

Prepared in cooperation with the U.S. Geological Survey Water Availability and Use Science Program

# Documentation for the MODFLOW 6 Groundwater Transport Model

Chapter 55 of  
Section A, Groundwater  
**Book 6, Modeling Techniques**

Techniques and Methods 6-AXX

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

DRAFT: December 18, 2019

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**Cover.** Binary computer code illustration.

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By Christian D. Langevin, Alden M. Provost, Sorab Panday, and Joseph D. Hughes

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William H. Werkheiser, Acting Director

**U.S. Geological Survey, Reston, Virginia: 2018**

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## Preface

The report describes the Groundwater Transport Model for the U.S. Geological Survey (USGS) modular hydrologic simulation program called MODFLOW 6. The program can be downloaded from the USGS for free. The performance of the Groundwater Flow 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/xx.xxx/XXXXXXX>).

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# **Documentation for the MODFLOW 6 Groundwater Transport Model**

By Christian D. Langevin, Alden M. Provost, Sorab Panday, and Joseph D. Hughes

## **Abstract**

This report documents the 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 the GWT Model represents a single chemical species, a MODFLOW 6 simulation may include multiple GWT Models, thereby allowing multi-species solute transport. The GWT Model is designed to work with the Groundwater Flow (GWF) Model for MODFLOW 6, which simulates transient, three-dimensional groundwater flow. The GWT model must use the same spatial discretization used by the GWF Model. The GWT Model simulates (1) advective transport, (2) the combined hydrodynamic dispersion processes of velocity-dependent mechanical dispersion and chemical diffusion, (3) sorption of solutes by the aquifer matrix, (4) transfer between one or more immobile domains, (5) solute decay or production, (6) mixing from groundwater sources and sinks, and (7) direct addition of solute mass. For some problems that have a steady-state solution, the solution can be obtained in a single time by specifying that the time step is steady state, but for most simulations, changes in solute concentration will be represented as a transient process.

# Chapter 1. Introduction

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. The GWT Model is designed to work with the Groundwater Flow (GWF) Model ([Langevin and others, 2017](#)), which simulates three-dimensional, transient, groundwater flow. The GWF and GWT Models operate simultaneously during a MODFLOW 6 simulation to represent coupled groundwater flow and solute transport. MODFLOW 6 is the latest version of the U.S. Geological Survey (USGS) model commonly called MODFLOW. MODFLOW 6 was designed so that new types of models could be added to the program, much like packages could be added to previous MODFLOW versions. The GWT Model is a new addition to the MODFLOW 6 framework ([Hughes and others, 2017](#)).

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 chemical 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 very low permeability aquifer material where it can be stored and later released, (5) 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.

## History

There are several solute transport models that are designed to work with MODFLOW. These include MT3DMS ([Zheng, 1990; Zheng and Wang, 1999](#)), MOC3D ([Konikow and others, 1996](#)), SEAWAT ([Langevin and others, 2008](#)), MT3D-USGS ([Bedekar and others, 2016](#)), and MODFLOW-USG beta (xxx). MT3DMS and MT3D-USGS are separate from MODFLOW. Instead of running simultaneously, MODFLOW writes a special flow file while it is running, as described by [Zheng and others \(2001\)](#), and then this file is read as input by MT3DMS and MT3D-USGS. Alternatively, GWT, SEAWAT, and MODFLOW-USG beta simulate flow and transport simultaneously during a simulation.

[MOC2D \(Konikow and Bredehoeft, 1978\)](#) [MT3D \(Zheng and Wang, 1999\)](#) [MT3D-USGS \(Bedekar and others, 2016\)](#) [MODFLOW-USG \(Panday and others, 2013\)](#)

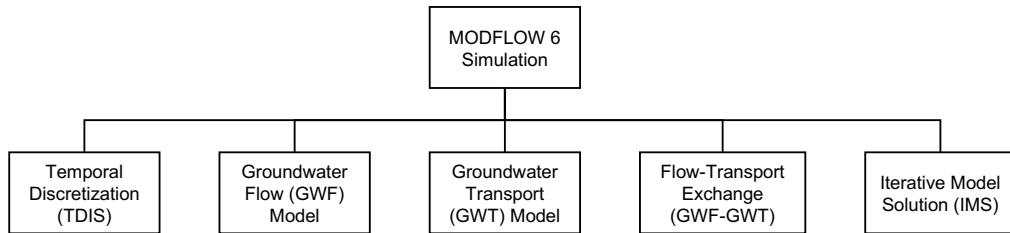
## Overview the Groundwater Transport Model

The GWT Model is designed to work with the Groundwater Flow (GWF) Model as part of a MODFLOW 6 simulation. As shown in Figure 1–1 for the most common use case, a GWT Model will run within a MODFLOW 6 simulation in conjunction with a GWF Model. 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 GWT Model by the Iterative Model Solution (IMS). Concentration and solute fluxes are also calculated by the IMS.

If transport-only mode working, add here and update figure...

The GWT Model described in this report is divided into “packages.” A package is the 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 diffusion. Some packages are required, whereas other packages are only activated if their capabilities are needed for a particular application.

## 1–2 Documentation for the MODFLOW 6 Groundwater Transport Model



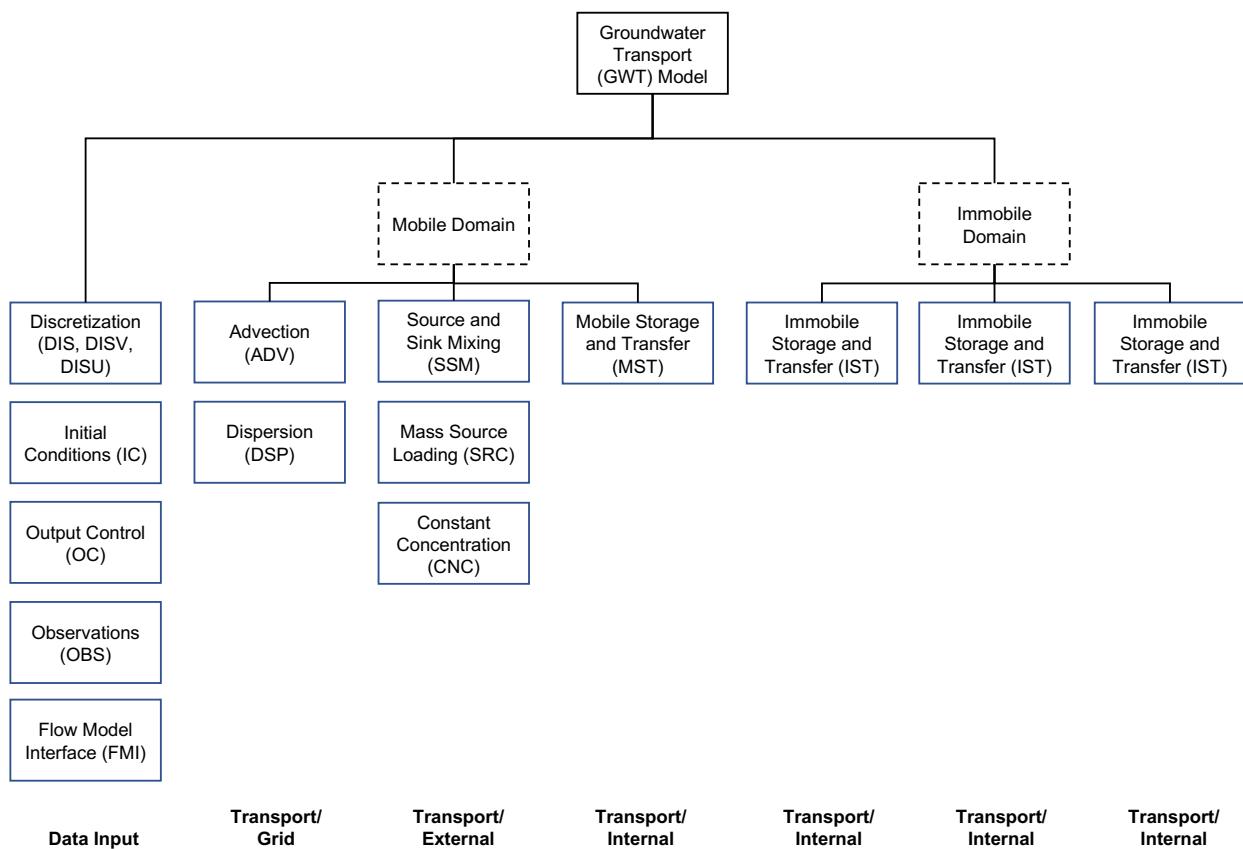
**Figure 1–1.** Diagram showing the structure of a MODFLOW 6 simulation.

