwater Transport (GWT) Model for MODFLOW 6. The GWT Model simulates three-dimensional transport of a single chemical species in flowing groundwater based on a generalized control-volume finite-difference approach. Although each GWT Model is only able to represent a single chemical species, multiple GWT Models may be invoked within a single MODFLOW 6 simulation to represent solute transport of multiple non-interacting chemical species. The GWT Model is designed to work with the Groundwater Flow (GWF) Model for MODFLOW 6, which simulates transient, three-dimensional groundwater flow. The version of the GWT model documented here must use the same spatial discretization used by the GWF Model; however, that spatial discretization can be represented by regular MODFLOW grids consisting of layers, rows, and columns, or by more general unstructured grids. The GWT Model simulates (1) advective transport, (2) the combined hydrodynamic dispersion processes of velocity-dependent mechanical dispersion and molecular diffusion, (3) adsorption and absorption (collectively referred to as sorption) of solutes by the aquifer matrix, (4) transfer between the mobile domain and one or more immobile domains, (5) first- or zero-order solute decay or production, (6) mixing from groundwater sources and sinks, and (7) direct addition of solute mass. The GWT Model can also represent advective solute transport through advanced package features, such as streams, lakes, multi-aquifer wells, and the unsaturated zone. If the GWF Model application uses the Water Mover (MVR) Package to connect flow packages, then solute transport between these packages can also be represented. The transport processes described in this report have been implemented in a fully implicit manner and are solved in a system of equations using iterative numerical methods. The present version of the GWT Model for MODFLOW 6 does not have an option to calculate steady-state transport solutions; if a steady-state solution is required, then transient evolution of the solute must be represented using multiple time steps until no further changes in solute concentrations are detected.

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Chapter 1. Introduction

MODFLOW 6 is the latest core version of the MODFLOW software. It was released by the U.S. Geological Survey (USGS) in 2017 (Hughes and others, 2017). This new version of MODFLOW was redesigned from scratch using an object-oriented design that allows for multiple models to be included in a single simulation. The new MODFLOW 6 framework facilitates more than one model of the same type in a simulation. For example, there may be a regional groundwater flow model and a locally refined inset model, and these models can be tightly coupled along their interface. A unique feature of the MODFLOW 6 framework allows these models to be coupled at the matrix solution level whereby a single system of equations is constructed and solved simultaneously for both models.

In addition to supporting multiple models of the same type in a single simulation, the MODFLOW 6 framework was also designed to support multiple models of different types in the same simulation. The first type of model introduced in MODFLOW 6 was the Groundwater Flow (GWF) Model (Langevin and others, 2017), which simulates three-dimensional, transient, groundwater flow. The GWF Model synthesizes many of the newer capabilities that were added to the MODFLOW-2005 program (Harbaugh, 2005). The following list summarizes select features available in the GWF Model for MODFLOW 6:

- The GWF Model includes a Newton flow formulation for handling cell wetting and drying that can occur in unconfined aquifers (Niswonger and others, 2011; Panday and others, 2013).
- The GWF Model can represent groundwater flow using a regular MODFLOW grid consisting of layers, rows, and columns, but the GWF Model also supports unstructured grids, following the approach implemented in Panday and others (2013).
- The GWF Model has a set of advanced stress packages for representing streams, lakes, multi-aquifer wells, and flow in the unsaturated zone.
- The GWF Model includes a rule-based approach to transfer water between the different stress packages. The approach is implemented in the Water Mover (MVR) Package (Morway and others, 2021) to transfer water from providers to receivers.
- Because of its object-oriented design a single GWF Model can contain multiple packages of the same type. This feature allows separate Well Package input files to be created for each well field, for example.

This report describes and documents a new Groundwater Transport (GWT) Model for MODFLOW 6. The GWT Model simulates three-dimensional transport of a single solute species in flowing groundwater. Simulation of changing solute concentrations requires the solution of a partial differential equation governing solute transport. The GWT Model solves the solute transport equation using numerical methods and a generalized control-volume finite-difference approach, which can be used with regular MODFLOW grids or with unstructured grids. The GWT Model is designed to work with most of the new capabilities released with the GWF Model, including the Newton flow formulation, unstructured grids, advanced packages, and the movement of water between packages. The GWF and GWT Models operate simultaneously during a MODFLOW 6 simulation to represent coupled groundwater flow and solute transport. The GWT Model can also run separately from a GWF Model by reading the heads (groundwater levels) and flows saved by a previously run GWF Model. The GWT model is also capable of working with the flows from another groundwater flow model, provided the flows from that model are written in the correct form to flow and head files.

The purpose of the GWT Model is to calculate changes in solute concentration in both space and time. Solute concentrations within an aquifer can change in response to multiple solute transport processes. These processes include (1) advective transport of solute with flowing groundwater, (2) the combined hydrodynamic dispersion processes of velocity-dependent mechanical dispersion and molecular diffusion, (3) sorption of solutes by the aquifer matrix either by adsorption to individual solid grains or by absorption into solid

grains, (4) transfer of solute into low permeability aquifer material (called an immobile domain) where it can be stored and later released, (5) first- or zero-order solute decay or production in response to chemical or biological reactions, (6) mixing with fluids from groundwater sources and sinks, and (7) direct addition of solute mass.

With the present GWT Model implementation, there can be multiple domains and multiple phases. There is a single mobile domain, which normally consists of flowing groundwater, and there can be one or more immobile domains. The GWT Model simulates the dissolved phase of chemical constituents in both the mobile and immobile domains. The dissolved phase is also referred to in this report as the aqueous phase. If sorption is represented, then the GWT Model also simulates the solid phase of the chemical constituent in both the mobile and immobile domains. The dissolved and solid phases of the chemical constituent are tracked in the different domains by the GWT Model and can be reported as output as requested by the user. There is no provision in the version of the GWT Model described here to calculate and track a vapor phase.

History

Numerical models are often used to simulate and predict the fate and transport of a dissolved chemical constituent in groundwater. These models range in complexity from simple particle tracking models to dispersive solute transport models. This section summarizes some of the popular particle tracking and solute transport models that have been developed for MODFLOW.

A first step in simulating and predicting the fate and transport of a dissolved chemical constituent is development and calibration of a groundwater flow model, such as MODFLOW, for the area of interest. If the objective of a transport investigation is merely to develop an understanding of groundwater flow directions and rates, then simple particle tracking methods can be used to simulate and predict predict groundwater travel times and paths. These groundwater travel times and paths are often a good first approximation of solute movement if the solute is conservative (it does not sorb or react with the aquifer) and transport is advection dominated such that hydrodynamic dispersion can be neglected. To this end, MODPATH offers a semi-analytical particle tracking method designed to work with simulated flows from a MODFLOW groundwater flow simulation. A recent version of MODPATH (Version 7), was designed to work with the simulated flows from MODFLOW 6, provided the model grid used for the flow simulation consisted of rectangular cells (Pollock, 2016) . Unstructured model grids consisting of quad-based refinement, such as quadpatch and quadtree grids, meet this criterion, and can be used with MODPATH Version 7. MODPATH Version 7 has several limitations that restrict its use with the GWF Model, including (1) simulated particle paths are not consistent with the Newton flow formulation if cells are dry, (2) the model grid used for flow must have rectangular cells, and (3) particles cannot be tracked through advanced model flow packages.

The USGS distributes a MODFLOW-based solute transport model, called the Groundwater Transport (GWT) Process. The GWT Process (not to be confused with the GWT Model for MODFLOW 6 described in this report) is implemented directly in MODFLOW-2000, and is referred to as MODFLOW-GWT. MODFLOW-GWT is based on the MOC2D (Konikow and Bredehoeft, 1978) and MOC3D (Konikow and others, 1996) programs and simulates advection, hydrodynamic dispersion, and simple reactions for a single chemical species. Winston and others (2018) document a volume-weighted particle tracking method for the most recent release of this solute transport model. MODFLOW-GWT has many advanced capabilities, including solute routing through lakes (Merritt and Konikow, 2000), streams (Prudic and others, 2004), and multi-node wells (Hornberger and Konikow, 2006). These advanced capabilities provided the impetus for many of the design features described in this report. MODFLOW-GWT does not work with some of the newer capabilities developed for MODFLOW, such as the Newton flow formulation and unstructured grids.

MT3D is another popular numerical model developed to simulate solute transport using flows from a MODFLOW simulation. MT3D is not implemented directly inside of MODFLOW. Rather, it reads heads and flows from a separate file that MODFLOW creates while the model is running. The flow and transport link file

has been updated over time to work with MODFLOW-2000 (Zheng and others, 2001) and newer MODFLOW versions. The original version of MT3D (Zheng, 1990) was a single species solute transport model, but MT3D was later extended to represent dual-domain transport and multiple chemical species under the MT3DMS name (Zheng and Wang, 1999) (where "MS" was added to indicate multiple species). Additional capabilities were added to MT3DMS to support more MODFLOW packages, simulate zero-order reactions, and solve for steady-state conditions, culminating in MT3DMS Version 5.3 (Zheng, 2010). MT3DMS has been widely used by consultants, academics, and government agencies to simulate complex groundwater transport problems. MT3DMS is used in other codes, such as SEAWAT, to solve the transport equation for variable-density flow problems (Guo and Langevin, 2002; Langevin and others, 2003, 2008), and RT3D and PHT3D to simulate reactive transport (Clement, 1997; Prommer and others, 2003). MT3DMS does not work with some of the newer capabilities developed for MODFLOW, such as the Newton flow formulation and unstructured grids.

Bedekar and others (2016) extended MT3DMS to work with the Newton flow formulation and transport in streams, lakes, and the unsaturated zone. Many other changes were also made as part of this extension, which resulted in a new version of the program called MT3D-USGS. At this time (2022), MT3D-USGS is continuing to receive updates and fixes in response to user requests. MT3D-USGS can be used with heads and flows from a MODFLOW 6 simulation with a GWF Model provided a regular MODFLOW grid is used for the flow simulation. MT3D-USGS cannot be used to simulate transport within the flow domains represented by the advanced stress packages of the GWF Model.

MODFLOW-USG is a popular unstructured grid version of MODFLOW (Panday and others, 2013) that can be used with regular MODFLOW grids or flexible unstructured grids. MODFLOW-USG has a robust Newton flow formulation for solving difficult unconfined aquifer problems, and it has the Connected Linear Network (CLN) Process for simulating flow in boreholes, fractures, and conduits. Since its release by the USGS, MODFLOW-USG has been updated to include many new capabilities, including the addition of a generalized control-volume solute transport model (Panday, 2020). The solute transport model in MODFLOW-USG runs concurrently with the flow model to simulate the fate and transport of multiple chemical species in response to advection, hydrodynamic dispersion, sorption, and zero- or first-order growth and decay. Many of the features and concepts developed for MODFLOW-USG have provided the foundation for the GWF and GWT Models in MODFLOW 6.

Overview of the Groundwater Transport Model

The GWT Model documented here builds on the successes of previous solute transport models and takes advantage of design and solver advances implemented in the MODFLOW 6 framework. Following the modular concepts developed by earlier MODFLOW developers, the GWT model is highly extensible so that new capabilities and packages can be added in the future. Because the GWT Model is part of the broader MODFLOW 6 framework, it conforms to a consistent design that should make it look, feel, and operate like the GWF Model and other models being developed for the framework. As the MODFLOW 6 framework evolves and new enhancements are made, these enhancements will also apply to the GWT Model.

The GWT Model works with the heads and flows generated by the GWF Model. These simulated heads and flows can be passed through memory from the GWF Model to a GWT Model running concurrently as part of a single MODFLOW 6 simulation. Alternatively, a GWF Model can be run first to save simulated heads and flows to binary files. Then, a second MODFLOW 6 simulation with a GWT Model can be used to represent solute transport, using the saved heads and flows from the first simulation with the GWF Model. There are advantages and disadvantages to both approaches.

For the single-simulation use case, a GWT Model will run within a MODFLOW 6 simulation in conjunction with a GWF Model (see figure 1–1a). The GWF Model will calculate heads and flows, which are made available to the GWT Model through the GWF-GWT Exchange. Time stepping is controlled by the Temporal Discretization (TDIS) Package. Heads and flows are calculated for the GWF Model by the Iterative Model

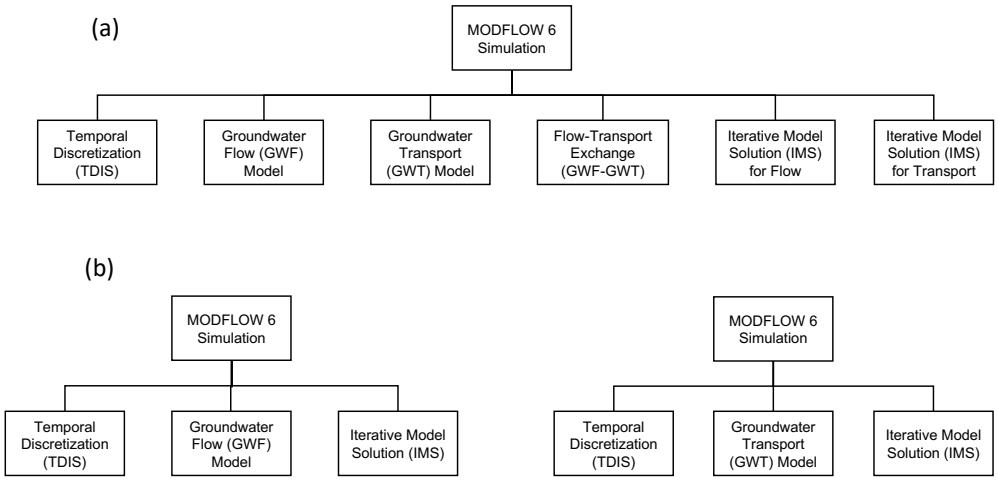

Figure 1–1. Structure of a MODFLOW 6 simulation. (a) Flow and transport models are part of the same simulation. (b) Flow and transport models are in separate simulations. In this case with separate simulations, GWF Model flows are saved to a binary file, which is read as input to the transport model.

Solution (IMS). A second IMS is used to solve for concentration and solute fluxes of the GWT Model. Alternatively, the GWF and GWT Models can be run as separate simulations (figure 1–1b). In this case, the user runs the GWF Model first and saves all heads and flows for every time step to binary files. The user then runs the GWT Model, which reads the heads and flows as input.

The GWT Model described in this report is divided into "packages." A package is a part of the model that deals with a single aspect of simulation. For example, the Advection Package simulates the transport process of advection, and the Dispersion Package simulates the transport processes of mechanical dispersion and molecular diffusion. Some packages are always required for a simulation, whereas other packages are only activated if their capabilities are needed for a particular application.

The GWT Model is comprised of the packages shown in figure 1–2. The packages shown on the left of figure 1–2 are used to provide data to the model, such as discretization information, initial concentrations, the frequency and type of output to save, locations and types of observations to save, and information on how the GWT Model interfaces with the GWF Model. These data input packages do not represent transport processes, but are needed to provide information for the GWT Model. The remaining packages shown in figure 1–2 are separated into mobile domain and immobile domain packages. The mobile domain represents the "fast" part of the groundwater system in which a dissolved constituent is transported through an aquifer with flowing groundwater. The immobile domain represents the "slow" part of the system in which groundwater movement can be considered negligible. Solute mass can move between the mobile and immobile domains in response to a transfer coefficient and the concentration difference between the mobile and immobile domains. A unique aspect of the GWT Model described here is that there can be any number of immobile domains, each with their own transfer coefficients, immobile domain porosity values, sorption and decay parameters, and calculated concentrations. The mobile domain has packages for representing solute sources and sinks, the direct addition of solute mass, and the specification of constant concentration conditions. Both the mobile and immobile domains have packages for entering properties for internal transport (such as porosity, and sorption and decay parameters). Specification of one or more immobile domains is optional; however, most simulations will require specification of mobile domain packages.

The various packages of the GWT Model documented in this report, the shortened character abbreviation used for each package, and the package category are listed in table 1–1.

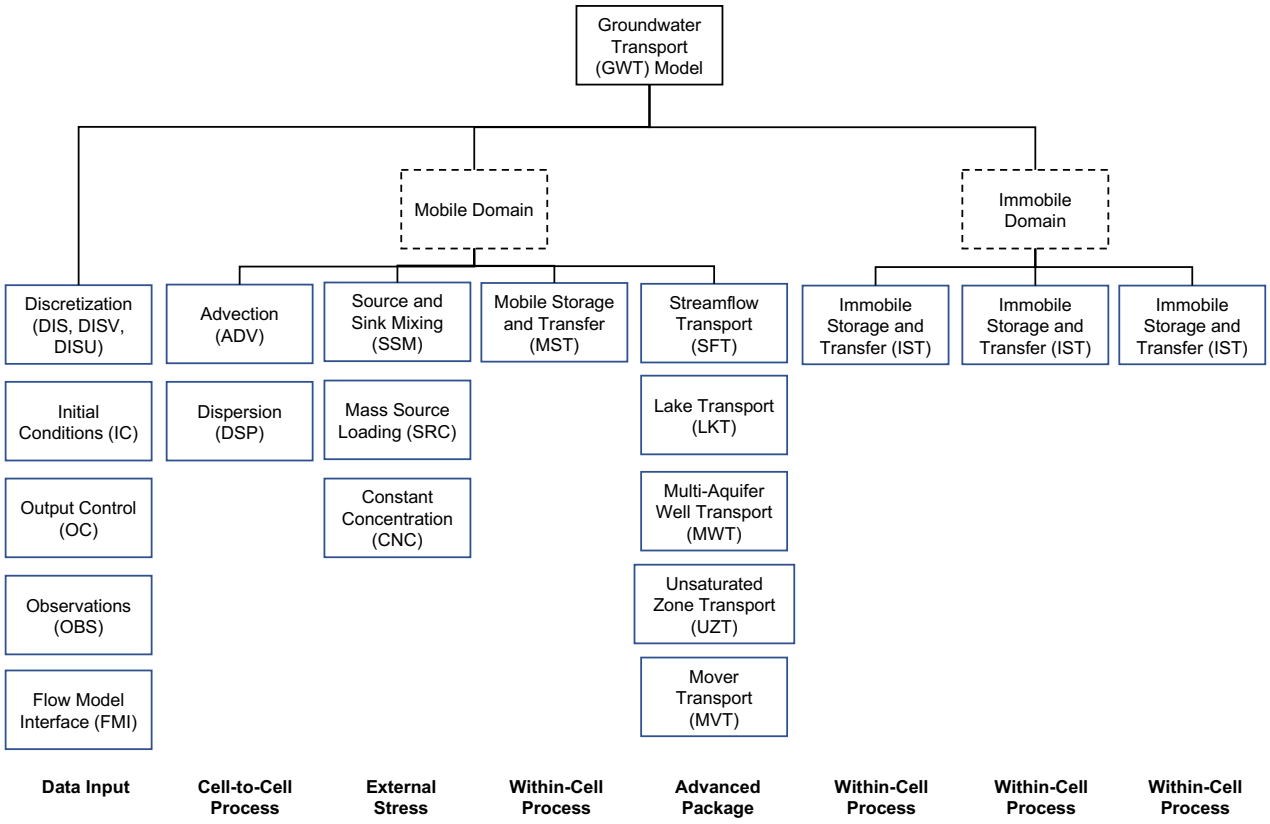

Figure 1–2. Domains and packages for the MODFLOW 6 Groundwater Transport (GWT) Model. There are three Immobile Storage and Transfer (IST) Packages shown here, however, the user can include as many IST Packages as needed for a model simulation.