The GWT Model and the packages that comprise it are 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 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 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 domain in response to a transfer coefficient and the concentration difference between the mobile and immobile domain. 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, 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 sorbtion and decay parameters). Specification of one or more immobile domains is optional; however, most simulations will require specification of mobile domain packages.

Table 1–1 lists the various packages that comprise the GWT Model documented in this report, the three-character abbreviation used for each package, and the package category.

**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	Transport/Grid
Dispersion	DSP	Transport/Grid
Source-Sink Mixing	SSM	Transport/External
Mass Source Loading	SRC	Transport/External
Constant Concentration	CNC	Transport/External
Mobile Storage and Transfer	MST	Transport/Internal
Immobile Storage and Transfer	IST	Transport/Internal



**Figure 1–2.** Diagram showing the domains and packages for the Groundwater Transport Model.

## 1-4 Documentation for the MODFLOW 6 Groundwater Transport Model

### Information for Existing MT3D Users

MODFLOW 6 contains most of the functionality of MT3D.

The following list summarizes the major differences between the GWT Model in MODFLOW 6 and previous MODFLOW-based transport programs.

Update when capabilities are finalized...

1. The GWT Model simulates transport of a single solute 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.
2. There is no flow-transport link file ([Zheng and others, 2001](#)) used to pass the simulated groundwater flows to the transport model. Instead, simulated flows from the GWF Model are passed in memory to the GWT Model while the program is running.
3. Transport can be simulated using regular MODFLOW grids or unstructured grids.
4. Advection can be simulated using central-in-space weighting, upstream weighting, or an implicit second-order 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 systems.
5. The GWT model includes the DCY, SRB, and IMD Packages, which collectively comprise the capabilities of the MT3D Reactions Package.
6. The SRB Package contains only the linear isotherm, and does not support the Langmuir, Freundlich and other nonlinear isotherms found in MT3D. Nonlinear isotherms are not commonly used in practice and require additional code complexity and numerical overhead.
7. The GWT model was designed so that the user can specify as many immobile domains and necessary to represent observed contaminant transport patterns. The effects of an immobile domain are represented using the Immobile Domain (IMD) Package, and the user can specify as many IMD Packages as necessary.
8. Here is the second one.
9. There are other differences between MODFLOW 6 and previous MODFLOW versions regarding input and output. Descriptions for the MODFLOW 6 input and output are described in a separate user guide, which is included with the distribution. One of the most visible changes to the input files is the use of keywords to label the individual input variables. This improvement makes the input files human readable, reduces the likelihood of input errors, and makes it easier to support backward compatibility as new capabilities are added to the program.

### Organization and Scope of This Report

This report documenting the GWT Model is similar to the MT3D-USGS documentation in that it describes the fundamental concepts for the GWF Model; however, the programmer information and user input instructions are not included in this report, as was done in [Bedekar and others \(2016\)](#). Instead, user input instructions are provided as a separate document with the program distribution. By distributing the input instructions separately, they can evolve with the program as new options are added. In some instances, users

may need to refer to additional reports for capabilities added to MODFLOW, including additions of processes and capabilities to simulate additional hydrologic features.

The purpose of this report is to describe the mathematical concepts used in the GWT Model of MODFLOW 6. [Chapter 2](#) derives the control-volume finite-difference (CVFD) equation upon which the GWT Model is based. Short summary of each chapter XXX. [Appendix A](#) contains a list of mathematical symbols used in this report. [Appendix B](#) describes the implementation of the GWT Model in the MODFLOW 6 framework. 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

Change the order so that SSM and SRC come at the end?

Change water saturation  $S_w$  to be the saturated fraction  $S_f$

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 groundwater transport model, discretization options, and the general forms of the finite-difference equations used to simulate groundwater transport.

### Mathematical Model

Transport of a solute dissolved in groundwater is described mathematically by a partial differential equation that dictates 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, which includes the transport mechanisms represented by the GWT Model:

$$\frac{\partial (S_w \theta C)}{\partial t} = -\nabla \cdot (\mathbf{q}C) + \nabla \cdot (S_w \theta \mathbf{D} \nabla C) + q'_s C_s + M_s + q'_e C - \lambda \theta S_w C^n - f_m \rho_b \frac{\partial (S_w \bar{C})}{\partial t} - \lambda_{\bar{C}} \rho_b \bar{C}^n - \sum_{im}^{nim} \zeta_{im} (C - C_{im}), \quad (2-1)$$

where  $S_w$  is the water saturation (dimensionless) defined as the volume of water per volume of voids,  $\theta$  is the effective porosity of the mobile domain (dimensionless),  $C$  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 flow flow into the aquifer) for sources and sinks ( $1/T$ ),  $C_s$  is the volumetric solute concentration of the source or sink fluid ( $M/L^3$ ),  $q'_e$  is a flow imbalance term that may arise from errors in the solution of the flow equation ( $1/T$ ),  $M_s$  is rate of solute mass loading per unit volume of aquifer ( $M/L^3 T$ ),  $\lambda$  is the first-order decay coefficient ( $1/T$ ) or zero-order decay coefficient ( $M/L^3 T$ ) for the aqueous dissolved phase,  $n$  is the order of the decay rate with a value of zero or one (dimensionless),  $f_m$  is the fraction of the total porosity, including the mobile and immobile porosities, that is in contact with mobile water,  $\rho_b$  is the bulk density of the aquifer material ( $M/L^3$ ),  $\bar{C}$  is the concentration of the solute mass that is sorbed to the aquifer solids ( $M/M$ ),  $\lambda_{\bar{C}}$  is the first-order decay coefficient ( $1/T$ ) or zero-order decay coefficient ( $M/L^3 T$ ) for the sorbed phase,  $nim$  is the number of immobile domains,  $\zeta_{im}$  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.

$$\underbrace{-\nabla \cdot (\mathbf{q}C) + \nabla \cdot (S_w \theta \mathbf{D} \nabla C)}_{ADV} + \underbrace{q'_s C_s + q'_e C + M_s}_{SSM} + \underbrace{-f_m \rho_b \frac{\partial (S_w \bar{C})}{\partial t} - \lambda_{\bar{C}} \rho_b \bar{C}^n - \sum_{im}^{nim} \zeta_{im} (C - C_{im})}_{MST} = 0. \quad (2-2)$$

## 2–2 Documentation for the MODFLOW 6 Groundwater Transport Model

In this form (eq. 2–2), the terms have been grouped and labeled according to the GWT transport package that contains them. 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 are represented with the Source and Sink Mixing (SSM) Package. The effects of a fluid mass balance error are compensated for by the Flow Model Interface (FMI) Package. The direct loading of solute mass can be represented with the Mass Source Loading (SRC) Package. The effects of solute storage, sorbtion, and decay on the mobile domain are represented with the Mass Storage and Transfer (MST) Package. The effects of a diffusive exchange of the mobile domain with 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 this manner 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

$$f^{ADV} + f^{DSP} + f^{SSM} + f^{FMI} + f^{SRC} + f^{MST} + f^{IST} = 0, \quad (2-3)$$

where

$$\begin{aligned} f^{ADV} &= -\nabla \cdot (\mathbf{q}C) \\ f^{DSP} &= \nabla \cdot (S_w \theta \mathbf{D} \nabla C) \\ f^{SSM} &= q'_s C_s \\ f^{FMI} &= q'_e C \\ f^{SRC} &= M_s \\ f^{MST} &= -\frac{\partial (S_w \theta C)}{\partial t} - f_m \rho_b \frac{\partial (\bar{S}_w \bar{C})}{\partial t} - \lambda \theta S_w C^n - \lambda \bar{C} \rho_b \bar{C}^n \\ f^{IST} &= -\zeta_{im} (C - C_{im}). \end{aligned} \quad (2-4)$$

## Control-Volume Finite-Difference Method

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. The GWT Model of MODFLOW 6 solves numerically for the solute concentration in each cell of MODFLOW 6 grid using the control-volume finite-difference (CVFD) method. The balance of solute mass is formulated for each 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.

Equation 2–1, together with any relevant boundary conditions, represents mathematically the solute mass balance at any point in the model domain. To approximate the corresponding concentration distribution using the CVFD method, MODFLOW 6 discretizes the model domain into cells, formulates a solute mass balance over each cell, and solves the resulting set of algebraic equations numerically.

## 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. Figure 2-1 shows an example of a groundwater model cell, with the size of individual sediment grains exaggerated to illustrate porosity concepts. The area of the cell 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

$$V_{cell} = A_n (TOP_n - BOT_n). \quad (2-5)$$

This is the equation used for 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

$$\theta = \frac{V_{void}}{(V_{void} + V_{solid})}. \quad (2-6)$$

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. And when a cell is partially saturated, the saturation is assumed to depend on the head value within the cell as

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

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

$$V_w = \theta V_{cell} S_w \quad (2-8)$$

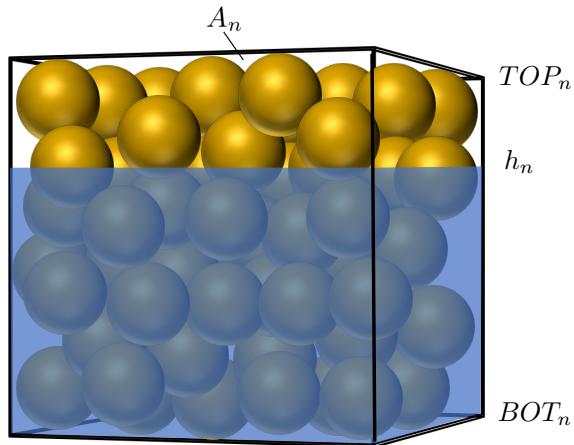
The volume of water in a cell may change during the simulation in response to inflows and outflows, as calculated by the flow model. An inherent assumption in the approximation of the volume of water in a cell using this approach is that the aquifer porosity does not change with time. As noted by [Goode \(1990\)](#) this is incorrect, because changes 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

$$\dot{M}_n^{STO} = \dot{M}_n^{ADV} + \dot{M}_n^{DSP} + \dot{M}_n^{SSM} + \dot{M}_n^{DCY} + \dot{M}_n^{SRB} + \dot{M}_n^{IMD} + \dot{M}_n^{SRC}, \quad (2-9)$$

## 2-4 Documentation for the MODFLOW 6 Groundwater Transport Model



**Figure 2-1.** Diagram of a partially saturated model cell. 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 in the cell.

where  $\dot{M}_n^{STO}$  is the rate of change of dissolved solute mass in the cell;  $\dot{M}_n^{ADV}$ ,  $\dot{M}_n^{DSP}$ ,  $\dot{M}_n^{SSM}$  are the net rates at which solute mass flows into the cell due to advection, dispersion, and mixing from external fluid sources and sinks,  $\dot{M}_n^{DCY}$  represents the loss of solute mass to first- or zero-order decay,  $\dot{M}_n^{SRB}$  is rate of change of solute mass in the cell due to sorption,  $\dot{M}_n^{IMD}$  is the rate of change of solute mass in the cell due to exchange with an immobile domain, and  $\dot{M}_n^{SRC}$  is the rate of solute mass loading added directly to a cell. 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 removal of solute from a cell is negative.

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 between two cells. This flow is expressed using  $F_{n,m}$ , where  $n$  and  $m$  are cells adjacent to one another.  $F_{n,m}$  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:

$$\dot{M}_n^{ADV} = \sum_{m \in \eta_n} F_{n,m}^{ADV} \quad (2-10)$$

where  $\eta_n$  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 on the right-hand side 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 neighbors:

$$\dot{M}_n^{DSP} = \sum_{m \in \eta_n} F_{n,m}^{DSP} \quad (2-11)$$

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 5.