Table 1–1. List of packages available for use with the Groundwater Transport Model.

Package Name	Abbreviation	Package Category
Spatial Discretization	DIS, DISV, or DISU	Data Input
Initial Conditions	IC	Data Input
Model Observations	OBS	Data Input
Output Control	OC	Data Input
Flow Model Interface	FMI	Data Input
Advection	ADV	Cell-to-Cell Process
Dispersion	DSP	Cell-to-Cell Process
Source-Sink Mixing	SSM	External Stress
Mass Source Loading	SRC	External Stress
Constant Concentration	CNC	External Stress
Mobile Storage and Transfer	MST	Within-Cell Process
Immobile Storage and Transfer	IST	Within-Cell Process
Streamflow Transport	SFT	Advanced Package
Lake Transport	LKT	Advanced Package
Multi-Aquifer Well Transport	MWT	Advanced Package
Unsaturated Zone Transport	UZT	Advanced Package
Mover Transport	MVT	Advanced Package

Information for Existing Solute Transport Modelers

The MODFLOW 6 GWT Model contains most of the functionality of MODFLOW-GWT, MT3DMS, MT3D-USGS and MODFLOW-USG. The following list summarizes major differences between the GWT Model in MODFLOW 6 and previous MODFLOW-based solute transport programs.

1. The GWT Model simulates transport of a single chemical species; however, because MODFLOW 6 allows for multiple models of the same type to be included in a single simulation, multiple species can be represented by using multiple GWT Models. A clear advantage of this design is that each chemical species has a dedicated GWT Model. The flexibility allows all transport input parameters to be specified separately for each species, including initial conditions, boundary conditions, output frequency, and so forth. A disadvantage of this approach is that the present implementation requires separate memory for each GWT Model, which may not be efficient.

2. There is no specialized flow and transport link file (Zheng and others, 2001) used to pass the simulated groundwater flows to the transport model, as is required by MT3D. Instead, simulated flows from the GWF Model are passed in memory to the GWT Model while the program is running. Alternatively, the GWT Model can read the standard binary head and flow files saved by the GWF Model during a preceding flow simulation. If the user intends to simulate transport through the advanced stress packages and Water Mover Package, then flows from these advanced packages must also be saved to binary files. Names for these binary files are provided as input to the Flow Model Interface (FMI) Package.

3. The GWT Model is based on a generalized control-volume finite-difference method, which means that solute transport can be simulated using regular MODFLOW grids (specified with the DIS Package), which consist of layers, rows, and columns, or unstructured MODFLOW grids (specified with the DISV or DISU Packages; table 1–1).

4. Advection can be simulated using central-in-space weighting, upstream weighting, or an implicit second-order Total Variation Diminishing (TVD) scheme. The GWT Model does not have the Method of Characteristics (particle-based approaches) or an explicit TVD scheme. Consequently, the GWT Model may require a higher level of spatial discretization than other transport models that use higher order terms for advection dominated groundwater systems. This can be an important limitation for some problems, which require the preservation of sharp solute fronts.

5. Variable-density flow and transport can be simulated by including a GWF Model and a GWT Model in the same MODFLOW 6 simulation. The Buoyancy Package should be activated for the GWF Model if density variations are expected to affect groundwater flow so that fluid density is calculated as a function of simulated concentration. If more than one chemical species is represented then the Buoyancy Package allows the simulated concentration for each species to be used in the density equation of state. Langevin and others (2020) describe the hydraulic-head formation that is implemented in the Buoyancy Package for variable-density groundwater flow and present results from MODFLOW 6 variable-density simulations. The variable-density capabilities available in MODFLOW 6 replicate and extend the capabilities available in SEAWAT to include, for example, the Newton flow formulation for unconfined aquifers, transport through advanced packages, and transport using unstructured grids.

6. The GWT model includes the MST and IST Packages (fig. 1–2). These two packages collectively comprise the capabilities of the MT3DMS Reaction Package.

7. The MST Package supports the linear isotherm for representation of sorption as well as the nonlinear Freundlich and Langmuir isotherms. The MST Package described in this report does not support the nonequilibrium sorption model that is available in MT3DMS. The IST Package supports only linear sorption.

8. The GWT Model was designed so that the user can specify as many immobile domains as necessary to represent observed contaminant transport patterns and solute breakthrough curves. The effects of an immobile domain are represented using the IST Package, and the user can specify as many IST Packages as necessary.

9. The GWT Model documented in this report does not support kinetic reactions between species, a feature that is available in MT3D-USGS. Interactions between species in separate GWT Models is an option that may be developed in the future through a GWT-GWT Exchange.

10. There is no option to automatically run the GWT Model to steady state using a single time step. This is an option available in MT3DMS (Zheng, 2010). Steady-state conditions must be determined by running the transport model under transient conditions until solute concentrations stabilize.

11. The GWT Model described in this report is capable of simulating solute transport in the advanced stress packages of MODFLOW 6, including the Lake, Streamflow Routing, Multi-Aquifer Well and Unsaturated Zone Transport Packages (Langevin and others, 2017). Solute transport between these advanced packages is also supported, such as the transport of solute from a stream into a lake. The present implementation simulates solute advection between package features, such as between two stream reaches, but dispersive transport between package features is not represented. Similarly, solute transport between the advanced packages and the aquifer is only through advection.

12. There are many other differences between the MODFLOW 6 GWT Model and other solute transport models that work with MODFLOW, especially with regards to program design and input and output.

MODFLOW 6 input and output are described in a separate user guide, which is included with the distribution. A full suite of test and example problems for the GWT Model is also included with the software distribution available on the internet for download.

Organization and Scope of This Report

This report documents the GWT Model for MODFLOW 6 and contains the underlying mathematical equations and fundamental concepts. The report focuses on foundational equations and concepts that are expected to persist even as new versions of the model are released. Equations and concepts that may change as the program evolves are mentioned only briefly here, and users should consult the release notes and supplementary information that is distributed with MODFLOW 6. Likewise, instructions for preparing input files, running the model, and post-processing the results are not included in this report. Instead, user input instructions are provided as a separate document with the program distribution. Distributing the input instructions separately allows them to evolve and change with the program as new options are added. In some instances, users may need to refer to additional reports that describe new capabilities added to MODFLOW 6, including capabilities to simulate additional solute transport processes. The MODFLOW 6 distribution also includes a rich set of example problems for the GWT Model. These example problems contain problem descriptions and model input files so that users can run the examples and evaluate the results.

This report is organized as follows. Chapter 2 describes the derivation of the control-volume finite-difference (CVFD) equation upon which the GWT Model is based. Chapter 3 describes the Mobile Storage and Transfer (MST) Package, which calculates changes in solute storage, sorption, and solute growth and decay processes. Chapter 4 describes the equations and approaches for simulating the transport of solute due to advection and dispersion. Chapter 5 describes the representation of simple solute sources and sinks, which can be represented with the Constant Concentration (CNC) Package, the Source and Sink Mixing (SSM) Package for sources and sinks associated with the groundwater flow model, and the mass source loading (SRC) Package, which represents the direct addition of solute mass to a model cell. Chapter 6 describes the advanced package transport capabilities, which can be used to simulate solute transport in streams, lakes, multi-aquifer wells, and in the unsaturated zone. Chapter 7 describes the Immobile Storage and Transfer (IST) Package, which can be used to represent one or more immobile domains embedded within the aquifer. These domains may correspond to silt or clay lenses, for example, that can store or release solute mass from or to the mobile domain. The GWT Model packages documented in this report are those listed in table 1–1.

Chapter 2. Formulation and Solution of the Control-Volume Finite-Difference Equation

The groundwater transport equation in MODFLOW 6 is discretized using a control-volume finite-difference (CVFD) method. This chapter describes the mathematical equations discretized in the GWT model, discretization options, and the general forms of the finite-difference equations used to simulate solute transport within an aquifer.

Mathematical Model

Transport of a solute dissolved in groundwater is described mathematically by a partial differential equation that represents the conservation of solute mass (Konikow and Grove, 1977; Zheng and Bennett, 2002). At any location, the accumulation of solute mass is equal to the difference between mass entering and mass leaving a specified volume of aquifer. Such an equation can be written in a variety of different forms, including the following form (eq. 2–1), which includes the transport mechanisms represented by the GWT Model:

$$\begin{aligned}\frac{\partial \left(S_w \theta C\right)}{\partial t} &= -\nabla \cdot (\mathbf{q}C) + \nabla \cdot (S_w \theta \mathbf{D} \nabla C) + q_s' C_s + M_s - \lambda_1 \theta S_w C - \gamma_1 \theta S_w \\ &- f_m \rho_b \frac{\partial \left(S_w \overline{C}\right)}{\partial t} - \lambda_2 f_m \rho_b S_w \overline{C} - \gamma_2 f_m \rho_b S_w - \sum_{im=1}^{nim} \zeta_{im} S_w \left(C - C_{im}\right),\end{aligned} \tag{2–1}$$

where S_w is the water saturation (dimensionless) defined as the volume of water per volume of voids, θ is the effective porosity of the mobile domain (dimensionless), defined as volume of voids participating in mobile transport per unit volume of aquifer, C is volumetric concentration of the mobile domain expressed as mass of dissolved solute per unit volume of fluid (M/L^3), t is time (T), $\mathbf{q}$ is the vector of specific discharge (L/T), $\mathbf{D}$ is the second-order tensor of hydrodynamic dispersion coefficients (L^2/T), q_s' is the volumetric flow rate per unit volume of aquifer (defined as positive for flow into the aquifer) for mass sources and sinks ($1/T$), C_s is the volumetric solute concentration of the source or sink fluid (M/L^3), M_s is rate of solute mass loading per unit volume of aquifer (M/L^3T), λ_1 is the first-order decay rate coefficient for the liquid phase ($1/T$), γ_1 is the zero-order decay rate coefficient for the liquid phase (M/L^3T), f_m is the fraction of aquifer solid material available for sorptive exchange with the mobile phase under fully saturated conditions, ρ_b is the bulk density of the aquifer material (M/L^3), $\overline{C}$ is the sorbed concentration of solute mass in the mobile domain (M/M), λ_2 is the first-order decay rate coefficient ($1/T$) for the sorbed phase of the mobile domain, γ_2 is the zero-order decay rate coefficient for the sorbed phase of the mobile domain (M/MT), nim is the number of immobile domains, ζ_{im} is the rate coefficient for the transfer of mass between the mobile domain and immobile domain im ($1/T$), and C_{im} is the solute concentration for immobile domain im (M/L^3).

Equation 2–1 can be rewritten in the following manner to correspond to the design of the GWT Model (see table 1–1 for package names and abbreviations).

$$\begin{aligned}&\underbrace{-\frac{\partial \left(S_w \theta C\right)}{\partial t} - f_m \rho_b \frac{\partial \left(S_w \overline{C}\right)}{\partial t} - \lambda_1 \theta S_w C - \gamma_1 \theta S_w - \lambda_2 f_m \rho_b S_w \overline{C} - \gamma_2 f_m \rho_b S_w}_{MST} \\ &\underbrace{-\nabla \cdot (\mathbf{q}C)}_{ADV} \underbrace{+\nabla \cdot (S_w \theta \mathbf{D} \nabla C)}_{DSP} \underbrace{+q_s' C_s}_{SSM} \underbrace{+M_s}_{SRC} \underbrace{- \sum_{im=1}^{nim} \zeta_{im} S_w \left(C - C_{im}\right)}_{IST} = 0.\end{aligned} \tag{2–2}$$

In this form (eq. 2–2), the terms have been grouped and labeled according to the GWT transport package that represents their effects. The effects of solute storage, sorption, and decay on the mobile domain are represented with the Mobile Storage and Transfer (MST) Package. The effects of advection are represented with the Advection (ADV) Package. The effects of hydrodynamic dispersion, which includes mechanical dispersion and molecular diffusion, are represented by the Dispersion (DSP) Package. Groundwater inflow and outflow from stress packages in the flow model are represented with the Source and Sink Mixing (SSM) Package. The direct loading of solute mass can be represented with the Mass Source Loading (SRC) Package (table 1–1). The effects of a diffusive exchange between the mobile domain and an immobile domain is represented with the Immobile Storage and Transfer (IST) Package or multiple instances of the IST Package if the intent is to represent multiple immobile domains.

Separating the transport equation in the manner described above is a common way of breaking the problem into individual terms that can be addressed independently of one another. Zheng (1990) and Zheng and Wang (1999) were among the first to write the transport equation in this manner, which allowed them to write "packages" to solve the individual terms. Their approach built on the MODFLOW concept of a package, which makes it relatively easy for a user to learn about individual processes, turn packages on and off, and develop new packages. A simplified form of equation 2–2 is

$$f^{MST} + f^{ADV} + f^{DSP} + f^{SSM} + f^{SRC} + f^{IST} = 0, \tag{2–3}$$

where

$$\begin{aligned}
f^{MST} &= -\frac{\partial \left(S_w \theta C\right)}{\partial t} - f_m \rho_b \frac{\partial \left(S_w \overline{C}\right)}{\partial t} - \lambda_1 \theta S_w C - \gamma_1 \theta S_w - \lambda_2 f_m \rho_b S_w \overline{C} - \gamma_2 f_m \rho_b S_w \\
f^{ADV} &= -\nabla \cdot (\mathbf{q} C) \\
f^{DSP} &= \nabla \cdot (S_w \theta \mathbf{D} \nabla C) \\
f^{SSM} &= q_s' C_s \\
f^{SRC} &= M_s \\
f^{IST} &= -\sum_{im=1}^{nim} \zeta_{im} S_w \left(C - C_{im}\right).
\end{aligned} \tag{2–4}$$

Control-Volume Finite-Difference Method

Equation 2–1, together with initial conditions and any relevant boundary conditions, represents mathematically the solute mass balance at any point in the model domain. In certain simple cases, equation 2–1 can be solved analytically to obtain a mathematical expression for the distribution of solute concentration throughout a model domain. For models of real-world field sites, which tend to be too complex to solve analytically, numerical solutions are often sought. Using the CVFD method, MODFLOW 6 discretizes the model domain into cells. The balance of solute mass is formulated for each model cell, taking into account the flows of solute to and from neighboring cells by advection and dispersion, as well as external sources and sinks. Taken together, the solute mass balance equations for all the cells form a system of linear equations that is solved iteratively using a linear matrix solver. Details of the CVFD implementation in the GWT Model are described below.

Characteristics of a Model Cell

As described by Langevin and others (2017) a MODFLOW 6 groundwater model cell is a prism with vertical sides and a horizontal top and bottom. An example of a groundwater model cell, with the size of individual sediment grains exaggerated to illustrate porosity concepts, is shown in figure 2–1. The area of cell n in plan view is defined as A_n. The top and bottom cell elevations are defined as TOP_n and BOT_n, respectively, and the head in the cell is defined as h_n. The total volume of the cell, including the solid and void space, is defined as

$$V_{cell} = A_n \left(TOP_n - BOT_n \right). \tag{2–5}$$

Equation 2–5 is used to calculate cell volume in MODFLOW 6 instead of one based on cell widths and depths, because although cells are prisms, they can have shapes other than rectangles in plan view. The volume of void space (V_{void}) and the volume of space occupied by solids (V_{solid}) within a cell is related to porosity by

$$\theta = \frac{V_{void}}{V_{cell}} = \frac{V_{void}}{(V_{void} + V_{solid})}. \tag{2–6}$$

In this context, porosity is intended to represent the pores available for mobile transport, also referred to as the effective porosity. This effective porosity is different from the immobile domain porosity, which is defined in chapter 7 “Immobile Domain Storage and Transfer”. Unless stated otherwise, porosity refers to effective porosity.

The volume of water is related to the cell saturation, S_w, which is calculated by the flow model. When a cell is fully saturated, it has a saturation of one, which means all of the pore space is filled with water. When a cell is completely dry, it has a saturation of zero. When a cell is partially saturated, the saturation is assumed to depend on the head value within the cell as

$$S_w = \frac{h - BOT}{(TOP - BOT)}. \tag{2–7}$$

If the Newton-Raphson formulation is used in the flow model, then the equation for cell saturation is slightly different in that the transitions from fully saturated to partially saturated and from partially saturated to dry are smoothed (Langevin and others, 2017).

From these equations, the volume of water in a cell, V_w, is expressed as

$$V_w = \theta V_{cell} S_w. \tag{2–8}$$

The volume of water in a cell may change during the simulation in response to inflows and outflows, as calculated by the flow model. An inherent assumption in the approximation of the volume of water in a cell using this approach is that the aquifer porosity does not change with time. As noted by Goode (1990), this is not strictly correct, because changes in head and the corresponding change in the volume of water in storage is normally associated with a change in porosity. The GWT Model, however, does not explicitly account for the change in aquifer porosity that results from water being added to or released from storage.