## Numerical Solution

Solution of the solute transport equation relies on the MODFLOW 6 framework described by [Hughes and others \(2017\)](#), which is customized to solve CVFD equations. The CVFD equation for solute transport can be written for model cell  $n$  as

$$A_{n,n}C_n + \sum_{m \in \eta_n} A_{n,m}C_m = b_n, \quad (2-12)$$

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  $m$ ,  $C_n$  and  $C_m$  are the concentrations ( $M/L^3$ ) in cells  $n$  and  $m$ , 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 any number of surrounding cell concentrations in  $\eta_n$ . 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 value in equation 2-12 are the sum of the contributions from the different 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 concentration terms in equation 2-12 are for the end of the time step. This means that the concentration terms 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. 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. This system of equations can be expressed in the following matrix form as

$$\mathbf{AC} = \mathbf{b}. \quad (2-13)$$

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 number of entries equal to the number of cells. For some GWT Model applications, equation 2-13 is linear in that  $\mathbf{A}$  and  $\mathbf{b}$  are not dependent on the dependent variable  $\mathbf{C}$ ; however, for some applications the balance equation is nonlinear, and solution of equation 2-13 must be repeated multiple times, each time with updated coefficients and right-hand-side values, until convergence is achieved.

## Initial Conditions

### Constant Concentration Boundary Condition

### Steady-State Solutions

### Time Stepping

## Chapter 3. Storage

This chapter documents the Storage (STO) Package, which simulates the change in the aqueous solute mass. There can be only one STO Package specified for a GWT Model. Unlike the STO Package for the GWF Model, which is optional, the STO Package is required for a GWT model because it contains the aquifer porosity term, which is required even for steady state simulations.

The rate of change of aqueous solute mass, as shown in the mathematic equations for solute transport (eqs. 2-1, 2-2, and 2-4), is expressed as

$$\dot{f}^{STO} = \frac{\partial (S_w \theta C)}{\partial t}. \quad (3-1)$$

### Numerical Solution

The change in aqueous solute mass during a time step can be approximated for a model cell using the following difference equation

$$\dot{M}^{STO} = \frac{C^{t+\Delta t} V_w^{t+\Delta t} - C^t V_w^t}{\Delta t}, \quad (3-2)$$

where  $t$  is time ( $T$ ),  $\Delta t$  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 pertain to cell  $n$ , has been omitted for clarity. Equation 3-2 can be derived by multiplying equation 3-1 by the cell volume ( $V_{cell}$ ), and then by using equation 2-8 to replace  $S_w \theta V_{cell}$  with the volume of water in the cell,  $V_w$ .

The equation for aqueous solute storage is added to the system of equations by updating the left-hand side coefficient ( $A_{n,n}$ ) and the right-hand side ( $b_n$ ) as

$$A_{n,n} \leftarrow A_{n,n} - \frac{V_w^{t+\Delta t}}{\Delta t}, \quad (3-3)$$

and

$$b_n \leftarrow b_n - \frac{C^t V_w^t}{\Delta t}. \quad (3-4)$$

## Chapter 4. Advection

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

$$\mathbf{f}^{ADV} = \mathbf{q}C. \quad (4-1)$$

This is 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,  $C_{n,m}$  ( $M/L^3$ ):

$$F_{n,m}^{ADV} = Q_{n,m}C_{n,m}, \quad (4-2)$$

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

Several 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 concentration at the cell face can be expressed as a weighted average of the concentrations in the two cells:

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

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

### Central-In-Space Weighting

The central-in-space weighting scheme uses simple distance-weighted linear interpolation between the center of cell  $n$  and the center of cell  $m$  to calculate concentration at the shared face between cell  $n$  and cell  $m$ . The value for  $\omega_{n,m}$  is a distance-weighted interpolation factor calculated based on cell dimensions:

$$\omega_{n,m} = \frac{L_{m,n}}{L_{n,m} + L_{m,n}}. \quad (4-4)$$

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, however, because it may be useful for 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

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$$\omega_{n,m} = \begin{cases} 0 & \text{for } Q_{n,m} > 0 \\ 1 & \text{for } Q_{n,m} \leq 0 \end{cases}. \quad (4-5)$$

### Total Variation Diminishing (TVD)

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

$$C_{n,m} = C_{n,m}^{ups} + C_{n,m}^{TVD}, \quad (4-6)$$

with

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

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

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

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

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

where  $C_{n,m}^{2up}$  is the concentration of the second upstream cell. The second upstream cell is determined by identifying the cell with the largest flow into the upstream cell.

The weighting factor  $\omega_{n,m}$  used for upstream weighting (equation 4–5) enters the advective flow expression, equation 4–2, through the term  $C_{n,m}^{ups}$  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,  $\sigma_{n,m}$ :

$$C_{n,m} = \omega_{n,m}^{TVD} + (1 - \omega_{n,m}^{TVD}) C_m, \quad (4-10)$$

where

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

## 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

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

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

$$A_{n,n} \leftarrow A_{n,n} + \omega_{n,m} Q_{n,m}, \quad (4-13)$$

The matrix coefficient in row  $n$  that corresponds to the connection between cell  $n$  and neighboring cell  $m$  is updated by adding the term  $\omega_{n,m} Q_{n,m} C_m$ :

$$A_{n,m} \leftarrow A_{n,m} + \omega_{n,m} Q_{n,m} C_m. \quad (4-14)$$

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

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

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,  $\mathbf{b}$ :

$$b_n \leftarrow b_n + Q_{n,m} C_{n,m}^{TVD}. \quad (4-16)$$

When upstream weighting or the TVD schemes 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.

## Chapter 5. Dispersion

Over time, a mass of solute dissolved in groundwater spreads by molecular diffusion. If the 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, [\(references\)](#)).

**Need to mention here that we are assuming that dispersion is proportional to the gradient in volumetric concentration, and not mass fraction. Cite Bird, Stewart, and Lightfoot and Zheng and Wang, and say that have picked the Zheng and want approach.**

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,  $\nabla C$  ( $M/L^4$ ), via 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:

$$\mathbf{f}^{DSP} = -S_w\theta\mathbf{D}\nabla C. \quad (5-1)$$

with

$$\mathbf{D} = \mathbf{D}^{mech} + D^{mol}\mathbf{I} \quad (5-2)$$

where  $\mathbf{D}^{mech}$  ( $L^2/T$ ) is the mechanical dispersion tensor, which may be anisotropic,  $D^{mol}$  ( $L^2/T$ ) is the molecular diffusion coefficient, and  $\mathbf{I}$  is the identity tensor (dimensionless). The second term on the right-hand side of equation 5-2 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. The factor  $S_w\theta$  in equation 5-1, where  $S_w$  is the water saturation and  $\theta$  is porosity (both dimensionless), accounts for the fact that hydrodynamic dispersion occurs only within the porespace (not within the solid matrix), and that the porespace may be only partially saturated. Equation 5-1 represents the dispersive solute flux that appears in parentheses in the second term on the right-hand side of equation 2-1.