Control-Volume Finite-Difference Equation

A general solute mass balance equation for a model cell n can be written as

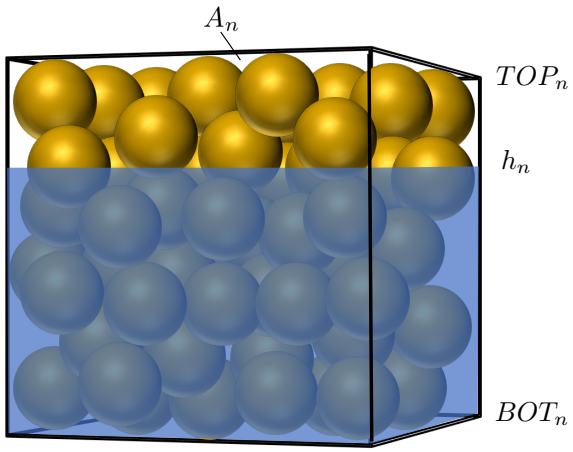

Figure 2–1. Porous media model cell that is partially saturated. The area of cell n in plan view is A_n; the cell top and bottom elevations are TOP_n and BOT_n, respectively; and h_n is the head (water level) in the cell. Above the water level, the cell is considered to be unsaturated.

$$\dot{M}_n^{MST} + \dot{M}_n^{ADV} + \dot{M}_n^{DSP} + \dot{M}_n^{SSM} + \dot{M}_n^{SRC} + \dot{M}_n^{IST} + \dot{M}_n^{FMI} + \dot{M}_n^{APT} = 0, \tag{2–9}$$

where $\dot{M}_n^{MST}$ is the rate of change of solute mass in the cell due to storage, sorption, and decay; $\dot{M}_n^{ADV}$, $\dot{M}_n^{DSP}$, $\dot{M}_n^{SSM}$ are the net rates at which solute mass flows into or out of the cell due to advection, dispersion, and mixing from external groundwater fluid sources and sinks, respectively; $\dot{M}_n^{SRC}$ is the rate of solute mass loading added directly to a cell; and $\dot{M}_n^{IST}$ is the rate of change of solute mass in the cell due to exchange with an immobile domain. Equation 2–9 contains two additional terms, $\dot{M}_n^{FMI}$ and $\dot{M}_n^{APT}$, which are not represented in equations 2–1 and 2–2. These terms represent the addition or subtraction of solute mass to or from a cell to account for errors in the flow solution and exchange with an advanced package, respectively. All of the terms in equation 2–9 have dimensions of M/T. The sign convention is chosen for equation 2–9 using a simple "change in storage is equal to inflow minus outflow" equation such that the addition of solute to a cell is positive and the subtraction (removal) of solute from a cell is negative. When expressed in this form, the $\dot{M}_n^{MST}$ term is the net rate at which solute mass enters the cell from groundwater storage and the sorbed phase and due to decay or production. A negative value for $\dot{M}_n^{MST}$ indicates a net uptake of solute mass into groundwater storage and the sorbed phase and by decay or production.

The advection and dispersion terms in equation 2–9 involve the transfer of solute mass between adjacent model cells. These terms require an expression for the flow of solute mass, $F_{n,m}$, between two adjacent cells, n and m. $F_{n,m}$ has dimensions of M/T and is positive when flow is from cell m and into cell n.

For the advection term, the net rate at which solute mass is entering or leaving cell n is the sum of the advective flows of solute mass between cell n and each of its neighbors:

$$\dot{M}_n^{ADV} = \sum_{m \in \eta_n} F_{n,m}^{ADV}, \tag{2–10}$$

where η_n is the set of neighbors of (cells connected to) cell n, and $F_{n,m}^{ADV}$ is the advective flow rate of solute mass (M/T) into cell n from cell m (the rates are positive for flow into cell n from cell m). Alternative formulations for $F_{n,m}^{ADV}$ are discussed in chapter 4.

The $\dot{M}_n^{DSP}$ term of equation 2–9 is the net rate at which solute mass is entering or leaving cell n due to hydrodynamic dispersion. This term is the sum of the hydrodynamic dispersive flows of solute mass between cell n and each of its surrounding cells:

$$\dot{M}_n^{DSP} = \sum_{m \in \eta_n} F_{n,m}^{DSP}, \tag{2–11}$$

where $F_{n,m}^{DSP}$ is the dispersive flow rate of solute mass (M/T) into cell n from cell m. Alternative formulations for $F_{n,m}^{DSP}$ are discussed in chapter 4.

All of the terms in equation 2–9 are discussed in more detail in subsequent chapters of this report.

Numerical Solution

Solution of the system of solute transport equations relies on the MODFLOW 6 framework described by Hughes and others (2017), which is customized to solve generalized CVFD equations in which a cell can be connected to any number of surrounding cells. The CVFD equation for solute transport can be written for model cell n as

$$A_{n,n}C_n + \sum_{m \in \eta_n} A_{n,m}C_m = b_n, \tag{2–12}$$

where $A_{n,n}$ is the coefficient (L^3/T) for the concentration in cell n, $A_{n,m}$ is the coefficient (L^3/T) for the concentration in cell m, a neighbor of cell n, C_n and C_m are the concentrations (M/L^3) in cells n and m, respectively, and b_n is the right-hand-side value of the balance equation (M/T). The summation term in equation 2–12 is written in a general way to indicate that the balance equation for cell n may depend on the concentrations in any number of surrounding cells. The set of cells surrounding cell n is denoted by η_n. The terms in equation 2–12 are assembled by the GWT Model piece-by-piece as each package adds contributions to the coefficients and right-hand-side terms. Once all of the assembly routines are complete, the concentration coefficients and the right-hand-side term in equation 2–12 are the sum of the contributions from the different packages. For example, the $A_{n,m}$ term may contain contributions from both the advection and dispersion packages. These contributions are described in detail in subsequent chapters on the different transport packages.

The solute balance equation in the GWT Model is written using an implicit formulation in which the concentrations in equation 2–12 represent values at the end of the time step. This approach means that the concentration values in equation 2–12 are unknown and must be solved simultaneously. The implicit formulation is often preferred over an explicit formulation, because it is generally stable and allows for relatively large time steps. Use of an explicit formulation would require a relatively small time step and flow expressions that use known concentrations from the end of the previous time step so that equation 2–12 could be solved directly.

Equation 2–12 is the solute balance equation for a single model cell. Application of this balance equation to every cell in the model grid results in a system of equations that can be expressed in matrix form as

$$\mathbf{AC} = \mathbf{b}. \tag{2–13}$$

In equation 2–13, $\mathbf{A}$ is a sparse square matrix with the number of rows and columns equal to the number of cells. $\mathbf{C}$ is a vector of cell concentrations with the number of entries equal to the number of cells. $\mathbf{b}$ is the right-hand-side vector also with the length equal to the number of cells. The number of cells here refers to the number of cells in the model grid plus the number of features represented with advanced packages. Depending

on the options selected by the user, the $\mathbf{A}$ matrix may be symmetric or asymmetric, which affects the type of linear solution methods that can be used. For some GWT Model applications, equation 2–13 is linear in that $\mathbf{A}$ and $\mathbf{b}$ are independent of the dependent variable $\mathbf{C}$. However, in many applications $\mathbf{A}$ and $\mathbf{b}$ depend on concentration, and the balance equation is, therefore, nonlinear. In such cases, solution of equation 2–13 must be repeated multiple times, each time with updated coefficients and right-hand-side values, until solution convergence is achieved.

Initial Conditions

Starting concentrations are required as input for all cells in the model grid. These starting concentrations represent the initial solute condition for the aquifer system. If one or more immobile domains are included in the model, then starting concentrations for each immobile domain are also required. Starting concentrations for the mobile domain are entered in the Initial Conditions (IC) Package. Starting concentrations for each immobile domain are specified in each IST Package.

Flow Model Interface

For most applications, the GWT Model is intended to work with a corresponding GWF Model. The GWF Model calculates (1) heads for all active model cells, (2) flows between all connected model cells, (3) flows between model cells and stress features, and (4) rates of storage changes in model cells. Flows calculated by the GWF model represent volumetric flow rates with dimensions of L^3/T. The FMI Package is used within the GWT Model to provide calculated groundwater flows. These calculated groundwater flows may come from a corresponding GWF Model that is run concurrently in the same simulation as the GWT Model, or the flows may be read from a file that was created from a previous GWF simulation or from some other program that is capable of writing files in the correct format.

Flow Imbalance Correction

The GWT Model of MODFLOW 6 uses numerical methods to solve for the water balance of a model cell. In most cases, there will be a small residual flow error Q^e for a cell, which can be controlled through the tolerances specified for the numerical solution. When Q^e is zero, the inflows and outflows for the cell are perfectly balanced. If Q^e is nonzero and flow into a model cell is greater than the outflow for the cell, then the calculated concentration may increase erroneously. Likewise, if the simulated flow out of a cell is larger than the flow into a cell, then calculated concentrations may erroneously decrease. In most cases, these small errors are inconsequential and go unnoticed. These errors can become more apparent in the results when simulated concentrations are larger or smaller than surrounding cell and boundary concentrations. In some situations, these errors can grow over time and complicate interpretation of calculated concentrations.

Panday and others (2018) developed a simple approach to help minimize the effects of these flow imbalance errors. The approach works by simply adding or removing solute mass at a rate equal to the product of the residual flow error Q_e and the calculated cell concentration,

$$\dot{M}_n^{FMI} = Q_n^e C_n. \tag{2–14}$$

In effect, the residual flow error is treated as a source or sink with the concentration equal to the calculated cell concentration. To represent this addition or subtraction of solute mass in the system of equations, the $\mathbf{A}$ coefficient matrix is updated as

$$A_{n,n} \leftarrow A_{n,n} - Q_n^e. \tag{2–15}$$

For most solute transport applications, the flow model is solved with sufficient accuracy that the residual flow error Q_e for a cell is so small as to not have a noticeable effect on the calculated concentration. In some cases, however, this optional correction available in the FMI Package can improve the accuracy of calculated concentrations, improve model stability, and minimize the presence of calculated concentrations that are above or below expected values (Panday and others, 2018).

Time Stepping

For the present implementation of the GWT Model, all terms in the solute transport equation are solved implicitly. With the implicit approach applied to the transport equation, it is possible to take relatively large time steps and efficiently obtain a stable solution. If the time steps are too large, however, accuracy of the model results will decline, so there is usually some compromise required between the desired level of accuracy and length of the time step. If an explicit method were to be added to the GWT Model in the future, such as the Method of Characteristics approach for solving the advection term, then time-step constraints would likely be required to ensure numerical stability.

In MODFLOW 6, time step lengths are controlled by the user and specified in the Temporal Discretization (TDIS) input file. When the flow model and transport model are included in the same simulation, then the length of the time step specified in TDIS is used for both models. If the GWT Model runs in a separate simulation from the GWF Model, then the time steps used for the transport model can be different, and likely shorter, than the time steps used for the flow solution. Instructions for specifying time steps are included in the input and output guide that is distributed with the MODFLOW 6 software.

Special Considerations for Dry Cells

There are special considerations for handling dry model cells. The MODFLOW 6 GWF Model has two alternatives for handling dry cells. With the traditional MODFLOW approach, a cell becomes dry when the calculated head is below the cell bottom. When this drying happens, the cell is marked as dry and is removed from flow calculations. In MODFLOW 6, a dry cell is assigned a special head value by the GWF Model. The GWT Model checks for this dry cell value and, if present, removes the cell from the transport calculations. Dry cells can be reactivated by the GWF Model if the rewetting option is selected by the user and if calculated heads in surrounding cells meet certain criteria (McDonald and others, 1992). The GWT Model checks to see if a dry cell has rewet, and will reactivate that cell for transport calculations if that situation is encountered. This procedure for handling dry model cells is consistent with the approach implemented in MT3DMS (Zheng, 1990; Zheng and Wang, 1999) and MT3D-USGS (Bedekar and others, 2016).

MODFLOW also has a Newton approach for handling dry cells (Painter and others, 2008), which has become the preferred approach for simulating aquifers with unconfined conditions. With the Newton approach, cells remain active, even if they are dry. Dry cells have calculated heads that are at or beneath the cell bottom elevation. Although cells with heads below the cell bottom are dry, they can still transmit water to underlying cells that are not dry. This vertical transmission happens instantaneously, as there is no water storage within a dry cell. The Newton approach is available in MODFLOW-NWT (Niswonger and others, 2011), MODFLOW-USG (Panday and others, 2013), and MODFLOW 6 (Langevin and others, 2017).

Bedekar and others (2016) implemented a method in MT3D-USGS to route solute mass through cells with a calculated head below the cell bottom. The method works by inactivating these dry cells in the transport model and accumulating mass fluxes in all overlying cells and then passing this mass directly to the high-

est cell that is not dry. The method has been shown to work for complicated groundwater modeling problems involving many dry cells (Bedekar and others, 2016).

The MODFLOW 6 GWT Model handles transport through dry cells in a different manner than MT3D-USGS. Instead of deactivating dry cells for solute transport, these cells remain active and a balance equation is solved. Because there is no water in the cell, and thus, there is no solute mass in the cell, the balance equation reduces to a steady state form in which all solute mass coming into the cell instantaneously exits the cell. Thus, for Newton models with dry cells, solute mass entering a dry cell is instantaneously transmitted down to the uppermost cell that is not dry. Because the calculated head is below the cell bottom for these cells, the calculated saturation is zero. Thus, whereas there may be an advective flux of solute through these model cells, there is no dispersive flux as the dispersive flux equation contains a saturation term (eqn. 4–17). The advantage of this approach is that solute transmission through dry cells is calculated as part of the matrix equations, rather than requiring a separate accumulation step. A disadvantage of this approach is that the calculated concentrations in these dry cells are meaningless, and should be removed as part of a post-processing step. This approach, as implemented in MODFLOW 6, has proven stable and robust for a variety of problems, including transport through an aquifer system with perched conditions (Keating and Zyvoloski, 2009), and a complicated water-table fluctuation problem reported by Langevin and others (2020).

Chapter 3. Mobile Storage and Transfer

The Mobile Storage and Transfer (MST) Package of the GWT Model for MODFLOW 6 represents solute mass storage, sorption, and first- or zero-order decay. The mathematical expression for these terms is grouped in equation 2–4 as f^{MST}. To isolate and describe these processes, the f^{MST} term is expanded as

$$f^{MST} = f^{storage} + f^{sorption} + f^{decay} + f^{decaysorbed}. \tag{3–1}$$

This chapter describes the mathematical expressions for these individual terms and shows how the terms are added to the system of equations. Because this chapter does not include equations describing flow between cells, for example, between cells n and m, the n subscript is not included for cell variables.

Storage

The $f^{storage}$ term in equation 3–1 describes the rate of change of dissolved solute mass as

$$f^{storage} = -\frac{\partial \left(S_w \theta C\right)}{\partial t}. \tag{3–2}$$

The backward-in-time finite-difference approximation of equation 3–2 for a model cell is

$$\dot{M}^{storage} = -\frac{C^{t+\Delta t} V_w^{t+\Delta t} - C^t V_w^t}{\Delta t}, \tag{3–3}$$

where t is time (T), Δt is the length of the transport time step (T), C is the solute concentration (M/L^3), and V_w is the volume of water in the cell (L^3). Superscripts indicate the discrete time level at which each quantity is evaluated, and the subscript n, which indicates that quantities M, C, and V pertain to cell n, has been omitted for clarity. Equation 3–3 is derived by multiplying the $f^{storage}$ term in equation 3–2 by the cell volume (V_{cell}), then using equation 2–8 to replace $S_w \theta V_{cell}$ with the volume of water in the cell, V_w. The expressions in equations 3–2 and 3–3 are preceded by negative signs because the $\dot{M}^{storage}$ term is on the left side of the cell balance equation (eq. 2–9). Thus, if more mass is added to a cell than is lost (and the volume of water remains the same), the concentration in the cell must increase.

The equation for aqueous solute storage is added to the system of equations by updating the diagonal position of the $\mathbf{A}$ matrix for row n with the coefficient of the $C^{t+\Delta t}$ term in equation 3–3 as

$$A_{n,n} \leftarrow A_{n,n} - \frac{V_w^{t+\Delta t}}{\Delta t}, \tag{3–4}$$

and by moving the remaining $\frac{C^t V_w^t}{\Delta t}$ term to the right-hand side to update b_n as

$$b_n \leftarrow b_n - \frac{C^t V_w^t}{\Delta t}. \tag{3–5}$$

Sorption

As a dissolved solute moves through an aquifer, some of the solute mass can bind to the surface of the solid material, a process known as adsorption, or penetrate into the solid material, a process known as absorp-

tion (Zheng and Bennett, 2002). Adsorption and absorption, collectively called sorption, can slow the movement of chemicals dissolved in groundwater. This apparent slowing of solute movement relative to water flow is also known as retardation. Sorption can be modeled as a transfer of solute mass from a dissolved state in the aqueous phase to a sorbed state in the solid phase, where it can no longer be transported by advection and dispersion. Desorption refers to the reverse process, whereby sorbed mass is released from the solid material and reenters the flow system.

The sorption capability of the MST Package simulates sorption and desorption by transferring solute mass between the groundwater and the solid material of the aquifer following the general approach implemented by Zheng and Wang (1999) in the RCT Package of the MT3DMS program. The sorption capability described here is similar to that of the MT3DMS RCT Package in that the MST Package also includes the linear equilibrium sorption model and the Freundlich and Langmuir isotherms, but it differs in that it does not presently include the nonequilibrium sorption model.

The concentration of sorbed mass, $\overline{C}$, is expressed as the mass of sorbed solute per mass of solid aquifer material available for sorption (M/M). When all of the solid aquifer material is available for sorption, the sorbed mass per volume of aquifer is $\rho_b\overline{C}$, where ρ_b is the bulk density of the solid in M/L^3, the mass of solid aquifer material per volume of aquifer. However, sorptive exchange between the mobile water and the solid aquifer material requires contact between the mobile water and the pore walls. When one or more immobile domains are present, only some fraction of the solid is available for sorptive exchange with the mobile phase. Under fully saturated conditions, this fraction of porosity that is mobile is defined as f_m, and the sorbed mass per volume of aquifer is $f_m\rho_b\overline{C}$. In the absence of immobile domains, f_m is internally assigned a value of one as there is no other domain for sorption to occur. If one or more immobile domains are present, then f_m is calculated internally by the program as one minus the sum of the immobile domain porosities. Under partially saturated conditions, the walls of desaturated pores are assumed to be effectively dry; any residual film of water that may remain on desaturated pore walls is assumed not to contribute appreciably to sorptive exchange. The fraction of solid aquifer material available for sorption is assumed to be proportional to the mobile water saturation, S_w, and the most general expression for sorbed mass per volume of aquifer is given as $f_m\rho_b S_w\overline{C}$.

The rate of change of the sorbed mass per volume of aquifer is

$$f^{sorption} = -\frac{\partial\left(f_m\rho_b S_w\overline{C}\right)}{\partial t}. \tag{3–6}$$

Assuming f_m and the bulk density do not change with time, equation 3–6 can be simplified to

$$f^{sorption} = -f_m\rho_b\frac{\partial\left(\overline{C}S_w\right)}{\partial t}. \tag{3–7}$$

Equation 3–7 is a convenient expression in some cases, such as when a simple linear expression can be used to relate the sorbed concentration to the aqueous concentration. For more complicated relations, however, it is beneficial to use the product rule to expand equation 3–7 into

$$f^{sorption} = -f_m\rho_b\left(S_w\frac{\partial\overline{C}}{\partial C}\frac{\partial C}{\partial t} + \overline{C}\frac{\partial S_w}{\partial t}\right). \tag{3–8}$$

Equations 3–7 and 3–8 are discretized and used with the linear, Freundlich, and Langmuir isotherms to develop finite-difference approximations that include the effect of sorption.

Linear Isotherm

There are several different conceptual models for relating the concentration of sorbed mass, $\overline{C}$, to the concentration of dissolved solute, C. The most common approach is to assume that the dissolved solute is in equilibrium with the sorbed solute, and that the concentration of sorbed mass is proportional to the concentration of dissolved solute mass. This equilibrium-controlled linear approach can be represented mathematically by the equation

$$\overline{C} = K_d C, \tag{3–9}$$

where K_d is the linear distribution coefficient (L^3/M), often referred to as the partition coefficient or the adsorption ratio. This equilibrium-controlled linear sorption model is one of three options available in the GWT Model for MODFLOW 6.

The sorption process is included in the system of equations by adding terms to the coefficient matrix $\mathbf{A}$ and the right-hand-side vector $\mathbf{b}$. For the linear isotherm, the transfer of mass to and from the solid phase can be approximated from the substitution of equation 3–9 into 3–7 and by multiplication by the volume of the model cell to give

$$\dot{M}^{sorption} = -\frac{f_m \rho_b V_{cell}}{\Delta t} K_d \left(S_w C\right)^{t+\Delta t} + \frac{f_m \rho_b V_{cell}}{\Delta t} K_d \left(S_w C\right)^{t}, \tag{3–10}$$

where K_d is assumed to be constant. The subscript n, which indicates that the quantities M, f_m, V_{cell}, K_d, S_w, and C pertain to cell n, has been omitted for clarity. The sorption mass transfer $\dot{M}^{sorption}$ is part of the $\dot{M}^{MST}$ term on the left side of equation 2–9. Thus, to place these terms into the matrix equation, the terms on the right side of equation 3–10 that are coefficients of $C^{t+\Delta t}$ are added to the diagonal position of the $\mathbf{A}$ matrix for row n as

$$A_{n,n} \leftarrow A_{n,n} - \frac{f_m \rho_b V_{cell}}{\Delta t} K_d S_w^{t+\Delta t}. \tag{3–11}$$

The remaining terms must be moved to the right-hand-side vector, $\mathbf{b}$, which requires that the signs of the terms be changed:

$$b_n \leftarrow b_n - \frac{f_m \rho_b V_{cell}}{\Delta t} K_d \left(S_w C\right)^{t}. \tag{3–12}$$

Freundlich Isotherm

The Freundlich isotherm is nonlinear with respect to the aqueous concentration and is written as

$$\overline{C} = K_f C^a, \tag{3–13}$$

where K_f is the Freundlich constant $(L^3/M)^a$ and a is the dimensionless Freundlich exponent. The Freundlich isotherm is implemented in the MST Package by writing a finite-difference expression for equation 3–8, which also requires an expression for $\frac{\partial \overline{C}}{\partial C}$. Equation 3–13 can be differentiated with respect to the aqueous concentration to give

$$\frac{\partial \overline{C}}{\partial C} = aK_f C^{a-1}. \tag{3–14}$$

The finite-difference approximation to equation 3–8 is

$$\begin{aligned} \dot{M}^{sorption} = &-\frac{f_m \rho_b V_{cell}}{\Delta t} \left(S_w \frac{\partial \overline{C}}{\partial C} \right)^{t+\frac{1}{2}\Delta t} \left(C^{t+\Delta t} - C^t \right) \\ &-\frac{f_m \rho_b V_{cell}}{\Delta t} \left(\overline{C} \right)^{t+\frac{1}{2}\Delta t} \left(S_w^{t+\Delta t} - S_w^t \right). \end{aligned} \tag{3–15}$$

To evaluate the $t + \frac{1}{2}\Delta t$ terms an average value over the time step is used. For $\overline{C}$ and $\frac{\partial \overline{C}}{\partial C}$, an average aqueous concentration is calculated using the concentration at the start of the time step, and the most recent iterate of the concentration at the end of the time step. This average aqueous concentration is then substituted into equations 3–13 and 3–14. Equation 3–15 is included in the system of equations by adding terms to the coefficient matrix $\mathbf{A}$ and the right-hand-side vector $\mathbf{b}$.

Langmuir Isotherm

The Langmuir isotherm is also nonlinear with respect to the aqueous concentration and written as

$$\overline{C} = \frac{K_l \overline{S} C}{1 + K_l C}, \tag{3–16}$$

where K_l is the Langmuir constant (L^3/M) and $\overline{S}$ is the total concentration of sorption sites available (M/M). The Langmuir isotherm is implemented in a manner similar to the Freundlich isotherm by using the finite-difference approximation shown in equation 3–15. For the Langmuir isotherm, the derivative term is

$$\frac{\partial \overline{C}}{\partial C} = \frac{K_l \overline{S}}{(1 + K_l C)^2}. \tag{3–17}$$

Considerations for Unconfined Conditions

The sorption formulation implemented in the GWT Model is mass conservative. A consequence of this sorption formulation described here, however, is that simulated concentrations may be higher than or lower than expected concentrations under unconfined conditions. When the water table decreases in a model cell, sorbed mass within the dewatered part of the cell is instantaneously applied to the saturated part of the cell at the end of the time step. Thus, in the absence of other solute inflows and outflows, solute is distributed over a smaller volume at the end of the time step than the volume at the start of the time step. In extreme cases this may cause the solute concentration to increase above expected concentrations simply due to the reduction in the volume of water in the cell. MT3D-USGS has options for treating this condition (Bedekar and others, 2016); however, these options are not available in the version of the GWT Model described in this report.

Decay

The decay capability of the MST Package simulates the effects of first- or zero-order decay and production of the dissolved aqueous phase. Decay and production can also be represented for the sorbed phase, as described in a following section (Decay of Sorbed Mass), and for the dissolved aqueous and sorbed phases in an immobile domain as described in chapter 7, "Immobile Domain Storage and Transfer". The mathematical expression for decay,

$$f^{decay} = -\lambda_1 \theta S_w C - \gamma_1 \theta S_w, \tag{3–18}$$

can be written to include first-order decay and zero-order decay, although only one can be active in the present GWT Model implementation. λ_1 is the first-order decay rate coefficient for the mobile domain (T^{-1}), and γ_1 is the zero-order decay rate coefficient for the mobile domain ($ML^{-3}T^{-1}$). Implementation of decay is handled differently depending on whether first-order or zero-order is selected.

First Order Decay

First-order decay is typically used to represent radioactive decay and biodegradation or chemical decomposition. When first-order decay is represented, f^{decay} can be written as

$$f^{decay} = -\lambda_1 \theta S_w C. \tag{3–19}$$

For first-order decay defined by equation 3–19, the rate of solute-mass decay in a cell of volume V_{cell} is

$$\dot{M}^{decay} = -\lambda_1 \theta V_{cell} \left(S_w C\right)^{t+\Delta t}. \tag{3–20}$$

To include the effect of first-order decay in the matrix equations, the coefficient term on the right side of equation 3–20 (that is a coefficient of the dependent variable $C^{t+\Delta t}$) is added to the diagonal position of the $\mathbf{A}$ matrix for row n as

$$A_{n,n} \leftarrow A_{n,n} - \lambda_1 \theta V_{cell} S_w^{t+\Delta t}. \tag{3–21}$$

First-order decay is commonly written in terms of a half life $t_{1/2}$, which is the length of time for the solute concentration to decrease by half. The half life is related to the first-order decay rate coefficient by

$$t_{1/2} = \frac{\ln 2}{\lambda_1}. \tag{3–22}$$

Zero-Order Decay

Under some transport conditions, zero-order decay may be used to mathematically represent the process of biodegradation in which the rate of biodegradation does not depend on concentration. Zero-order decay can also be used to model groundwater age mathematically as a solute "concentration," as described by Goode (1996). When groundwater age is simulated in this way, a zero-order (constant) growth rate of one (a decay rate of minus one) causes the groundwater age to increase by one unit of time for every unit of time simulated. Thus, during each time step the groundwater age increases by the length of the time step.

When zero-order decay is represented, f^{decay} is

$$f^{decay} = -\gamma_1 \theta S_w, \tag{3–23}$$

which is expressed in finite-difference form as

$$\dot{M}^{decay} = -\gamma_1 \theta V_{cell} S_w^{t+\Delta t}. \tag{3–24}$$

Unlike in the case of first-order decay (eq. 3–20), the dependent variable C does not appear in the expression for zero-order decay (eq. 3–24), so the zero-order term is moved to the right-hand-side vector, $\mathbf{b}$, which requires that the sign of the term be changed:

$$b_n \leftarrow b_n + \gamma_1 \theta V_{cell} S_w^{t+\Delta t}. \tag{3–25}$$

Zero-order decay can result in negative concentrations unless the decay rate is automatically reduced by the program based on simulated solute concentrations. A simple method was implemented to reduce the user-specified zero-order decay rate if that rate would result in negative concentrations. This reduced rate is estimated by comparing the user-specified decay rate with the solute concentration divided by the length of the time step. If the user-specified decay rate is larger than the solute concentration divided by the time step, then the program replaces γ_1 with the solute concentration divided by the time step. Because this approach requires the current concentration, which is estimated as the previous concentration iterate, additional outer iterations may be required for solution convergence.

Decay of Sorbed Mass

When sorption is represented in the GWT Model, separate terms are included in the mass balance equation to represent decay of the sorbed mass. Decay of the sorbed mass can be expressed with the following mathematical expression (Toride and others, 1993),

$$f^{sorbeddecay} = -\lambda_2 f_m \rho_b S_w \overline{C} - \gamma_2 f_m \rho_b S_w. \tag{3–26}$$

Linear Isotherm

For first-order decay with the linear sorption isotherm, the rate of decay of sorbed mass in a cell is

$$\dot{M}^{sorbeddecay} = -\lambda_2 f_m \rho_b S_w K_d V_{cell} C^{t+\Delta t}, \tag{3–27}$$

and for zero-order decay, the rate of decay of sorbed mass in a cell is

$$\dot{M}^{sorbeddecay} = -\gamma_2 f_m \rho_b S_w V_{cell}. \tag{3–28}$$

The decay of sorbed mass is added to the system of equations differently depending on whether the decay is first or zero order. For first-order decay, in which the mass transfer rate depends on concentration, the coefficient of $C^{t+\Delta t}$ in equation 3–27 is added to the diagonal position of the $\mathbf{A}$ matrix for row n as

$$A_{n,n} \leftarrow A_{n,n} - \lambda_2 f_m \rho_b S_w K_d V_{cell}. \tag{3–29}$$

For zero-order decay, in which the mass transfer rate is independent of solute concentration, the mass transfer rate is moved to the right-hand-side vector, $\mathbf{b}$, as

$$b_n \leftarrow b_n + \gamma_2 f_m \rho_b S_w V_{cell}. \tag{3–30}$$

Additional precautions are also necessary, as described in the previous section, to ensure that zero-order decay does not result in negative concentrations.

Nonlinear Freundlich and Langmuir Isotherms

For the nonlinear Freundlich and Langmuir isotherms, zero-order decay is also represented using equations 3–28 and 3–30 as the rate is not a function of the sorbed concentration (except when the rate must be reduced to prevent negative concentrations). For first-order decay, however, sorbed mass is expressed using $\overline{C}$ as

$$\dot{M}^{sorbeddecay} = -\lambda_2 f_m \rho_b S_w V_{cell} \overline{C}^{t+\Delta t}, \tag{3–31}$$

where $\overline{C}^{t+\Delta t}$ is approximated using the isotherm equation (eq. 3–13 for the Freundlich isotherm or 3–16 for the Langmuir isotherm) and the most recent iterate for the aqueous concentration. Unlike for the linear isotherm with first-order decay, which can be added to the $\mathbf{A}$ matrix, the term resulting from first-order decay with the nonlinear isotherms must be added to the right-hand-side vector. Additional outer iterations are often required for solution convergence when the Freundlich isotherm or the Langmuir isotherm is used to represent sorption.

Chapter 4. Advective and Dispersive Solute Transport

The Advection (ADV) and Dispersion (DSP) Packages add terms to the system of equations to represent advective transport and the combined effects of mechanical dispersion and molecular diffusion. These two transport processes are represented in the GWT Model by transferring mass between adjacent model cells according to groundwater flow rates and solute concentration gradients.

Advection (ADV) Package

Advection is the movement of a dissolved solute as it is transported through an aquifer at the average linear velocity of the groundwater flow. The advective flux $\mathbf{f}^{ADV}$ (M/L^2T) of a solute of concentration C (M/L^3) transported by a specific discharge of groundwater $\mathbf{q}$ (L/T) is

$$\mathbf{f}^{ADV} = \mathbf{q}C. \tag{4–1}$$

This advective flux term comprises the advective solute flux that appears in parentheses in the first term on the right-hand side of equation 2–1. As indicated in equation 2–10, the discrete analog of equation 4–1 used by the CVFD method in the GWT Model expresses the total advective flow rate of solute mass across the interface between cells n and m, $F_{n,m}^{ADV}$ (M/T), as the product of the volumetric groundwater flow rate across the interface, $Q_{n,m}$ (L^3/T), and a representative solute concentration of groundwater crossing the interface, $C_{n,m}$ (M/L^3):

$$F_{n,m}^{ADV} = Q_{n,m}C_{n,m}, \tag{4–2}$$

where $F_{n,m}^{ADV}$ and $Q_{n,m}$ are defined to be positive for flow into cell n from cell m.

Three options are available for calculating the concentration at the cell face, $C_{n,m}$: central-in-space weighting, upstream weighting, and a total variation diminishing (TVD) scheme. In each case, the solute concentration at the cell face can be expressed as a weighted average of the concentrations in the two cells:

$$C_{n,m} = \omega_{n,m}C_n + (1 - \omega_{n,m})\, C_m, \tag{4–3}$$

where $\omega_{n,m}$ is a dimensionless weighting factor.

Central-In-Space Weighting

The central-in-space weighting scheme is based on a simple distance-weighted linear interpolation between the center of cell n and the center of cell m to calculate solute concentration at the shared face between cell n and cell m. Although "central-in-space" is a misnomer for grids without equal spacing between connected cells, it is retained here for consistency with nomenclature used by other MODFLOW-based transport programs, such as MT3D. The value for $\omega_{n,m}$ is a distance-weighted interpolation factor calculated based on cell dimensions:

$$\omega_{n,m} = \frac{L_{m,n}}{L_{n,m} + L_{m,n}}, \tag{4–4}$$

where $L_{n,m}$ and $L_{m,n}$ are the distance (L) from the center of cell n to its shared face with cell m and the distance from the center of cell m to its shared face with cell n, respectively. Central-in-space weighting is not often used because it can result in spurious oscillations in the simulated concentrations. It is included as an option in the ADV Package, however, because it may be useful for model testing and comparison purposes.

Upstream Weighting

Upstream weighting is a commonly used approach for calculating the interface concentration. For upstream weighting, the weighting factor, $\omega_{n,m}$, depends on the sign of the flow between cell n and m according to

$$\omega_{n,m} = \begin{cases} 0 & \text{for } Q_{n,m} > 0 \\ 1 & \text{for } Q_{n,m} \leq 0 \end{cases}. \tag{4–5}$$

Total Variation Diminishing (TVD)

A TVD expansion of $C_{n,m}$ can be expressed as

$$C_{n,m} = C_{n,m}^{ups} + C_{n,m}^{TVD}, \tag{4–6}$$

with

$$C_{n,m}^{TVD} = \frac{\sigma_{n,m}}{2}\left(C_{n,m}^{dwn} - C_{n,m}^{ups}\right), \tag{4–7}$$

where $C_{n,m}^{ups}$ is the concentration of the upstream cell, $C_{n,m}^{dwn}$ is the concentration of the downstream cell, $C_{n,m}^{TVD}$ is an additional flux-limiting concentration term, and $\sigma_{n,m}$ is the flux limiter. The van Leer flux limiter (Forsyth and others, 1998) can be written as

$$\sigma_{n,m} = \begin{cases} 0 & \text{for } r_{n,m} \leq 0 \\ \frac{2r_{n,m}}{1+r_{n,m}} & \text{for } r_{n,m} > 0. \end{cases} \tag{4–8}$$

$r_{n,m}$ is the smoothness sensor defined as

$$r_{n,m} = \frac{C_{n,m}^{ups} - C_{n,m}^{2up}}{L_{ups,2up} + L_{2up,ups}} \cdot \frac{L_{n,m} + L_{m,n}}{C_{n,m}^{dwn} - C_{n,m}^{ups}}, \tag{4–9}$$

where $C_{n,m}^{2up}$ is the concentration of the second upstream cell, and $L_{ups,2up}$ and $L_{2up,ups}$ are the distance (L) from the center of the upstream cell to its shared face with the second upstream cell and the distance from the center of the second upstream cell to its shared face with the upstream cell, respectively. The second upstream cell is determined by identifying the cell with the largest flow into the upstream cell. If a second upstream cell cannot be identified because of flow conditions or because the upstream cell is on the edge of the grid, then the TVD adjustment is not applied.

As shown in equation 4–6 the interface concentration $C_{n,m}$ consists of two terms for the TVD expansion. The first term $C_{n,m}^{ups}$ is simply an upstream-weighted concentration calculated using equations 4–3 and 4–5. Thus, the upstream weighting factor $\omega_{n,m}$ (eq. 4–5) enters the advective flow expression, equation 4–2, through the $C_{n,m}^{ups}$ term in equation 4–6. The contribution to the advective flow associated with $C_{n,m}^{TVD}$ is treated separately, as described below in the discussion of the numerical solution procedure. However, for the purpose of comparison with other weighting schemes, the TVD scheme can be expressed entirely in terms of its own weighting factor, $\omega_{n,m}^{TVD}$, which depends on the flux limiter, $\sigma_{n,m}$:

$$C_{n,m} = \omega_{n,m}^{TVD} C_n + \left(1 - \omega_{n,m}^{TVD}\right) C_m, \tag{4–10}$$

where

$$\omega_{n,m}^{TVD} = \begin{cases} \frac{\sigma_{n,m}}{2} & \text{for } Q_{n,m} > 0 \\ 1 - \frac{\sigma_{n,m}}{2} & \text{for } Q_{n,m} \leq 0 \end{cases}. \tag{4–11}$$

Numerical Solution

When the central-in-space or upstream weighting scheme is used, the advective-transport term for the face shared by cells n and m is incorporated into the system of linear equations, equation 2–13, as follows. Substitution of equation 4–3 into equation 4–2 gives

$$F_{n,m}^{ADV} = \omega_{n,m} Q_{n,m} C_n + (1 - \omega_{n,m}) Q_{n,m} C_m. \tag{4–12}$$

The matrix coefficient in the diagonal position for row n is updated by adding the term $\omega_{n,m} Q_{n,m}$ as

$$A_{n,n} \leftarrow A_{n,n} + \omega_{n,m} Q_{n,m}. \tag{4–13}$$

The matrix coefficient in row n that corresponds to the connection between cell n and neighboring cell m is updated by adding the coefficient part of the term $(1 - \omega_{n,m}) Q_{n,m} C_m$ as

$$A_{n,m} \leftarrow A_{n,m} + (1 - \omega_{n,m}) Q_{n,m}. \tag{4–14}$$

When the TVD option is used, the expression for $F_{n,m}^{ADV}$ includes the additional TVD term $Q_{n,m} C_{n,m}^{TVD}$ as

$$F_{n,m}^{ADV} = \omega_{n,m} Q_{n,m} C_n + (1 - \omega_{n,m}) Q_{n,m} C_m + Q_{n,m} C_{n,m}^{TVD}, \tag{4–15}$$

where the weighting factor $\omega_{n,m}$ is evaluated as for upstream weighting (equation 4–5), and $C_{n,m}^{TVD}$ is the flux-limiting concentration introduced in equation 4–6. The terms in equation 4–15 that involve $\omega_{n,m}$ are incorporated in the coefficient matrix just as they would be for upstream weighting. The TVD term is added to b_n, the row-n entry in the right-hand-side vector, $\mathbf{b}$:

$$b_n \leftarrow b_n - Q_{n,m} C_{n,m}^{TVD}. \tag{4–16}$$

When upstream weighting or the TVD scheme is used, the dependence of $\omega_{n,m}$ on the flow direction causes the coefficient matrix, $\mathbf{A}$, to be nonsymmetric, that is, $A_{n,m} \neq A_{m,n}$. Solution of the resulting matrix problem requires use of a linear solver that can accommodate nonsymmetric matrices.