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 spreading pattern. For example, in "isotropic" dispersion, an initially spherical solute mass will retain a spherical shape as it advects with the flow and disperses. The model of Scheidegger (1961) ([live reference](#)), 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"

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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 5–1 tends to produce unrealistic backdispersion, and the dispersion coefficients are scale-dependent, particularly in applications involving estimation of effective dispersion coefficients in heterogeneous aquifers ([references](#)). 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 \(2002\)](#) ([live reference](#)) 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 neighbors (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 5–1. The "simplified" formulation is mathematically analogous to the "conductance-based" formulation of groundwater flow across cell faces in MODFLOW 6. Like 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 ([reference to gwf report](#)) and summarized below. Use of the simplified formulation when these requirements are not met 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 ([reference to xt3d report](#)), can be helpful because it automatically accounts for irregularities in the grid and tensor anisotropy, albeit at the expense of longer simulation times.

Add note exercising caution when flow model has the Horizontal Flow Barrier (HFB) Package active as the dispersive flux may be estimated to be too large, as described by [Hornberger and others \(2002\)](#).

## 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. 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

$$\mathbf{D}^{mech} = \begin{pmatrix} \alpha_L v & 0 & 0 \\ 0 & \alpha_{T1} v & 0 \\ 0 & 0 & \alpha_{T2} v \end{pmatrix}, \quad (5–3)$$

where  $\alpha_L$ ,  $\alpha_{T1}$ , and  $\alpha_{T2}$  are called the longitudinal and first and second transverse dispersivities ( $L$ ), and  $v$  is the groundwater flow velocity ( $L/T$ ). The longitudinal and transverse dispersivities vary with the groundwater flow direction as follows:

$$\begin{aligned}\alpha_L &= \alpha_{LH} \cos^2 \theta_2 + \alpha_{LV} \sin^2 \theta_2 = \alpha_{LH} \left(1 - \frac{v_z^2}{v^2}\right) + \alpha_{LV} \frac{v_z^2}{v^2} \\ \alpha_{T1} &= \alpha_{TH1} \cos^2 \theta_2 + \alpha_{TV} \sin^2 \theta_2 = \alpha_{TH1} \left(1 - \frac{v_z^2}{v^2}\right) + \alpha_{TV} \frac{v_z^2}{v^2}, \\ \alpha_{T2} &= \alpha_{TH2} \cos^2 \theta_2 + \alpha_{TV} \sin^2 \theta_2 = \alpha_{TH2} \left(1 - \frac{v_z^2}{v^2}\right) + \alpha_{TV} \frac{v_z^2}{v^2}\end{aligned}\quad (5-4)$$

where  $\theta_2$  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,  $\alpha_{LH}$  and  $\alpha_{LV}$ , and three transverse dispersivities,  $\alpha_{TH1}$ ,  $\alpha_{TH2}$ , and  $\alpha_{TV}$ , all with dimensions of  $(L)$ . Note that equation 5-3 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 5-4.

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 ( $\theta_2 = 0^\circ; v_z = 0$ ), the longitudinal dispersivity ( $\alpha_L$ ) is  $\alpha_{LH}$ , the transverse dispersivity for horizontal spreading ( $\alpha_{T1}$ ) is  $\alpha_{TH1}$ , and the transverse dispersivity for vertical spreading ( $\alpha_{T2}$ ) is  $\alpha_{TH2}$ . When flow is in the vertical direction ( $\theta_2 = 90^\circ; v_x = v_y = 0, v_z = v$ ), the longitudinal dispersivity ( $\alpha_L$ ) is  $\alpha_{LV}$ , and the transverse dispersivities ( $\alpha_{T1}$  and  $\alpha_{TH1}$ ), which represent horizontal spreading, are both  $\alpha_{TV}$ . For groundwater flow directions between horizontal and vertical, the longitudinal and transverse dispersivities vary smoothly with flow direction according to equation 5-4.

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

$$\begin{aligned}D_{xx}^{mech} &= \alpha_L \frac{v_x^2}{v} + \alpha_{TH1} \frac{v_y^2}{v} + \alpha_{Tx} \frac{v_z^2}{v} \\ D_{yy}^{mech} &= \alpha_{TH1} \frac{v_x^2}{v} + \alpha_L \frac{v_y^2}{v} + \alpha_{Ty} \frac{v_z^2}{v} \\ D_{zz}^{mech} &= \alpha_{T2} \frac{v_x^2}{v} + \alpha_{T2} \frac{v_y^2}{v} + \alpha_L \frac{v_z^2}{v}, \\ D_{xy}^{mech} &= (\alpha_L - \alpha_{T2} + \alpha_{TH2} - \alpha_{TH1}) \frac{v_x v_y}{v} \\ D_{xy}^{mech} &= (\alpha_L - \alpha_{T2}) \frac{v_x v_z}{v} \\ D_{xy}^{mech} &= (\alpha_L - \alpha_{T2}) \frac{v_y v_z}{v}\end{aligned}\quad (5-5)$$

where

$$\begin{aligned}\alpha_{Tx} &= \alpha_{TH2} \frac{v_x^2}{v^2} + \alpha_{TV} \left(1 - \frac{v_x^2}{v^2}\right) \\ \alpha_{Ty} &= \alpha_{TH2} \frac{v_y^2}{v^2} + \alpha_{TV} \left(1 - \frac{v_y^2}{v^2}\right).\end{aligned}\quad (5-6)$$

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Setting

$$\begin{aligned}\alpha_{LH} &= \alpha_L \\ \alpha_{LV} &= \alpha_L \\ \alpha_{TH1} &= \alpha_T^H, \\ \alpha_{TH2} &= \alpha_T^V \\ \alpha_{TV} &= \alpha_T^V\end{aligned}\tag{5–7}$$

where  $\alpha_L$  is a constant, gives the model of [Burnett and Frind \(1987\)](#):

$$\begin{aligned}D_{xx}^{mech} &= \alpha_L \frac{v_x^2}{v} + \alpha_T^H \frac{v_y^2}{v} + \alpha_T^V \frac{v_z^2}{v} \\ D_{yy}^{mech} &= \alpha_T^H \frac{v_x^2}{v} + \alpha_L \frac{v_y^2}{v} + \alpha_T^V \frac{v_z^2}{v} \\ D_{zz}^{mech} &= \alpha_T^V \frac{v_x^2}{v} + \alpha_T^V \frac{v_y^2}{v} + \alpha_L \frac{v_z^2}{v} \\ D_{xy}^{mech} &= (\alpha_L - \alpha_T^H) \frac{v_x v_y}{v} \\ D_{xz}^{mech} &= (\alpha_L - \alpha_T^V) \frac{v_x v_z}{v} \\ D_{yz}^{mech} &= (\alpha_L - \alpha_T^V) \frac{v_y v_z}{v}\end{aligned}\tag{5–8}$$

with

$$\begin{aligned}\alpha_L &= \alpha_L^H \left(1 - \frac{v_z^2}{v^2}\right) + \alpha_L^V \frac{v_z^2}{v^2} \\ \alpha_{Tx} &= \alpha_T^V \frac{v_x^2}{v^2} + \alpha_T^H \left(1 - \frac{v_x^2}{v^2}\right) \\ \alpha_{Ty} &= \alpha_T^V \frac{v_y^2}{v^2} + \alpha_T^H \left(1 - \frac{v_y^2}{v^2}\right) \\ \alpha_{T2} &= \alpha_T^V \left(1 - \frac{v_z^2}{v^2}\right) + \alpha_T^H \frac{v_z^2}{v^2}\end{aligned}\tag{5–9}$$