Dispersion (DSP) Package

Over time, a mass of solute dissolved in groundwater spreads by molecular diffusion. If groundwater is flowing, solute spreads also by mechanical dispersion, which is caused by "[v]ariations in local velocity, both in magnitude and direction, along the tortuous paths and between adjacent flow paths" within the pores of the porous medium (Bear, 1972). The combination of molecular diffusion and mechanical dispersion is called hydrodynamic dispersion.

Although mechanical dispersion originates from pore-scale processes, it is generally not feasible to simulate its effects at the pore scale. Mathematical representation of mechanical dispersion at the macroscopic scale, which is of interest in practical applications, has been the subject of active research for decades, and various "macrodispersion" models have been developed (for example, Scheidegger (1961), Burnett and Frind (1987), and Lichtner and others (2002)).

The simple "Fickian" model of hydrodynamic dispersion conceptualizes mechanical dispersion as being analogous to molecular diffusion. In the Fickian model, the flux of solute mass due to hydrodynamic dispersion, $\mathbf{f}^{DSP}$ (M/L^2T), is related to the solute concentration gradient, ∇C (M/L^4), through a tensorial "constant of proportionality," the hydrodynamic dispersion tensor, $\mathbf{D}$ (L^2/T), which is the sum of contributions from mechanical dispersion and molecular diffusion:

$$\mathbf{f}^{DSP} = -S_w \theta \mathbf{D} \nabla C, \tag{4–17}$$

with

$$\mathbf{D} = \mathbf{D}^{mech} + D^{mol}\mathbf{I}, \tag{4–18}$$

where $\mathbf{D}^{mech}$ (L^2/T) is the mechanical dispersion tensor, which may be anisotropic, D^{mol} (L^2/T) is an effective molecular diffusion coefficient that takes into account the effect of porous medium tortuosity, $\mathbf{I}$ is the identity tensor (dimensionless), and θ is effective porosity (dimensionless). Equation 4–17 represents the dispersive solute flux that appears in parentheses in the second term on the right-hand side of equation 2–1. The second term on the right-hand side of equation 4–18 places the contribution from the molecular diffusion coefficient on the diagonal of the hydrodynamic dispersion tensor, which corresponds to assuming that molecular diffusion is isotropic. Following Zheng and Wang (1999), θ is included explicitly in equation 4–17 to account for the fact that hydrodynamic dispersion occurs only within the pore space, not within the solid matrix. Similarly, inclusion of the saturation, S_w, in equation 4–17 accounts for the fact that hydrodynamic dispersion occurs only within the portion of the porespace that contains water.

Equation 4–17 shows the dispersive flux as proportional to the gradient of the solute concentration. This relation is consistent with the dispersion model presented by Zheng and Bennett (2002) and implemented in popular solute transport modeling codes such as MODFLOW-GWT and MT3DMS. Other literature suggests, however, that the dispersive flux should be proportional to the gradient of solute mass fraction (Bird and others, 2006), which is the dispersion model implemented in the SUTRA program (Voss and Provost, 2010). For most transport problems with slight density variations, the difference between the two approaches is expected to be negligible.

The mechanical dispersion tensor, $\mathbf{D}^{mech}$, is typically assumed to be characterized by three mutually perpendicular "principal" directions of spreading, which implies that the tensor is defined by a real, symmetric

matrix. In a homogeneous aquifer, a solute mass that is initially spherical will assume an ellipsoidal shape as it advects with the groundwater flow and spreads due to mechanical dispersion, and the principal axes of the ellipsoid will coincide with the principal directions of the dispersion tensor. The entries in the matrix, or "dispersion coefficients," control the rates and directions of spreading. The dispersion coefficients can vary with flow direction, and different models for the dispersion coefficients lead to different symmetries in the solute spreading pattern. For example, "isotropic" dispersion is controlled by two dispersion coefficients that do not vary with flow direction, and the rates of spreading along and perpendicular to the flow direction are independent of the flow direction. The model of Scheidegger (1961), which in its most general form admits nonsymmetric matrices and is defined by 61 dispersion coefficients, encompasses a wide variety of symmetries. In practice, however, the mechanical dispersion model is typically simplified considerably by assuming that one of the principal directions of the dispersion tensor, called the "longitudinal" direction, is always aligned with the flow direction. The remaining two principal directions, called the "transverse" directions, are then perpendicular to the flow direction. Special cases of this "flow-aligned" dispersion tensor have been developed by incorporating additional simplifying assumptions. For example, the popular model of Burnett and Frind (1987), which is defined by two longitudinal and three transverse dispersion coefficients, allows different spreading behavior for vertical flow than for flow within the horizontal plane and includes isotropic dispersion as a special case. For flow within the horizontal plane, the rates of longitudinal and transverse dispersion are independent of flow direction, but the rate of horizontal transverse dispersion can be different from the rate of vertical transverse dispersion. For vertical flow, transverse dispersion is horizontal and is axially symmetric about the vertical direction. For intermediate flow directions, dispersion coefficients are interpolated a specific way between their horizontal-flow and vertical-flow values.

The Fickian model described by equation 4–17 tends to produce unrealistic back dispersion, and the dispersion coefficients are scale-dependent, particularly in applications involving estimation of effective dispersion coefficients in heterogeneous aquifers (Konikow, 2010). Nevertheless, conceptual simplicity, ease of integration into conventional groundwater flow and transport models, and the ability to simulate varying degrees and directions of solute spreading make the Fickian model a popular tool for representing mechanical dispersion in practical applications. The GWT Model of MODFLOW 6 offers a Fickian dispersion model that includes isotropic dispersion and the mechanical dispersion models of Burnett and Frind (1987) and Lichtner and others (2002) as special cases.

The CVFD method used in the GWT Model is based on a solute mass balance over each cell (equation 2–9), which includes dispersive flows of solute between each cell and its surrounding cells (equation 2–11). The GWT Model offers two choices for formulating $F_{n,m}^{DSP}$, the dispersive flow rate of solute mass (M/T) into cell n from cell m across their shared face, which is a discrete analog of equation 4–17. The "simplified" formulation is mathematically analogous to the "conductance-based" formulation of groundwater flow across cell faces in MODFLOW 6. Similar to the conductance-based groundwater flow formulation, the simplified solute-mass flow formulation works well when the model grid and governing tensor—in this case the dispersion tensor—satisfy certain requirements, as discussed in Langevin and others (2017) and summarized below. When these requirements are not met use of the simplified formulation introduces numerical error (in addition to the usual discretization error), which may or may not be significant in a given application. In such cases the alternative XT3D formulation of the solute-mass flow, which is mathematically analogous to the XT3D formulation of groundwater flow in MODFLOW 6 (Provost and others, 2017), can be helpful because it automatically accounts for irregularities in the grid and tensor anisotropy, albeit at the expense of longer simulation times. The XT3D formulation is used by default for solute-mass flow in MODFLOW 6, but the simplified flow formulation can be activated by the user to evaluate model performance and accuracy.

When the GWT Model is used with a GWF Model that uses the Horizontal Flow Barrier (HFB) Package, transport results should be evaluated with caution as noted by Hornberger and others (2002), especially if the intent of the flow barrier is to impede solute movement. Flow barriers are not explicitly represented in the GWF Model. Instead, their effects are implicitly incorporated in the flow equations by adjusting the con-

ductance between two model cells to account for lower permeability material. A consequence of the implicit incorporation of a flow barrier is that the simulated dispersive flux through the barrier will be too large as it does not have any thickness or storage capacity. Therefore, the effectiveness of the barrier to contain a solute plume or impede solute movement will be underrepresented by the GWT Model in this situation.

Mechanical Dispersion Model

In the MODFLOW 6 GWT Model, the mechanical dispersion tensor, $\mathbf{D}^{mech}$, is assumed to be characterized by three mutually perpendicular "principal" directions of spreading, one of which, called the "longitudinal" direction, is always aligned with the direction of groundwater flow. The remaining two principal directions, called the "transverse" directions, are then perpendicular to the flow direction and to each other. One of the transverse directions lies within the (x, y) (horizontal) plane. Expressed in coordinates (x_L, x_{T1}, x_{T2}) that align with the longitudinal and two transverse directions, respectively, the mathematical form of the mechanical dispersion tensor used in the GWT Model is

$$\mathbf{D}^{mech} = \begin{pmatrix} \alpha_L v & 0 & 0 \\ 0 & \alpha_{T1} v & 0 \\ 0 & 0 & \alpha_{T2} v \end{pmatrix}, \tag{4–19}$$

where α_L, α_{T1}, and α_{T2} are called the longitudinal and first and second transverse dispersivities (L), and v is the groundwater flow velocity (L/T) or "seepage velocity" calculated as the specific discharge divided by the porosity. Although the equations presented here are based on groundwater velocity, implementation of these equations in the Dispersion Package is based on specific discharge (instead of velocity) by including the porosity term in equation 4–17 in the dispersion tensor and by replacing $v\theta$ with q.

The longitudinal and transverse dispersivities vary with the groundwater flow direction as follows:

$$\begin{aligned} \alpha_L &= \alpha_{LH} \cos^2\theta_2 + \alpha_{LV} \sin^2\theta_2 = \alpha_{LH}\left(1 - \frac{v_z^2}{v^2}\right) + \alpha_{LV}\frac{v_z^2}{v^2} \\ \alpha_{T1} &= \alpha_{TH1} \cos^2\theta_2 + \alpha_{TV} \sin^2\theta_2 = \alpha_{TH1}\left(1 - \frac{v_z^2}{v^2}\right) + \alpha_{TV}\frac{v_z^2}{v^2}, \\ \alpha_{T2} &= \alpha_{TH2} \cos^2\theta_2 + \alpha_{TV} \sin^2\theta_2 = \alpha_{TH2}\left(1 - \frac{v_z^2}{v^2}\right) + \alpha_{TV}\frac{v_z^2}{v^2} \end{aligned} \tag{4–20}$$

where θ_2 is the angle at which the groundwater velocity vector, $\mathbf{v}$, is inclined upward from the (x, y) (horizontal) plane, and v_z is the z (vertical) component of $\mathbf{v}$. The model has five parameters that can be specified by the user: two longitudinal dispersivities, α_{LH} and α_{LV}, and three transverse dispersivities, α_{TH1}, α_{TH2}, and α_{TV}, all with dimensions of (L).

Note that equation 4–19 expresses $\mathbf{D}^{mech}$ in (x_L, x_{T1}, x_{T2}) coordinates, but velocity is expressed relative to (x, y, z) model coordinates in equation 4–20. The "horizontal plane" relative to which the dispersion tensor is defined is the (x, y) model coordinate plane, and the "vertical" direction is the model coordinate z direction. Allowing the "horizontal" and "vertical" directions to be rotated relative to the model coordinates would allow the definition of the dispersion tensor to align with dipping beds; for example, in much the same way that three user-specified angles allow the conductivity tensor to be defined with respect to coordinates rotated relative to (x, y, z) model coordinates (Langevin and others, 2017). However, an option to set the reference coordinates for the dispersion tensor to be other than the model coordinates is not available in the current implemention.

The behavior of the mechanical dispersion model can be understood by considering the values assumed by the longitudinal and transverse dispersivities when the groundwater flow is either horizontal or vertical. When flow is in the horizontal plane ($\theta_2 = 0°; v_z = 0$), the longitudinal dispersivity (α_L) is α_{LH}, the transverse dispersivity for horizontal spreading (α_{T1}) is α_{TH1}, and the transverse dispersivity for vertical spreading (α_{T2}) is α_{TH2}. When flow is in the vertical direction ($\theta_2 = 90°; v_x = v_y = 0, v_z = v$), the longitudinal dispersivity (α_L) is α_{LV}, and the transverse dispersivities (α_{T1} and α_{TH1}), which represent horizontal spreading, are both α_{TV}. For groundwater flow directions between horizontal and vertical, the longitudinal and transverse dispersivities vary smoothly with flow direction according to equation 4–20.

When transformed entirely into (x, y, z) model coordinates, the mechanical dispersion tensor has the following form:

$$\begin{aligned} D_{xx}^{mech} &= \alpha_L \frac{v_x^2}{v} + \alpha_{TH1} \frac{v_y^2}{v} + \alpha_{Tx} \frac{v_z^2}{v} \\ D_{yy}^{mech} &= \alpha_{TH1} \frac{v_x^2}{v} + \alpha_L \frac{v_y^2}{v} + \alpha_{Ty} \frac{v_z^2}{v} \\ D_{zz}^{mech} &= \alpha_{T2} \frac{v_x^2}{v} + \alpha_{T2} \frac{v_y^2}{v} + \alpha_L \frac{v_z^2}{v} \\ D_{xy}^{mech} &= (\alpha_L - \alpha_{T2} + \alpha_{TH2} - \alpha_{TH1}) \frac{v_x v_y}{v} \\ D_{xz}^{mech} &= (\alpha_L - \alpha_{T2}) \frac{v_x v_z}{v} \\ D_{yz}^{mech} &= (\alpha_L - \alpha_{T2}) \frac{v_y v_z}{v} \end{aligned} \tag{4–21}$$

where

$$\begin{aligned} \alpha_{Tx} &= \alpha_{TH2} \frac{v_x^2}{v^2} + \alpha_{TV} \left(1 - \frac{v_x^2}{v^2}\right) \\ \alpha_{Ty} &= \alpha_{TH2} \frac{v_y^2}{v^2} + \alpha_{TV} \left(1 - \frac{v_y^2}{v^2}\right) \end{aligned}. \tag{4–22}$$

The generalized mechanical dispersion tensor, written in model coordinates (eq. 4–21), can be recast to correspond to other popular dispersion models, such as the models of Burnett and Frind (1987), Lichtner and others (2002), and the isotropic dispersion model. Setting

$$\begin{aligned} \alpha_{LH} &= \alpha_L \\ \alpha_{LV} &= \alpha_L \\ \alpha_{TH1} &= \alpha_T^H, \\ \alpha_{TH2} &= \alpha_T^V \\ \alpha_{TV} &= \alpha_T^V \end{aligned} \tag{4–23}$$

where α_L, α_T^H, and α_T^V are constants introduced for simplification purposes, gives the model of Burnett and Frind (1987):

$$
\begin{aligned}
D_{xx}^{mech} &= \alpha_L \frac{v_x^2}{v} + \alpha_T^H \frac{v_y^2}{v} + \alpha_T^V \frac{v_z^2}{v} \\
D_{yy}^{mech} &= \alpha_T^H \frac{v_x^2}{v} + \alpha_L \frac{v_y^2}{v} + \alpha_T^V \frac{v_z^2}{v} \\
D_{zz}^{mech} &= \alpha_T^V \frac{v_x^2}{v} + \alpha_T^V \frac{v_y^2}{v} + \alpha_L \frac{v_z^2}{v} \\
D_{xy}^{mech} &= \left(\alpha_L - \alpha_T^H\right) \frac{v_x v_y}{v} \\
D_{xz}^{mech} &= \left(\alpha_L - \alpha_T^V\right) \frac{v_x v_z}{v} \\
D_{yz}^{mech} &= \left(\alpha_L - \alpha_T^V\right) \frac{v_y v_z}{v}
\end{aligned}
\tag{4–24}
$$

Setting

$$
\begin{aligned}
\alpha_{LH} &= \alpha_L^H \\
\alpha_{LV} &= \alpha_L^V \\
\alpha_{TH1} &= \alpha_T^H, \\
\alpha_{TH2} &= \alpha_T^V \\
\alpha_{TV} &= \alpha_T^H
\end{aligned}
\tag{4–25}
$$

where α_L^H, α_L^V, α_T^H, and α_T^V are constants, gives a form of the model of Lichtner and others (2002):

$$
\begin{aligned}
D_{xx}^{mech} &= \alpha_L \frac{v_x^2}{v} + \alpha_T^H \frac{v_y^2}{v} + \alpha_{Tx} \frac{v_z^2}{v} \\
D_{yy}^{mech} &= \alpha_T^H \frac{v_x^2}{v} + \alpha_L \frac{v_y^2}{v} + \alpha_{Ty} \frac{v_z^2}{v} \\
D_{zz}^{mech} &= \alpha_{T2} \frac{v_x^2}{v} + \alpha_{T2} \frac{v_y^2}{v} + \alpha_L \frac{v_z^2}{v}, \\
D_{xy}^{mech} &= \left(\alpha_L - \alpha_{T2} + \alpha_{TH2} - \alpha_T^H\right) \frac{v_x v_y}{v} \\
D_{xz}^{mech} &= \left(\alpha_L - \alpha_{T2}\right) \frac{v_x v_z}{v} \\
D_{yz}^{mech} &= \left(\alpha_L - \alpha_{T2}\right) \frac{v_y v_z}{v}
\end{aligned}
\tag{4–26}
$$

with

$$\begin{aligned}
\alpha_L &= \alpha_L^H \left(1 - \frac{v_z^2}{v^2}\right) + \alpha_L^V \frac{v_z^2}{v^2} \\
\alpha_{Tx} &= \alpha_T^V \frac{v_x^2}{v^2} + \alpha_T^H \left(1 - \frac{v_x^2}{v^2}\right) \\
\alpha_{Ty} &= \alpha_T^V \frac{v_y^2}{v^2} + \alpha_T^H \left(1 - \frac{v_y^2}{v^2}\right) \\
\alpha_{T2} &= \alpha_T^V \left(1 - \frac{v_z^2}{v^2}\right) + \alpha_T^H \frac{v_z^2}{v^2}
\end{aligned} \quad . \tag{4–27}$$

Setting

$$\begin{aligned}
\alpha_{LH} &= \alpha_L \\
\alpha_{LV} &= \alpha_L \\
\alpha_{TH1} &= \alpha_T, \\
\alpha_{TH2} &= \alpha_T \\
\alpha_{TV} &= \alpha_T
\end{aligned} \tag{4–28}$$

where α_L and α_T are constants, gives an isotropic mechanical dispersion tensor, which is a special case of both the Burnett and Frind (1987) model and the Lichtner and others (2002) model:

$$\begin{aligned}
D_{xx}^{mech} &= \alpha_L \frac{v_x^2}{v} + \alpha_T \frac{v_y^2}{v} + \alpha_T \frac{v_z^2}{v} \\
D_{yy}^{mech} &= \alpha_T \frac{v_x^2}{v} + \alpha_L \frac{v_y^2}{v} + \alpha_T \frac{v_z^2}{v} \\
D_{zz}^{mech} &= \alpha_T \frac{v_x^2}{v} + \alpha_T \frac{v_y^2}{v} + \alpha_L \frac{v_z^2}{v} \\
D_{xy}^{mech} &= (\alpha_L - \alpha_T) \frac{v_x v_y}{v} \\
D_{xz}^{mech} &= (\alpha_L - \alpha_T) \frac{v_x v_z}{v} \\
D_{yz}^{mech} &= (\alpha_L - \alpha_T) \frac{v_y v_z}{v}
\end{aligned} \quad . \tag{4–29}$$

With the isotropic dispersion model, the rate of longitudinal spreading (along the flow direction) is controlled by α_L, and the rate of transverse spreading (symmetrically about an axis oriented with the flow direction) is controlled by α_T. The rates of longitudinal and transverse spreading are independent of the flow direction. In general, an initially spherical patch of solute in a uniform flow field spreads into a diffuse ellipsoid that is symmetric about an axis oriented with the flow direction. In the special case $\alpha_T = \alpha_L$, an initially spherical patch of solute in a uniform flow field spreads into a diffuse sphere.

Simplified Formulation

Hydrodynamic dispersion results in solute spreading from areas of higher concentration to areas of lower concentration. In an anisotropic porous medium, however, dispersive transport is not necessarily in the direc-

tion of the concentration gradient; that is, the solute mass flux vector is not necessarily aligned with the concentration gradient vector. In the Fickian dispersion model (equation 4–17) in three dimensions (3D), each of the three components of the solute mass flux vector is related, by way of the hydrodynamic dispersion tensor, to each of the three components of the concentration gradient:

$$\begin{aligned} f_x^{DSP} &= -S_w\theta\left(D_{xx}\frac{\partial C}{\partial x} + D_{xy}\frac{\partial C}{\partial y} + D_{xz}\frac{\partial C}{\partial z}\right) \\ f_y^{DSP} &= -S_w\theta\left(D_{xy}\frac{\partial C}{\partial x} + D_{yy}\frac{\partial C}{\partial y} + D_{yz}\frac{\partial C}{\partial z}\right), \\ f_z^{DSP} &= -S_w\theta\left(D_{xz}\frac{\partial C}{\partial x} + D_{yz}\frac{\partial C}{\partial y} + D_{zz}\frac{\partial C}{\partial z}\right) \end{aligned} \tag{4–30}$$

where D_{xx}, D_{xy}, D_{xz}, D_{yy}, D_{yz}, and D_{zz} (L/T) are the elements (dispersion coefficients) of the hydrodynamic dispersion tensor $\mathbf{D}$, which is assumed to be symmetric ($D_{yx} = D_{xy}$, $D_{zx} = D_{xz}$, and $D_{zy} = D_{yz}$). Thus, in the most general case, the solute mass flux component along a particular direction cannot be computed solely based on the component of the concentration gradient along that one direction; three independent components of the gradient are required. However, in certain special cases that are discussed later in this section, flux components reduce to the simplified form

$$f_s^{DSP} = -S_w\theta D_{ss}\frac{\partial C}{\partial s}, \tag{4–31}$$

where s represents the direction along which the concentration gradient is evaluated and the flux component is computed. Direction s may represent one of the coordinate directions, x, y, or z, or another direction, depending on the special case.

The "simplified formulation" of the dispersive solute mass flow rate between adjacent cells n and m is a discrete analog of equation 4–31 and has the form

$$F_{n,m}^{DSP} = \tilde{D}_{n,m}\left(C_m - C_n\right). \tag{4–32}$$

The coefficient $\tilde{D}_{n,m}$ (L^3/T) is analogous to a "conductance" for flow of solute mass driven by a concentration difference and incorporates the effects of the dispersion coefficients and porosities in the two model cells, the interfacial area over which the dispersive flux occurs, and the distance between the nodes at which the cell concentrations are calculated.

For the simplified formulation, a dispersion conductance is defined as a coefficient, that when multiplied by a concentration difference, will result in the dispersive mass flux. The dispersion conductance is calculated based on the harmonic mean of two half-cell dispersion conductances as

$$\tilde{D}_{n,m} = \frac{\tilde{d}_n\tilde{d}_m}{\tilde{d}_n + \tilde{d}_m}, \tag{4–33}$$

where $\tilde{d}_n$ is the calculated half-cell dispersion conductance for cell n in the direction of cell m and $\tilde{d}_m$ is the calculated half-cell dispersion conductance for cell m in the direction of cell n. The half-cell dispersion conductance is calculated for cell n (in the direction of cell m) as

$$\tilde{d}_n = \frac{D_{n,m} A_{n,m}}{L_{n,m}}, \tag{4–34}$$

and for cell m in the direction of cell n as

$$\tilde{d}_m = \frac{D_{m,n} A_{m,n}}{L_{m,n}}. \tag{4–35}$$

In equations 4–34 and 4–35, the effective dispersion coefficients, $D_{n,m}$ and $D_{m,n}$, are interpolated from the principal flow-aligned dispersion components D_{11}, D_{22}, and D_{33}. D_{11} is aligned with the flow direction, and D_{22} and D_{33} are aligned with the two orthogonal transverse directions. $A_{n,m}$ and $A_{m,n}$ are equal and are calculated as the area for flow between cells n and m. For a horizontal connection, the flow area is a function of cell saturation. The distance between cell n and its shared face with cell m is denoted by $L_{n,m}$. Likewise, the distance between cell m and its shared face with cell n is denoted by $L_{m,n}$.

With the simplified formulation, the value for the effective dispersion coefficient $D_{n,m}$ in the n-m direction is calculated from D_{11}, D_{22}, and D_{33}. For the NPF Package (Langevin and others, 2017) the simplified approach interpolates an effective hydraulic conductivity value from a hydraulic conductivity ellipsoid. For the dispersion coefficient, however, the following simple linear equation is used to calculate an effective value as

$$D_{n,m} = \nu_{D1}^2 D_{11} + \nu_{D2}^2 D_{22} + \nu_{D3}^2 D_{33}, \tag{4–36}$$

where ν_{D1}, ν_{D2}, and ν_{D3} define the three components of a unit vector pointing in the n-m direction and referenced in the local x_L, x_{T1}, x_{T2} flow-aligned coordinate system for cell n. A separate calculation is made for $D_{m,n}$, which is the effective dispersion coefficient for model cell m in the n direction.

The simplified formulation defined by equation 4–32 can provide an accurate estimate of the solute mass flow if (1) all the flux expressions that need to be evaluated reduce to the simplified form in equation 4–31, and (2) the model grid satisfies certain geometric requirements. The MODFLOW 6 GWF Model documentation (Langevin and others, 2017) discusses these "CVFD requirements" in detail and summarizes them as follows:

> "For accurate solutions, the standard CVFD formulation requires that a line drawn between the centers of two connected cells should intersect the shared face at a right angle ... . Furthermore, the intersection point should coincide with an appropriate mean position on the shared face (Narasimhan and Witherspoon, 1976). ... Although this CVFD requirement is met for a simple grid of regular polygons, equilateral triangles, and rectangles, it is violated for nested grids and may be violated for grids with nonregular polygon-shaped cells. ... The smaller the deviation from this CVFD requirement, the smaller the loss of accuracy in the groundwater flow solution. In addition, the errors generally decrease as resolution increases, but they are difficult to quantify."

The constraints on the flux expressions and grid geometry described above imply that the simplified formulation defined by equation 4–32 can provide an accurate estimate of the solute mass flow in the following special cases:

1. **The MODFLOW grid is regular and aligned with the model coordinates, and flow is unidirectional along one of the grid directions.** In this case, every flux component calculation is performed along a grid direction and depends only on the concentration gradient component along that same grid direction.

For example, if flow is uniformly in the x direction in a three-dimensional transport simulation, the y and z components of velocity are zero, the hydrodynamic dispersion tensor is diagonal ($D_{xy} = D_{xz} = D_{yz} = 0$), and the flux components in equation 4–30 simplify to

$$\begin{aligned} f_x^{DSP} &= -S_w \theta D_{xx} \frac{\partial C}{\partial x} \\ f_y^{DSP} &= -S_w \theta D_{yy} \frac{\partial C}{\partial y} \\ f_z^{DSP} &= -S_w \theta D_{zz} \frac{\partial C}{\partial z}. \end{aligned} \tag{4–37}$$

Each of the three flux expressions in equation 4–37 is of the form given in equation 4–30, with s set to x, y, or z. Furthermore, because the grid is regular, it satisfies the CVFD requirements.

2. **The MODFLOW grid satisfies the CVFD requirements, and the longitudinal and relevant transverse dispersivities are always equal to each other, regardless of the flow direction.** Satisfaction of the CVFD requirements is stipulated, so it remains only to discuss the ramifications of equal longitudinal and transverse dispersivities, which are defined in equation 4–20. For a three-dimensional simulation, both transverse dispersivities are relevant, and the requirement is that $\alpha_L = \alpha_{T1} = \alpha_{T2}$ for all flow directions, in which case the hydrodynamic dispersion tensor is diagonal ($D_{xy} = D_{xz} = D_{yz} = 0$) and the flux components in equation 4–30 simplify to the forms in equation 4–37 (with $D_{xx} = D_{yy} = D_{zz}$). This is accomplished by setting $\alpha_{LH} = \alpha_{TH1} = \alpha_{TH2}$ and $\alpha_{LV} = \alpha_{TV}$. For a two-dimensional simulation within the (x, y) (horizontal) plane, α_{T2} is irrelevant, and the requirement that $\alpha_L = \alpha_{T1}$ for all flow directions is satisfied by setting $\alpha_{LH} = \alpha_{TH1}$; the values of α_{LV}, α_{TV}, and α_{TH2} have no effect. For a two-dimensional simulation within either the (x, z) or (y, z) (vertical) plane, α_{T1} is irrelevant, and the requirement that $\alpha_L = \alpha_{T2}$ for all flow directions is satisfied by setting $\alpha_{LH} = \alpha_{TH2}$ and $\alpha_{LV} = \alpha_{TV}$; the value of α_{TH1} has no effect. For a one-dimensional simulation in either the x, y, or z direction, neither transverse dispersivity is relevant, and the constraint on the dispersivities is satisfied by default.

The special cases listed above may apply to an entire grid or to portions of a grid. In cases in which the conditions described above are not met, the XT3D option discussed below can provide a more accurate estimate of the solute mass flow rate. Although it may be possible to implement some type of ghost-node correction, as implemented for flow by Panday and others (2013) and Langevin and others (2017), the XT3D option provides an easier way to improve the flux calculation and is the only method implemented as an alternative to the simple flux calculation.

XT3D Formulation

The XT3D formulation overcomes the limitations of the simplified formulation described above by relating each component of solute mass flux to all three components of the solute concentration gradient vector (equation 4–30). In doing so, XT3D accounts for anisotropy of the dispersion tensor and irregularities in the model grid. The solute concentration gradient vector is estimated by spatial interpolation of concentration values at the nodes of model cells. The implementation of the XT3D formulation for solute mass flow in the GWT Model is mathematically analogous to its implementation for groundwater flow in the GWF Model. The following description of the XT3D formulation is adapted and summarized from the detailed discussion in Provost and others (2017).

The XT3D method produces an expression for the solute mass flow between two model cells, n and m, as a function of the solute concentrations in those two cells and their surrounding cells. Conceptually, the method is the result of three main mathematical steps listed below:

1. On each side of the interface between cells n and m, construction of an expression for the concentration-gradient vector. The expression for the "cell n" side is a function of the concentrations in cell n and its neighbors, and an unknown concentration at the interface. The expression for the "cell m" side is a function of the solute concentrations in cell m and its neighbors, and the unknown concentration at the interface.

2. On each side of the interface between cells n and m, application of the Fickian dispersion equation (equation 4–17) and calculation of an expression for the component of the solute mass flux normal to the interface in terms of the concentrations mentioned above. $\mathbf{D}$ can be anisotropic and different on each side of the interface.

3. Application of the continuity principle, which requires that the solute mass flow crossing the interface between cells n and m be the same on each side of the interface. This allows the unknown concentration at the interface to be solved for and leads to a single expression for the solute mass flow across the interface in terms of the concentrations in cells n and m and their neighbors.

Implementation of the steps enumerated above is based on the following concepts:

- the use of weighted averaging to incorporate gradient information from neighboring connections,
- dependence of weights on distances and orientations, and
- combining information from both sides of the interface.

Figure 4–1 shows the connections used by the XT3D method to estimate the concentration gradient at the interface between two cells, n and its neighbor m, on an unstructured grid. (Although the grid shown in figure 4–1 consists of regular hexagons, the XT3D method is applicable to more general unstructured grids, as well.) In this context, the connection between cells n and m is the "primary connection," and the corresponding interface is the "primary interface." The gradient is estimated at the point at which the primary connection intersects the primary interface, which is marked with an "X." The component of the gradient along the primary connection is estimated simply by differencing along the primary connection. An obvious approach would be to difference over the entire length of the primary connection; that is, between the nodes n and m. Instead, an "unknown" concentration value is temporarily assigned to the point on the primary interface, and differencing along the primary connection is performed between node n and the interface, and between node m and the interface. The unknown solute concentration is eventually eliminated as a variable by enforcing continuity of the normal flux at the primary interface.

In the simplified formulation, the solute mass flow from cell m into cell n (equation 4–32) involves concentrations only at nodes n and m. In contrast, the spatial interpolation (weighted averaging) performed by XT3D results in a solute mass flow expression that involves concentration values from all neighbors of cells n and m:

$$F_{n,m}^{DSP} = D_{n,m,(n,m)}\left(C_m - C_n\right) + \sum_{\substack{p\in\eta_n \\ p\neq m}} D_{n,p,(n,m)}\left(C_p - C_n\right) - \sum_{\substack{q\in\eta_m \\ q\neq n}} D_{m,q,(n,m)}\left(C_q - C_m\right), \qquad (4\text{–}38)$$

where the first summation is over neighbors of cell n, excluding cell m, the second summation is over neighbors of cell m, excluding cell n. The "D" coefficients are analogous to "conductances" for flow of solute mass

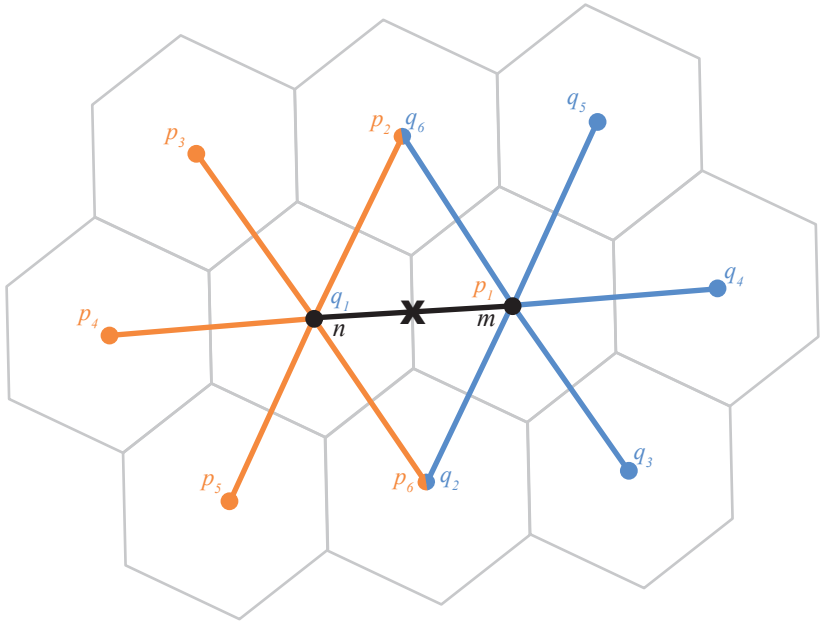

Figure 4–1. The connections used by the XT3D method, in two dimensions, to estimate the concentration gradient at a point ("X") on the interface between cells n and m (the "primary" interface). A separate estimate of the concentration gradient at point X is formulated using information from each side of the primary interface. On the "node n" side of the primary interface, the component of the gradient along the primary connection (black line) is estimated by finite differencing the concentrations at node n and point X, and the component of the gradient perpendicular to the primary connection is estimated using gradient-component information from connections between node n and its neighbors p_2, ..., p_6 (orange lines). An analogous procedure involving node m and its connections with its neighbors q_2, ..., q_6 (blue lines) is used to formulate an estimate of the concentration gradient for the "node m" side of the primary interface. Modified from Provost and others (2017).

driven by concentration differences and incorporate the effects of the dispersion coefficients in cells n and m, the saturation-dependent interfacial area over which the dispersive flux occurs, and other geometric information. Formulation of the "D" coefficients for dispersive transport is directly analogous to the formulation of the XT3D conductance-like "C" coefficients for groundwater flow described in Provost and others (2017). Subscripts on the "D" coefficients indicate the cell-cell connection from which the coefficient derives and the cell-cell interface to which it applies. For example, $D_{n,p,(n,m)}$ is the coefficient that derives from the connection between cell n and neighboring cell p and applies to calculating the solute mass flow at the interface between cells n and m.

The XT3D option is applicable to both regular and irregular model grids, whether the dispersion tensor is isotropic or anisotropic. The XT3D option is on by default for transport (XT3D is not on by default for the GWF model). The simplified formulation can be activated by turning off the XT3D option. The XT3D option tends to be more computationally intensive than using the simplified formulation. Before deciding whether to use the simplified formulation or XT3D option for production runs, the user should consider whether the simplified formulation alone can provide acceptable accuracy for the particular problem being solved. Trial runs that compare solution accuracy and run times for different formulations can be helpful in this regard.

When the concentration gradient is uniform in the vicinity of a cell interface and its neighboring connections, the XT3D estimate of solute mass flow across the interface is exact. When the concentration gradient is nonuniform, as is typically the case in practice, and anisotropy of the dispersion tensor is not aligned with the model-coordinate axes, XT3D handles the gradient nonuniformity by weighted averaging of gradient-component information. Such averaging is conceptually similar to the averaging done in standard finite differencing on a rectangular grid. If accuracy is a concern when simulating dispersion with anisotropy that is not aligned with the model coordinates and driven by substantially nonuniform gradients, such as the gradients associated with strong sources and sinks of solute mass, grid refinement can be used to estimate the discretization error.