Setting

$$\begin{aligned}\alpha_{LH} &= \alpha_L^H \\ \alpha_{LV} &= \alpha_L^V \\ \alpha_{TH1} &= \alpha_T^H \\ \alpha_{TH2} &= \alpha_T^V \\ \alpha_{TV} &= \alpha_T^H\end{aligned}\tag{5–10}$$

gives the model of Lichnter and others (reference) (NOTE: This is not the form in which they presented their model, so probably should show some more math):

$$\begin{aligned}
 D_{xx}^{mech} &= \alpha_L \frac{v_x^2}{v} + \alpha_T^H \frac{v_y^2}{v} + \alpha_{Tx} \frac{v_z^2}{v} \\
 D_{yy}^{mech} &= \alpha_T^H \frac{v_x^2}{v} + \alpha_L \frac{v_y^2}{v} + \alpha_{Ty} \frac{v_z^2}{v} \\
 D_{zz}^{mech} &= \alpha_{T2} \frac{v_x^2}{v} + \alpha_{T2} \frac{v_y^2}{v} + \alpha_L \frac{v_z^2}{v} \\
 D_{xy}^{mech} &= (\alpha_L - \alpha_{T2} + \alpha_{TH2} - \alpha_T^H) \frac{v_x v_y}{v} \\
 D_{xy}^{mech} &= (\alpha_L - \alpha_{T2}) \frac{v_x v_z}{v} \\
 D_{xy}^{mech} &= (\alpha_L - \alpha_{T2}) \frac{v_y v_z}{v}
 \end{aligned} \tag{5-11}$$

with

$$\begin{aligned}
 \alpha_L &= \alpha_L^H \left( 1 - \frac{v_z^2}{v^2} \right) + \alpha_L^V \frac{v_z^2}{v^2} \\
 \alpha_{Tx} &= \alpha_T^V \frac{v_x^2}{v^2} + \alpha_T^H \left( 1 - \frac{v_x^2}{v^2} \right) \\
 \alpha_{Ty} &= \alpha_T^V \frac{v_y^2}{v^2} + \alpha_T^H \left( 1 - \frac{v_y^2}{v^2} \right) \\
 \alpha_{T2} &= \alpha_T^V \left( 1 - \frac{v_z^2}{v^2} \right) + \alpha_T^H \frac{v_z^2}{v^2}
 \end{aligned} \tag{5-12}$$

Setting

$$\begin{aligned}
 \alpha_{LH} &= \alpha_L \\
 \alpha_{LV} &= \alpha_L \\
 \alpha_{TH1} &= \alpha_T, \\
 \alpha_{TH2} &= \alpha_T \\
 \alpha_{TV} &= \alpha_T
 \end{aligned} \tag{5-13}$$

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where  $\alpha_L$  and  $\alpha_T$  are constants, gives an isotropic mechanical dispersion tensor, which is a special case of both the [Burnett and Frind \(1987\)](#) model and the Lichnter and others ([reference](#)) model:

$$\begin{aligned} D_{xx}^{mech} &= \alpha_L \frac{v_x^2}{v} + \alpha_T \frac{v_y^2}{v} + \alpha_T \frac{v_z^2}{v} \\ D_{yy}^{mech} &= \alpha_T \frac{v_x^2}{v} + \alpha_L \frac{v_y^2}{v} + \alpha_T \frac{v_z^2}{v} \\ D_{zz}^{mech} &= \alpha_T \frac{v_x^2}{v} + \alpha_T \frac{v_y^2}{v} + \alpha_L \frac{v_z^2}{v}. \\ D_{xy}^{mech} &= (\alpha_L - \alpha_T) \frac{v_x v_y}{v} \\ D_{xz}^{mech} &= (\alpha_L - \alpha_T) \frac{v_x v_z}{v} \\ D_{yz}^{mech} &= (\alpha_L - \alpha_T) \frac{v_y v_z}{v} \end{aligned} \quad (5-14)$$

## Simplified Formulation

Hydrodynamic dispersion transports solute from areas of higher concentration to areas of lower concentration, but in an anisotropic porous medium, dispersive transport is not necessarily in the direction 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 5–1) in three dimensions (3D), each of the three components of the solute mass flux vector is related, via the dispersion tensor, to each of the three components of the concentration gradient:

$$\begin{aligned} f_x^{DSP} &= -S_w \theta \left( D_{xx} \frac{\partial C}{\partial x} + D_{xy} \frac{\partial C}{\partial y} + D_{xz} \frac{\partial C}{\partial z} \right) \\ f_y^{DSP} &= -S_w \theta \left( D_{xy} \frac{\partial C}{\partial x} + D_{yy} \frac{\partial C}{\partial y} + D_{yz} \frac{\partial C}{\partial z} \right) \\ f_z^{DSP} &= -S_w \theta \left( D_{xz} \frac{\partial C}{\partial x} + D_{yz} \frac{\partial C}{\partial y} + D_{zz} \frac{\partial C}{\partial z} \right) \end{aligned} \quad (5-15)$$

where  $D_{xx}$ ,  $D_{xy}$ ,  $D_{xz}$ ,  $D_{yy}$ ,  $D_{yz}$ , and  $D_{zz}$  ( $L/T$ ) are the elements (dispersion coefficients) of  $\mathbf{D}$ , 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 in along a particular direction cannot be computed solely based on the component of the concentration gradient in that one direction; three independent components of the gradient are required. However, if the principal directions of the dispersion tensor are aligned with the coordinate directions, that is, if the dispersion tensor is diagonal ( $D_{xy} = D_{xz} = D_{yz} = 0$ ), equation 5–15 simplifies to

$$\begin{aligned} f_x^{DSP} &= -S_w \theta D_{xx} \frac{\partial C}{\partial x} \\ f_y^{DSP} &= -S_w \theta D_{yy} \frac{\partial C}{\partial y} \\ f_z^{DSP} &= -S_w \theta D_{zz} \frac{\partial C}{\partial z} \end{aligned} \quad (5-16)$$

In this case, which includes the case of an isotropic tensor ( $D_{xx} = D_{yy} = D_{zz}$ ), each component of the solute mass flux depends only on the component of the concentration gradient along the same direction; for example,  $f_x^{DSP}$  depends on the  $x$  component, but not on the  $y$  and  $z$  components, of the concentration gradient.

The simplified formulation of the dispersive solute mass flow rate is

$$F_{n,m}^{DSP} = D_{n,m} (C_m - C_n), \quad (5-17)$$

where  $D_{n,m}$  ( $L^3/T$ ) is analogous to a "conductance" for flow of solute mass driven by a concentration difference. Equation 5-17 is a discrete analog of equation 5-16 and can provide a accurate estimate of the solute mass flow if the model grid is regular and the principal directions of the dispersion tensor,  $\mathbf{D}$ , coincide with the grid-aligned global model-coordinate system, or if  $\mathbf{D}$  is isotropic and the model grid is irregular but satisfies certain geometric requirements. The MODFLOW 6 GWF Model documentation ([reference to GWF report](#)) 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 ref](#)). . . 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."