If a cell is inactive or the head is below the cell bottom, as is possible with the Newton flow formulation, the XT3D method for the GWT Model is not used and the dispersive flux is set to zero.

Numerical simulations of highly anisotropic flow or transport based on CVFD and finite-element discretizations can exhibit "spurious oscillations" in the solution (Pal and Edwards, 2011). Although it can be difficult to distinguish spurious oscillations from legitimate variations in concentration in complex flow and transport systems, solutions calculated using XT3D for highly anisotropic systems should be evaluated critically for evidence of unrealistic patterns in concentration or solute mass flow. For example, in a steady-state groundwater flow and transport problem, the concentration solution should not exhibit a local maximum or minimum within the interior of the model domain unless there is a corresponding source or sink of solute mass at that location or solute decay or production that can explain the pattern.

Chapter 5. Sources and Sinks of Solute Mass

There are three different packages in the MODFLOW 6 GWT Model that can be used to represent sources and sinks of solute mass. These packages include the Constant-Concentration (CNC), Source-Sink Mixing (SSM), and the Source Mass Loading (SRC) Packages, which are described in this chapter.

Constant-Concentration (CNC) Package

The CNC Package for the MODFLOW 6 GWT Model allows a cell to be marked as a constant-concentration cell in which the solute concentration is fixed at a user-specified value for the duration of a time step. Users may change the value of this fixed concentration for each time step, and so it is important to emphasize that "constant" means that the concentration is fixed for the time step. Furthermore, the user may change the cell status from a constant-concentration condition to an active cell or from an active cell to a constant-concentration condition.

A constant-concentration cell is handled differently from other types of sources and sinks in that the solute concentration for the cell is not solved. Instead, the cell is marked to be handled in a special way by the solution routine. When a cell is marked as a constant concentration cell, the balance equation is manipulated such that

$$A_{n,n} = 1, \tag{5–1}$$

$$b_n = C_s, \tag{5–2}$$

and

$$A_{n,m \neq n} = 0, \tag{5–3}$$

where C_s is the concentration specified by the user. With this approach, the concentration for the cell is calculated ($C_n = b_n / A_{n,n}$) to be the concentration specified by the user. Adjacent active cells connected to a constant-concentration cell n will likely have non-zero $\mathbf{A}$ coefficients in their balance equations, because of advection and dispersion terms added by the ADV and DSP Packages, respectively. Upon solution of the system of equations, those active cells will show a non-zero mass flow to or from the connected constant-concentration cell. These mass flows are tabulated and provided to the user as model output.

Although constant-concentration conditions are easy to implement and specify for a solute transport model, they are not often used in practice, because they can result in unrealistically large mass fluxes. For most applications, users are encouraged to use the SSM or SRC Packages to represent solute sources and sinks.

Flow Model Source and Sink Mixing (SSM) Package

The Source and Sink Mixing (SSM) Package simulates the change in the solute mass caused by groundwater inflows and outflows from GWF stress and advanced stress packages. Stress boundaries can be assigned a user-specified solute concentration so that a solute mass flux can be calculated for inflow to a model cell. The addition of water from a stress boundary may increase or decrease the concentration in the cell, depending on

whether the user-specified concentration is greater than or less than the cell concentration. Flow packages that can act as sources or sinks within the SSM Package are shown in table 5–1.

Table 5–1. List of Groundwater Flow Model Packages that can act as a solute source or sink for the MODFLOW 6 Groundwater Transport Model.

Package Name	Abbreviation	Package Category
Specified Head	CHD	Stress
Well	WEL	Stress
Recharge	RCH	Stress
River	RIV	Stress
General-Head Boundary	GHB	Stress
Drain	DRN	Stress
Evapotranspiration	EVT	Stress
Stream-Flow Routing	SFR	Advanced Stress
Lake	LAK	Advanced Stress
Multi-Aquifer Well	MAW	Advanced Stress
Unsaturated Zone Flow	UZF	Advanced Stress

There are two alternative ways in which the advanced stress packages (SFR, LAK, MAW, and UZF; table 5–1) can be represented in the GWT Model. The simplest way is for the user to assign a concentration for any inflow into the GWT Model domain from the advanced stress package. This simpler approach is part of the SSM Package described here. Alternatively, solute transport can be explicitly simulated within these advanced stress packages using a more sophisticated approach, as described in the next chapter (chapter 6). When this more sophisticated approach is used, solute concentrations are calculated for the individual advanced stress package features, and these calculated concentrations are assigned to flows into the connected model cells.

The effect of groundwater sources and sinks, as shown in the mathematical equations for solute transport (eqs. 2–1, 2–2, and 2–4), is expressed as

$$f^{SSM} = q'_s C_s. \tag{5–4}$$

In the GWT Model, the user is allowed to assign multiple solute sources and sinks to a single model cell, and the concentrations for these individual sources and sinks also may vary. The fourth term on the left-hand side of equation 2–9, the net rate at which solute mass is entering or leaving cell n due to external sources and sinks associated with stress packages, is simply the sum of all $nssm$ sources and sinks, defined as

$$\dot{M}_n^{SSM} = \sum_{issm=1}^{nssm} Q_{n,issm} C_{n,issm} \tag{5–5}$$

where $Q_{n,issm}$ is the volumetric groundwater flow rate (L^3/T) into or out of cell n by way of a stress package source and sink. The variable $issm$ is included here to indicate that the formulation works for multiple groundwater sources and sinks assigned to the same cell. For inflow to cell n, $C_{n,issm}$ is the solute concentration of the stress package source. For outflow from cell n into a stress package feature, $C_{n,issm}$ is the calculated solute concentration in cell n.

The effects of the mass inflow or outflow due to stress package sources and sinks are added to the system of equations differently, depending on the sign of each $Q_{n,issm}$ term. For flow into model cell n ($Q_{n,issm}$ >0), the right-hand-side term is updated as

$$b_n \leftarrow b_n - Q_{n,issm}C_{n,issm}. \tag{5–6}$$

If flow is out of the model cell n ($Q_{n,issm}$ <0), then the SSM Package has two different options for how to determine the concentration that is assigned to the outflow. The default option is to remove the water at the same concentration as the cell. For this condition, the **A** matrix is updated as

$$A_{n,n} \leftarrow A_{n,n} + Q_{n,issm}. \tag{5–7}$$

The other option is for the user to specify a concentration for the outflow as $C_{n,issm}$. If this user-specified concentration is less than the concentration of the cell, then the right-hand-side term is updated according to equation 5–6. If the user-specified concentration is greater than the cell concentration, then water is withdrawn at the cell concentration and equation 5–7 is used.

Source Mass Loading (SRC) Package

Solute mass inflow or outflow not associated with the inflow or outflow from a GWF Model stress package can be specified by the user through the $\dot{M}_n^{SRC}$ term. This term allows users to add or remove solute mass directly to or from a model cell without an associated addition or withdrawal of water. The SRC Package is flexible in that multiple source and sink terms can be specified, including multiple terms for a single cell, as

$$\dot{M}_n^{SRC} = \sum_{isrc=1}^{nsrc} M_{n,isrc}^{SRC}, \tag{5–8}$$

where $nsrc$ is the number of source terms for cell n. Values for $M_{n,isrc}^{SRC}$ are specified by the user, and can be negative to remove solute mass or positive to add solute mass. If a negative value is specified by the user for $M_{n,isrc}^{SRC}$, then it is possible that the calculated solute concentration could be also negative. This cannot be determined before the start of the simulation, however.

The effect of the mass source term is included in the system of equations by simply updating the right-hand side as

$$b_n \leftarrow b_n - M_{n,isrc}^{SRC}. \tag{5–9}$$

This update is simply the addition of the user-specified mass inflow or removal rate to the balance equation, which is written in terms of M/T.

Use of this source and sink rate can be problematic in some instances. If $\dot{M}_n^{SRC}$ is specified as negative, then it is possible that the simulated concentrations will be negative, and there is no mechanism to prevent this other than the user adjusting the removal rate. Likewise, large source rates can result in concentrations that may not be reasonable. It is important that the user ensures that realistic rates are used.

Chapter 6. Transport for Advanced Stress Packages

The GWT Model has two different options for representing the effects of advanced stress packages (SFR, LAK, MAW, UZF, and MVR; table 5–1) on solute transport in an aquifer. The first option is to treat features in the advanced stress packages as sources and sinks with user-specified concentrations and use the SSM Package described in the previous chapter. With this SSM approach, the user can assign a solute concentration to features in the advanced stress packages. If water flows into a model cell from the feature, then that water enters the cell at the concentration specified by the user. If water leaves the model cell, then water exits the cell at the calculated concentration of the cell. With this approach, solute is not transported or tracked once it leaves the GWT Model cell and enters an advanced package feature.

In the second option, solute transport can be explicitly simulated for the advanced stress packages of the GWF Model (Langevin and others, 2017) by solving solute balance equations for each feature. For example, if the Streamflow Routing (SFR) Package is used to simulate flow in a stream network, then the GWT Model can simulate solute transport within the stream network itself, and transport between the stream and underlying aquifer. The approach presented here tightly couples solute transport in the aquifer with solute transport in the advanced package features. Tight coupling is implemented by adding additional rows to the matrix equations to solve a solute concentration for each advanced package feature. Specialized transport packages were written for each of the advanced stress packages and the Water Mover Package. These transport packages include the Streamflow Transport (SFT), Lake Transport (LKT), Multi-Aquifer Well Transport (MWT), Unsaturated Zone Transport (UZT), and Mover Transport (MVT) Packages. For the SFR Package, a feature is an individual stream reach. For the LAK Package a feature is a single lake. For the MAW Package, a feature is a single multi-aquifer well, and for the UZF Package, a feature is a single unsaturated zone flow cell.

The advanced package transport routines formulate a separate control-volume finite-difference equation for each feature in a way that is similar to what is done for a single model cell. The advanced package transport routines follow the same general pattern, which involves solving a form of the following equation,

$$\dot{M}_n^{storage} + \dot{M}_n^{advection} + \dot{M}_n^{to-mover} + \dot{M}_n^{from-mover} + \dot{M}_n^{sinks/sources} = 0, \tag{6–1}$$

where the n subscript indicates that the equation is for feature n, $\dot{M}_n^{storage}$ is the rate of change of solute mass in feature n per time (a positive value for $\dot{M}_n^{storage}$ indicates that solute mass in feature n is decreasing), $\dot{M}_n^{advection}$ is the sum of all advective inflow and outflow, $\dot{M}_n^{to-mover}$ is the rate of mass transfer to the water mover, $\dot{M}_n^{from-mover}$ is the rate of solute mass added to the feature from the water mover, and $\dot{M}_n^{sinks/sources}$ is the rate of solute mass added to or removed from the feature due to sources and sinks, which are defined separately for each advanced transport package (SFT, LKT, MWT, and UZT).

In the version of the GWT Model described here, the advanced package transport routines do not represent sorption, decay, or a dispersive flux between adjacent features or a feature and adjacent GWT Model cells. Although these terms could be added to these advanced transport packages in the future, the focus of the present implementation is on advective transport of a conservative dissolved constituent.

The terms in equation 6–1 are described in the remainder of this chapter. The storage and advection terms are solved using generalized routines that work with all of the advanced packages, including SFT, LKT, MWT, and UZT. The source and sink term in equation 6–1 has different implementations depending on the advanced package. For example, SFT and LKT can both be affected by rainfall, which may have an associated solute concentration, whereas rainfall is not a source term for MWT. Accordingly, the sink and source term, which may contain multiple types for an advanced package, is described in subsequent sections for those packages. The mover terms in equation 6–1 are described in the "Water Mover Terms and the Mover Transport (MVT) Package" section of this chapter.

Storage Term

The storage term in equation 6–1 is expressed as

$$\dot{M}^{storage} = \frac{1}{\Delta t}\left(-C^{t+\Delta t}V_w^{t+\Delta t} + C^t V_w^t\right), \tag{6–2}$$

where the solute concentration (C) and volume (V_w) terms represent the concentration and water volume of feature n at the start (t) and end ($t + \Delta t$) of the time step.

The equation for aqueous solute storage is added to the system of equations by updating the diagonal position of the $\mathbf{A}$ matrix for row n, corresponding to a specific feature within an advanced package, with the coefficient of the $C^{t+\Delta t}$ term in equation 6–2 as

$$A_{n,n} \leftarrow A_{n,n} - \frac{V_w^{t+\Delta t}}{\Delta t}, \tag{6–3}$$

and by moving the remaining $\frac{C^t V_w^t}{\Delta t}$ term to the right-hand side to update b_n as

$$b_n \leftarrow b_n - \frac{C^t V_w^t}{\Delta t}. \tag{6–4}$$

Implementation of this generic storage term allows the solute concentration to be calculated within each feature based on changes in water volume and the solute balance for each feature.

Advection Term

The advection term in equation 6–1 includes flows to and from adjacent features in an advanced package as well as flows to and from connected GWT Model cells. Following the weighted advective flux equation 4–12, this advection term is expressed as

$$\dot{M}^{advection} = \sum_{m \in \eta_n} \omega_{n,m} Q_{n,m} C_n + \left(1 - \omega_{n,m}\right) Q_{n,m} C_m, \tag{6–5}$$

where m is an adjacent advanced package feature or connected GWT Model cell, η_n is a list of all connected features and GWT model cells, $\omega_{n,m}$ is the upstream weighting factor determined using equation 4–5, and $Q_{n,m}$ is the volumetric flow rate between n and m defined as positive into n.

As shown in equations 4–13 and 4–14, the matrix coefficient in the diagonal position for row n is updated by adding the term $\omega_{n,m} Q_{n,m}$ as

$$A_{n,n} \leftarrow A_{n,n} + \omega_{n,m} Q_{n,m}. \tag{6–6}$$

The matrix coefficient in row n that corresponds to the connection between cell n and neighboring cell m is updated by adding the term $\left(1 - \omega_{n,m}\right) Q_{n,m}$ as

$$A_{n,m} \leftarrow A_{n,m} + \left(1 - \omega_{n,m}\right) Q_{n,m}. \tag{6–7}$$

Water Mover Terms and the Mover Transport (MVT) Package

The Water Mover (MVR) Package of the MODFLOW 6 GWF Model can be used to dynamically transfer water from a provider package to a receiver package, based on rules described by (Langevin and others, 2017). Providers can include regular stress package features, such as a drain, a general-head boundary, or a river cell, for example. Providers may also include a feature in an advanced stress package, such as a stream, lake, multi-aquifer well, or an unsaturated zone cell. Receivers are restricted to a feature in an advanced stress package; there is no way to transfer water to one of the regular stress packages, because they do not solve a continuity equation. The $\dot{M}_n^{to-mover}$ and $\dot{M}_n^{from-mover}$ terms in equation 6–1 represent the solute mass flux removed and added by the mover, respectively. The present mover transport implementation does not include dispersive transport as part of this mass transfer; only advective transport is represented.

When a feature in a regular or advanced stress package acts as a provider to the water mover, solute leaves the feature at a rate equal to the product of the water mover flow rate and the solute concentration of the feature:

$$\dot{M}_n^{to-mover} = Q_n^{to-mover} C_n, \tag{6–8}$$

where $Q_n^{to-mover}$ is the volumetric rate of water transferred to the water mover (which is negative in sign as water is being removed from feature n), and C_n is the simulated concentration of the feature in the stress package. The effect of the transferred water is included in the system of equations by updating the diagonal position of the $\mathbf{A}$ matrix for row n as

$$A_{n,n} \leftarrow A_{n,n} + Q_n^{to-mover}. \tag{6–9}$$

When a feature in an advanced stress package acts as a receiver, then the water that it receives can have an associated solute concentration. The Water Mover Transport (MVT) Package was implemented for the MODFLOW 6 GWT Model to facilitate the transfer of solute from providers to receivers. Because the GWF Model MVR Package is generalized and allows multiple providers to transfer water to a single receiver, the GWT Model MVT Package accumulates these solute mass fluxes into a $\dot{M}_n^{from-mover}$ term (which is positive in sign) for each feature of an advanced package as the system of equations is formulated. The advanced package then adds the accumulated solute mass flux as a source of mass from the mover by updating the right-hand-side vector as

$$b_n \leftarrow b_n - \dot{M}_n^{from-mover}. \tag{6–10}$$

Thus, the $\dot{M}_n^{to-mover}$ terms are handled in a fully implicit manner and added to the left-hand side, whereas the $\dot{M}_n^{from-mover}$ terms are added to the right-hand side. A fully implicit approach could be added in the future for the $\dot{M}_n^{from-mover}$ terms as a way to improve convergence of the numerical solution; however, this addition of an implicit approach would require adding matrix-level connections for all provider and receiver combinations.

Streamflow Transport (SFT) Package

The Streamflow Transport (SFT) Package simulates solute concentrations in each stream reach based on a numerical solution of the solute transport balance equation (eq. 2–12). Because the corresponding SFR Package simulates one-dimensional vertically averaged flow within a stream channel, the SFT Package simulates a

single solute concentration for each reach. This approach assumes that all of the water entering a reach instantaneously mixes with water in the stream reach. Thus, there is no way to represent stratification or variations of solute concentration with depth using the current SFT Package implementation.

The generalized balance equation 6–1 for an advanced package feature, which is a reach for SFT, includes a source and sink term, $\dot{M}_n^{sinks/sources}$. Source and sink terms for the SFT Package include rainfall, evaporation, external inflow, and external outflow. These source and sink terms are included in the balance equation by updating the diagonal position of the $\mathbf{A}$ matrix and the right-hand-side vector element for row n according to the equations in table 6–1.

Table 6–1. Source and sink equations for Streamflow Transport Package of the MODFLOW 6 Groundwater Transport Model.

[The $A_{n,n} \leftarrow$ column represents the term that is added to the diagonal position of the $\mathbf{A}$ matrix; $b_n \leftarrow$ column represents the term that is added to the right-hand-side vector; C_s is the user specified concentration for this source or sink term; Q_s is the volumetric flow rate provided by the corresponding Groundwater Flow Model stress package for this source or sink term; C_n is the solute concentration of the stream reach; ω is a weighting factor used to shift between the left-hand-side and right-hand-side implementations based on solute concentration]

Source or Sink	$\dot{M}_n^{sinks/sources}$	$A_{n,n} \leftarrow$	$b_n \leftarrow$	Note
Rainfall (source)	$C_s Q_s$	zero	$-C_s Q_s$	-
Evaporation (sink)	$\omega Q_s C_n + (1-\omega) Q_s C_s$	ωQ_s	$-(1-\omega) Q_s C_s$	$\omega = \begin{cases} 1 & \text{if } C_n < C_s \\ 0 & \text{if } C_n \geqslant C_s \end{cases}$
External inflow (source)	$C_s Q_s$	zero	$-C_s Q_s$	-
External outflow (sink)	$C_n Q_s$	Q_s	zero	-

Lake Transport (LKT) Package

The Lake Transport (LKT) Package simulates solute concentrations in each lake based on a numerical solution of the solute transport balance equation (eq. 2–12). Because the corresponding LAK Package simulates a single stage for the entire lake and does not represent flow within the lake, the LKT Package simulates a single concentration for each lake. This approach assumes that all of the water entering a lake instantaneously and thoroughly mixes with lake water. Thus, there is no way to represent stratification or variations of solute concentration with depth using the current LKT Package implementation.