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. ([Mention ghost nodes? Do they work for GWT?](#))

## 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 5-15). 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 ([reference to XT3D report](#)).

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

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 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 5-1) 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.

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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 (reproduce the XT3D stencil figure from the XT3D report) 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 (stencil figure) 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 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 5–17) 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  $m$ :

$$F_{n,m}^{DSP} = D_{n,m,(n,m)} (C_m - C_n) + \sum_{\substack{p \in \eta_n \\ p \neq m}} D_{n,p,(n,m)} (C_p - C_n) - \sum_{\substack{q \in \eta_m \\ q \neq n}} D_{m,q,(n,m)} (C_q - C_m), \quad (5-18)$$

where the first summation is over neighbors of cell  $n$ , excluding cell  $m$ , the second summation is over neighbors of cell  $m$ , excluding cell  $n$ , and the “ $D$ ” coefficients are analogous to “conductances” for flow of solute mass driven by concentration differences. 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 works with the existing model grid and is simple to activate, but it tends to be more computationally intensive than using the simplified formulation with or without the Ghost-Node Connection (GNC) Package (are ghost nodes relevant to GWT?). Before deciding whether to use the GNC Package 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. Note that the XT3D option and the GNC Package should not be used simultaneously.

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 flow 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.

For vertical connections, the XT3D method does not correct for partial dewatering. In that regard, its behavior is similar to the default behavior of MODFLOW 6 for calculating vertical "conductances" in the simplified formulation ([is this correct?](#)).

Numerical simulations of highly anisotropic flow based on CVFD and finite-element discretizations can exhibit "spurious oscillations" in the solution ([Edwards and Pal references, as in XT3D report](#)). Although it can be difficult to distinguish spurious oscillations from legitimate variations in concentration in complex flow 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 ([is this true?](#)).

## Chapter 6. Sources and Sinks

Might make more sense to include that flow error term in this package, and allow it to be turned on as an option. Then this package is responsible for adding solute terms to flow terms that come from the flow model. Then FMI can just become internal routines in the code that are not described in this report as a separate package. But it's not clear what this package should be called. SSM is nice because it is relatable to MT3D users, but it does behave rather differently, so maybe it needs to be renamed? Not sure.

This chapter documents the Source and Sink Mixing (SSM) Package, which simulates the change in the solute mass caused by groundwater inflows and outflows. The addition of fluid from a groundwater source may add solute based on a user-prescribed concentration, or the addition of a low-concentration fluid may dilute the solute concentration within an aquifer. There can be only one SSM Package specified for a GWT Model. Packages that

**Table 6-1.** List of Groundwater Flow Model Packages that can act as a solute source or sink.

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

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

$$f^{SSM} = q'_s C_s. \quad (6-1)$$

Need to describe the flow balance error here and how we are dealing with it. Should mention the moc3d report where it talks about the divergent versus convective equations and how they assume that this error term is zero. Should also cite Panday's paper as what we are doing to mitigate the effects.

## Numerical Solution

In the GWT Model, the user is allowed to assign multiple sources and sinks to a single model cell, and the concentrations for these individual sources and sinks may also vary. The third term on the right-hand side of

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equation 2–9, the net rate at which solute mass is entering or leaving cell  $n$  due to external sources and sinks, is simply the sum of all  $nssm$  sources and sinks:

$$\dot{M}_n^{SSM} = \sum_{issm=1}^{nssm} F_{n,issm}^{SSM} \quad (6-2)$$

with

$$F_{n,issm}^{SSM} = Q_{n,issm} C_{n,issm}, \quad (6-3)$$

where  $F_{n,issm}^{SSM}$  and  $Q_{n,issm}$  are the flow rate of solute mass ( $M/T$ ) and the volumetric groundwater flow rate ( $L^3/T$ ), respectively, into or out of cell  $n$  via groundwater source/sink  $issm$ . For inflow to cell  $n$ ,  $C_{n,issm}$  is the solute concentration of the source. For outflow from cell  $n$ ,  $C_{n,issm}$  is the solute concentration in cell  $n$ .

## Chapter 7. Decay

The Decay (DCY) 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 and for the dissolved aqueous and sorbed phase in an immobile domain; however, those processes are described separately in the SRB and IMD Packages.

$$f^{DCY} = -\lambda_1 \theta S_w C - \gamma_1 \theta S_w, \quad (7-1)$$

The DCY Package can simulate the decay or production of solute mass using either a first order or a zero order equation. First-order decay is typically used to represent radioactive decay and also biodegradation or chemical decomposition. 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 one half. The half life is related to the decay rate by

$$t_{1/2} = \frac{\ln 2}{\lambda_1}. \quad (7-2)$$

Zero-order decay may be used to represent biodegradation, but it can also be used when groundwater age is represented as a solute species. In this case, a zero-order growth rate, with a value of one (a decay rate of minus one) causes the groundwater age to increase by a rate equal to the length of the time step. Simulation of groundwater age in this manner is described by [Goode \(1996\)](#).

### Numerical Solution

Decay processes are included in the system of equations by adding terms to the coefficient matrix **A** and the right-hand side vector **b**.

$$\dot{M}_n^{DCY} = -\lambda_1 \theta V_{cell} (S_w C)^{t+\Delta t} - \gamma_1 \theta V_{cell} S_w^{t+\Delta t}. \quad (7-3)$$

The decay mass flux rate  $\dot{M}_n^{DCY}$  is on the left side of equation 2-9. Thus to put these terms into the matrix equation, the terms on the right side of equation 7-3 that are coefficients of  $C^{t+\Delta t}$  are added to the diagonal position of the **A** matrix for row  $n$  as

$$A_{n,n} \leftarrow A_{n,n} - \lambda_1 \theta V_{cell} S_w^{t+\Delta t}. \quad (7-4)$$

The remaining zero-order term must be moved to the right-hand side vector, **b**, which requires that the sign of the term be changed:

$$b_n \leftarrow b_n + \gamma_1 \theta V_{cell} S_w^{t+\Delta t}. \quad (7-5)$$

## Chapter 8. Sorbtion

The Sorbtion (SRB) Package simulates the effects of solute mass that bound to the aquifer solid material, including the possible decay of that sorbed mass. The sorbtion process was designed following the approach implemented by [Zheng and Wang \(1999\)](#) for the MT3DMS program, but the approach has been extended to work for unstructured grids. The SRB Package described here is simpler than the sorbtion processes simulated by the MT3DMS RCT Package in that the SRB Package does not represent the Freundlich, Langmuir, and nonequilibrium sorbtion equations as those equations are not often used in practice.

$$M_r = -f_m \rho_b \frac{\partial (S_w \bar{C})}{\partial t} - \lambda_2 \rho_b \bar{C} - \gamma_2 \rho_b, \quad (8-1)$$

where  $f_m$  is the fraction of the total porosity that is in contact with mobile water. Unless the dual domain approach is used,  $f_m$  has a value of one.