The generalized balance equation 6–1 for an advanced package feature, which is a lake for LKT, includes a source and sink term, $\dot{M}_n^{sinks/sources}$. Source and sink terms for the LKT Package include rainfall, evaporation, external inflow, external outflow, and withdrawal. These source and sink terms are included in the balance equation by updating the diagonal position of the $\mathbf{A}$ matrix and the right-hand-side vector element for row n according to the equations in table 6–2.

Table 6–2. Source and sink equations for Lake Transport Package of the MODFLOW 6 Groundwater Transport Model.

[The $A_{n,n} \leftarrow$ column represents the term that is added to the diagonal position of the $\mathbf{A}$ matrix; $b_n \leftarrow$ column represents the term that is added to the right-hand-side vector; C_s is the user specified concentration for this source or sink term; Q_s is the volumetric flow rate provided by the corresponding Groundwater Flow Model stress package for this source or sink term; C_n is the solute concentration of the lake; ω is a weighting factor used to shift between the left-hand-side and right-hand-side implementations based on solute concentration]

Source or Sink	$\dot{M}_n^{sinks/sources}$	$A_{n,n} \leftarrow$	$b_n \leftarrow$	Note
Rainfall (source)	$C_s Q_s$	zero	$-C_s Q_s$	-
Evaporation (sink)	$\omega Q_s C_n + (1-\omega) Q_s C_s$	ωQ_s	$-(1-\omega) Q_s C_s$	$\omega = \begin{cases} 1 & \text{if } C_n < C_s \\ 0 & \text{if } C_n \geqslant C_s \end{cases}$
External inflow (source)	$C_s Q_s$	zero	$-C_s Q_s$	-
External outflow (sink)	$C_n Q_s$	Q_s	zero	-
Withdrawal (sink)	$C_n Q_s$	Q_s	zero	-

Multi-Aquifer Well Transport (MWT) Package

The Multi-Aquifer Well Transport (MWT) Package simulates solute concentrations in each well based on a numerical solution of the solute transport balance equation (eq. 2–12). The MWT Package simulates a single concentration for each well. This approach assumes that all of the water entering a multi-aquifer well is instantaneously and thoroughly mixed with well water. There is no option at present to represent stratification or variations of solute concentration with depth in a well.

The generalized balance equation 6–1 for an advanced package feature, which is a multi-aquifer well for MWT, includes a source and sink term, $\dot{M}_n^{sinks/sources}$. Source and sink terms for the MWT Package include withdrawal and flowing well rate (rate of free flowing discharge due to artesian conditions). These source and sink terms are included in the balance equation by updating the diagonal position of the $\mathbf{A}$ matrix and the right-hand-side vector element for row n according to the equations in table 6–3.

Table 6–3. Source and sink equations for Multi-Aquifer Well Transport Package of the MODFLOW 6 Groundwater Transport Model.

[The $A_{n,n} \leftarrow$ column represents the term that is added to the diagonal position of the $\mathbf{A}$ matrix; $b_n \leftarrow$ column represents the term that is added to the right-hand-side vector; C_s is the user specified concentration for this source or sink term; Q_s is the volumetric flow rate provided by the corresponding Groundwater Flow Model stress package for this source or sink term; C_n is the solute concentration of the multi-aquifer well; ω is a weighting factor used to shift between the left-hand-side and right-hand-side implementations based on the sign of the well flow rate]

Source or Sink	$\dot{M}_n^{sinks/sources}$	$A_{n,n} \leftarrow$	$b_n \leftarrow$	Note
Well rate (source or sink)	$\omega Q_s C_n + (1-\omega) Q_s C_s$	ωQ_s	$-(1-\omega) Q_s C_s$	$\omega = \begin{cases} 1 & \text{if } Q_s < 0 \\ 0 & \text{if } Q_s \geqslant 0 \end{cases}$
Flowing well rate (sink)	$C_n Q_s$	Q_s	zero	-

Unsaturated Zone Transport (UZT) Package

The Unsaturated Zone Transport (UZT) Package simulates solute concentrations in each UZT cell based on a numerical solution of the solute transport balance equation (eq. 2–12). Although the corresponding UZF Package simulates individual wetting fronts, the UZT Package calculates an average concentration for the entire UZT cell. Individual wetting front concentrations are not calculated or tracked, although this feature could be implemented in the future.

The generalized balance equation 6–1 for an advanced package feature, which is an unsaturated zone cell for UZT, includes a source and sink term, $\dot{M}_n^{sinks/sources}$. Source and sink terms for the UZT Package include infiltration, rejected infiltration, and unsaturated zone evapotranspiration. These source and sink terms are included in the balance equation by updating the diagonal position of the $\mathbf{A}$ matrix and the right-hand-side vector element for row n according to the equations in table 6–4.

Table 6–4. Source and sink equations for Unsaturated Zone Transport Package of the MODFLOW 6 Groundwater Transport Model.

[The $A_{n,n} \leftarrow$ column represents the term that is added to the diagonal position of the $\mathbf{A}$ matrix; $b_n \leftarrow$ column represents the term that is added to the right-hand-side vector; C_s is the user specified concentration for this source or sink term; Q_s is the volumetric flow rate provided by the corresponding Groundwater Flow Model stress package for this source or sink term; C_n is the solute concentration of the unsaturated zone feature; ω is a weighting factor used to shift between the left-hand-side and right-hand-side implementations based on solute concentration]

Source or Sink	$\dot{M}_n^{sinks/sources}$	$A_{n,n} \leftarrow$	$b_n \leftarrow$	**Note**
Infiltration (source)	$C_s Q_s$	zero	$-C_s Q_s$	-
Rejected infiltration (sink)	$C_s Q_s$	zero	$-C_s Q_s$	-
Evapotranspiration (sink)	$\omega Q_s C_n + (1-\omega) Q_s C_s$	ωQ_s	$-(1-\omega) Q_s C_s$	$\omega = \begin{cases} 1 & \text{if } C_n < C_s \\ 0 & \text{if } C_n \geqslant C_s \end{cases}$

Chapter 7. Immobile Domain Storage and Transfer

Models of solute transport in heterogeneous groundwater systems often rely on conceptual models that involve multiple domains. For example, if a system can be conceptualized as having a fast (mobile) domain and a slow (immobile) domain, then advection and dispersion can be represented in the mobile domain and assumed to be negligible in the immobile domain. Under this conceptual model, the exchange between the mobile and immobile domains can be represented as a diffusive process with a simple linear exchange coefficient. Solute moves through the system in the mobile domain and can diffuse into or out of the immobile domain based on concentration differences. If the concentration in the mobile domain is higher than the concentration in the immobile domain, then solute mass will diffuse into the immobile domain. Alternatively, if the concentration in the mobile domain is less than the concentration in the immobile domain, then solute mass will diffuse into the mobile domain. This conceptual model has been implemented in many solute transport modeling programs, including MOC3D (Goode, 1999) and MT3DMS (Zheng and Wang, 1999).

Conceptual models for mobile and immobile domains are shown in figure 7–1. In figure 7–1A, an idealized sand aquifer is shown to contain evenly distributed and isolated clay and silt nodules. If the size of these nodules is similar or greater than the size of a model cell, then these low permeability features should be explicitly represented in the flow model as cells with reduced hydraulic conductivity compared to aquifer cells. If these nodules are much smaller than a model cell and are evenly distributed, then their effects on solute transport can be represented using immobile domain concepts. Likewise, fractured aquifers (fig. 7–1B) that can be approximated as an equivalent porous medium for groundwater flow may benefit from immobile domain concepts for solute transport. The fractures represent the fast moving mobile domain, and the less permeable rock matrix acts as an immobile domain that is capable of storing and releasing solute mass.

With the immobile domain conceptual model, groundwater does not flow through these nodules, and thus, their pore water is immobile. This conceptual model dictates that mobile domain porosity be calculated as the volume of voids in the mobile domain divided by the total volume. Likewise, the immobile domain porosity θ_{im} is defined as the volume of immobile domain pores divided by the total volume. Concentration within the mobile domain is tracked separately from the concentration in the immobile domain. For a model cell, an average concentration is calculated for the mobile domain, and an average concentration is calculated for each immobile domain. The flux of solute mass between the mobile domain and immobile domain im is represented as a diffusive process that can be expressed in the form

$$f^{IST} = -\zeta_{im} S_w \left(C - C_{im} \right), \tag{7–1}$$

where S_w is the mobile-domain saturation, and the immobile domain is assumed to be fully saturated. The transfer rate is calculated based on the concentration difference between the mobile and immobile domains and a mass transfer coefficient, ζ_{im} $(1/T)$, and the area available for mass transfer is assumed to be proportional to S_w. Under idealized conditions, values for ζ_{im} can be calculated based on the surface area of the immobile domain in contact with the mobile domain at full saturation and other geometric properties of the immobile domain, but in practice, ζ_{im} and other immobile domain properties are estimated through model calibration.

The Immobile domain Storage and Transfer (IST) Package in MODFLOW 6 simulates the effects of mass transfer between the mobile domain and an immobile domain. In the present implementation, there can be as many immobile domains as necessary, with each immobile domain being represented by a separate instance of an IST Package. For example, one immobile domain package can represent the clay nodules in figure 7–1A, and another immobile domain package can be used to represent the silt nodules. Each immobile domain can be assigned different properties and exchange coefficients, and these values can vary throughout the model grid. In this case, a separate concentration is also calculated for each immobile domain. Immobile domains do not interact with other immobile domains; an immobile domain can only interact with the mobile domain.

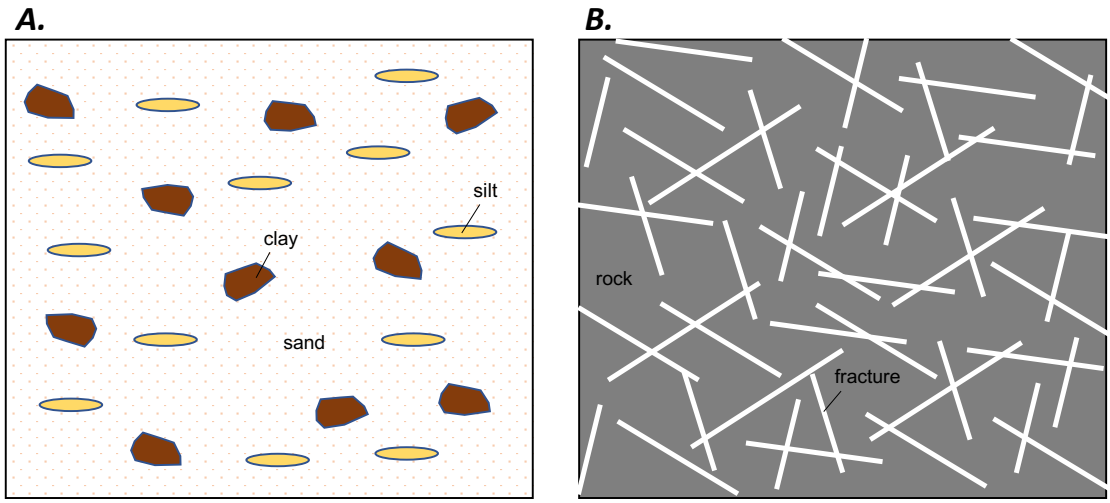

Figure 7–1. Two conceptualizations for mobile and immobile domains: (A) sand aquifer containing clay and silt nodules, and (B) fractured aquifer.

The immobile domain terms in equations 2–1, 2–2, and 2–4 contribute to the mass balance equation for solute in the mobile domain. In order to represent the dual domain mass transfer process, a separate governing equation must be written for the immobile domain (Zheng and Wang, 1999; Zheng and Bennett, 2002). If written to include the effects of sorption and decay in the immobile domain, as well as the transfer with the mobile domain, the governing equation for the immobile domain is

$$\theta_{im}\frac{\partial C_{im}}{\partial t} + f_{im}\rho_b\frac{\partial \overline{C}_{im}}{\partial t} = -\lambda_{1,im}\theta_{im}C_{im} - \lambda_{2,im}f_{im}\rho_b\overline{C}_{im} - \gamma_{1,im}\theta_{im} - \gamma_{2,im}f_{im}\rho_b + \zeta_{im}S_w\left(C - C_{im}\right), \tag{7–2}$$

where θ_{im} is the volume of the immobile pores per volume of aquifer, f_{im} is the fraction of aquifer solid material available for sorptive exchange with the immobile domain under fully saturated conditions, $\overline{C}_{im}$ is the sorbed concentration of the immobile domain, expressed as the mass of the sorbed chemical per mass of solid, $\lambda_{1,im}$ is the first-order reaction rate coefficient for the liquid phase of the immobile domain ($1/T$), $\lambda_{2,im}$ is the first-order reaction rate coefficient for the sorbed phase of the immobile domain ($1/T$), $\gamma_{1,im}$ is the zero-order reaction rate coefficient for the liquid phase of the immobile domain ($ML^{-3}T^{-1}$), and $\gamma_{2,im}$ is the zero-order reaction rate coefficient for the sorbed phase of the immobile domain ($MM^{-1}T^{-1}$). As noted by Zheng and Bennett (2002) f_{im}, can be approximated as $f_{im} = \theta_{im}/\theta$. This approximation is the default approach implemented in MODFLOW 6 and can be shown to be restricted to cases where the immobile domain porosity is the same as the mobile domain porosity and half of the domain is mobile and the other half is immobile, for example. The MODFLOW 6 program may be modified in the future so that users can specify values for f_{im} based on the fractions and porosities of the domains.

As noted by Ma and Zheng (2011) different forms of ζ_{im} have been reported in the literature. Ma and Zheng (2011) define classic and alternate forms, which differ by a factor of θ_{im}. With the approach developed here, based on equations 7–1 and 7–2, the definition of ζ_{im} in this report corresponds to the classic form, which is the form implemented in the various versions of MT3D.

Care should be taken when using the IST Package for simulations in which cells can become dry. When a cell becomes dry, the cell is removed from the solution and no transport calculations are made. Thus, if there is solute mass in the immobile domain, the mass may become trapped, and unable to reenter the groundwater

flow system. Any mass trapped in the immobile domain for a dry cell also will not be subjected to first-order or zero-order decay or production, though this may be supported in future versions. These issues do not occur if the flow model uses the Newton formulation. With the Newton formulation, model cells are not removed from the solution; instead, these cells remain active and subject to decay and production processes.

Following the solution approach outlined in Zheng and Bennett (2002), a discretized form of equation 7–1 can be written for a model cell as

$$\dot{M}_n^{IST} = -V_{cell} S_w^{t+\Delta t} \zeta_{im} C^{t+\Delta t} + V_{cell} S_w^{t+\Delta t} \zeta_{im} C_{im}^{t+\Delta t}, \tag{7–3}$$

where a positive value indicates solute transfer from the immobile domain into the mobile domain. The second term on the right side of equation 7–3, which contains the immobile domain concentration, is recast as a function of the mobile domain concentration. In order to express $C_{im}^{t+\Delta t}$ as a function of mobile domain solute concentrations and other known terms, an implicit finite-difference approximation can be applied to equation 7–2, the balance equation for the immobile domain. The implicit finite-difference equation for the immobile domain is

$$\begin{aligned} \frac{\theta_{im} V_{cell}}{\Delta t} C_{im}^{t+\Delta t} - \frac{\theta_{im} V_{cell}}{\Delta t} C_{im}^{t} + \frac{f_{im} \rho_b V_{cell}}{\Delta t} K_d C_{im}^{t+\Delta t} - \frac{f_{im} \rho_b V_{cell}}{\Delta t} K_d C_{im}^{t} \\ = \\ -\lambda_{1,im} \theta_{im} V_{cell} C_{im}^{t+\Delta t} - \lambda_{2,im} f_{im} V_{cell} \rho_b K_d C_{im}^{t+\Delta t} \\ -\gamma_{1,im} \theta_{im} V_{cell} - \gamma_{2,im} f_{im} \rho_b V_{cell} \\ +V_{cell} S_w^{t+\Delta t} \zeta_{im} C^{t+\Delta t} - V_{cell} S_w^{t+\Delta t} \zeta_{im} C_{im}^{t+\Delta t}. \end{aligned} \tag{7–4}$$

From this equation, an expression for $C_{im}^{t+\Delta t}$ as a function of $C^{t+\Delta t}$ and other known terms can be written as

$$C_{im}^{t+\Delta t} = \frac{V_{cell} S_w^{t+\Delta t} \zeta_{im}}{F} C^{t+\Delta t} + \frac{\frac{\theta_{im} V_{cell}}{\Delta t} + \frac{f_{im} \rho_b V_{cell}}{\Delta t} K_d}{F} C_{im}^{t} - \frac{\gamma_{1,im} \theta_{im} V_{cell}}{F} - \frac{\gamma_{2,im} f_{im} \rho_b V_{cell}}{F}, \tag{7–5}$$

where F is defined as

$$F = \frac{\theta_{im} V_{cell}}{\Delta t} + \frac{f_{im} \rho_b V_{cell}}{\Delta t} K_d + \lambda_{1,im} \theta_{im} V_{cell} + \lambda_{2,im} f_{im} V_{cell} \rho_b K_d + V_{cell} S_w^{t+\Delta t} \zeta_{im}. \tag{7–6}$$

This expression for $C_{im}^{t+\Delta t}$ in equation 7–5 can be substituted into the last term on the right side of equation 7–3. The diagonal position of the $\mathbf{A}$ matrix and the right-hand-side vector element for row n are then updated to include the transfer with the immobile domain as

$$A_{n,n} \leftarrow A_{n,n} - V_{cell} S_w^{t+\Delta t} \zeta_{im} + \frac{\left(V_{cell} S_w^{t+\Delta t} \zeta_{im}\right)^2}{F}, \tag{7–7}$$

and

$$b_n \leftarrow b_n - \frac{V_{cell} S_w^{t+\Delta t} \zeta_{im}}{F} \left[\left(\frac{\theta_{im} V_{cell}}{\Delta t} + \frac{f_{im} \rho_b V_{cell}}{\Delta t} K_d \right) C_{im}^t - \gamma_{1,im} \theta_{im} V_{cell} - \gamma_{2,im} f_{im} \rho_b V_{cell} \right]. \tag{7–8}$$

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