### Linear Isotherm

As a solute moves through an aquifer, some of the solute mass can adhere to the aquifer material or be absorbed into the rock or sediment matrix. This process is collectively referred adsorption, and can slow or impede the movement of chemicals dissolved in groundwater.

Adsorption can be represented as a transfer of some of the solute mass in the aqueous form into the adsorbed form, where it can no longer move through advection and dispersion. This rate of change of the sorbed mass is expressed as

$$f^{SRB} = \frac{\partial (f_m \rho_b S_w \bar{C})}{\partial t}, \quad (8-2)$$

where  $\rho_b$  is the bulk density of the solid in  $M/M$ . The water saturation  $S_w$  is included in equation 8-2 so that adsorption only occurs over that volume of aquifer where there is water in contact with the matrix. Equation 8-2 can be simplified, assuming the bulk density does not change, as

$$f^{SRB} = f_m \rho_b \frac{\partial (\bar{C} S_w)}{\partial t}. \quad (8-3)$$

There several different conceptual models for representing sorption in transport models. The most common approach is to assume that the dissolved solute is in equilibrium with the aquifer matrix, and that the concentration of the sorbed mass is linearly related to the concentration of the dissolved solute mass. This equilibrium-controlled linear approach can be represented by the following equation

$$\bar{C} = K_d C \quad (8-4)$$

where  $\bar{C}$  is the concentration of the sorbed mass ( $M/M$ ) expressed as the mass of solute per mass of aquifer material, and  $K_d$  is the distribution coefficient,  $L^3/M$ . The distribution coefficient is also referred to as the partition coefficient or the adsorption ratio. This equilibrium-controlled linear sorption model is the only approach available in the GWT Model for MODFLOW 6. This is more restrictive than other solute transport models, including MOC ([Konikow and Bredehoeft, 1978](#)), MOC3D ([Goode and Konikow, 1989](#)), MT3D

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(Zheng, 1990; Zheng and Wang, 1999; Bedekar and others, 2016), and SUTRA (Voss and Provost, 2010), for example, which contain the Langmuir, Freundlich, and other other more complex sorption models.

### Numerical Solution

The sorption process is included in the system of equations by adding terms to the coefficient matrix **A** and the right-hand side vector **b**. For the linear isotherm the transfer of mass to the solid phase can be approximated, from the substitution of equation 8–4 into 8–1, as

$$\dot{M}_n^{SRB} = -\frac{f_m \rho_b V_{cell}}{\Delta t} K_d (S_w C)^{t+\Delta t} + \frac{f_m \rho_b V_{cell}}{\Delta t} K_d (S_w C)^t - \lambda_2 f_m V_{cell} \rho_b K_d C^{t+\Delta t} - \gamma_2 f_m \rho_b V_{cell}. \quad (8-5)$$

The sorption mass flux  $\dot{M}_n^{SRB}$  is on the left side of equation 2–9. Thus to put these terms into the matrix equation, the terms on the right side of equation 8–5 that are coefficients of  $C^{t+\Delta t}$  are added to the diagonal position of the **A** matrix for row  $n$  as

$$A_{n,n} \leftarrow A_{n,n} - \frac{f_m \rho_b V_{cell}}{\Delta t} K_d S_w^{t+\Delta t} - \lambda_2 f_m V_{cell} \rho_b K_d. \quad (8-6)$$

The remaining terms must be moved to the right-hand side vector, **b**, which requires that the signs of the terms be changed:

$$b_n \leftarrow b_n - \frac{f_m \rho_b V_{cell}}{\Delta t} K_d (S_w C)^t + \gamma_2 f_m \rho_b V_{cell}. \quad (8-7)$$

## Chapter 9. Immobile Domain

The Immobile Domain (IMD) Package simulates the effects of mass transfer between the mobile domain and an immobile domain.

The transfer of solute mass between the mobile and immobile domain is represented as a diffusive process that can be expressed with the following mass transfer equation,

$$f^{IMD} = -\zeta (C - C_{im}). \quad (9-1)$$

With the dual domain approach, the aquifer is conceptualized as having a fast domain and a slow, immobile domain. Transfer of mass between the mobile and immobile domains occurs through a diffusive process in which the transfer rate is calculated based on the concentration difference between the mobile and immobile domains and a mass transfer coefficient,  $\zeta$ .

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). The governing equation for the immobile domain is

$$\theta_{im} \frac{\partial (S_w C_{im})}{\partial t} + f_{im} \rho_b \frac{\partial \bar{C}_{im}}{\partial t} = -\lambda_{1,im} \theta_{im} C_{im} - \lambda_{2,im} f_{im} \rho_b \bar{C}_{im} \\ -\gamma_{1,im} \theta_{im} - \gamma_{2,im} f_{im} \rho_b + \zeta (C - C_{im}), \quad (9-2)$$

where  $\theta_{im}$  is the volume of the immobile pores divided by the bulk volume of aquifer,  $f_{im}$  is the fraction of the mass of solid grains with their surface in contact with immobile water under fully saturated conditions.  $f_{im}$  can be approximated as  $f_{im} = \theta_{im}/\theta$ .

## Numerical Solution

The immobile domain is conceptualized as very low permeability material that is distributed evenly from top to bottom within a model cell. One such conceptualization is shown in Figure 9–1.

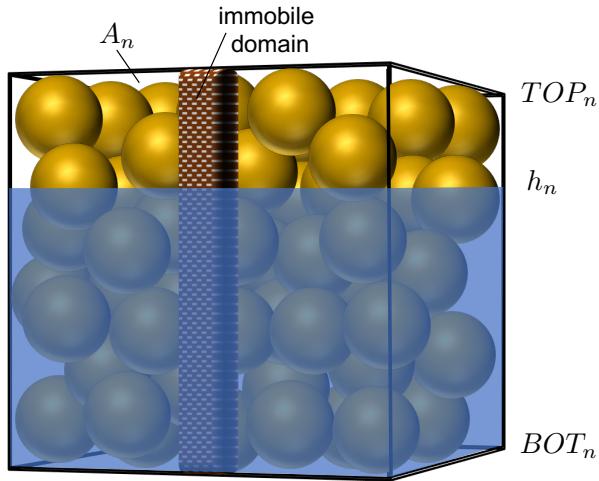
$$\dot{M}_n^{IMD} = -V_{cell} S_w^{t+\Delta t} \zeta C^{t+\Delta t} + V_{cell} S_w^{t+\Delta t} \zeta C_{im}^{t+\Delta t}. \quad (9-3)$$

The mass transfer  $\dot{M}_n^{IMD}$  is on the left side of equation 2–9. Thus to put these terms into the matrix equation, the terms on the right side of equation 9–3 that are coefficients of  $C^{t+\Delta t}$  are added to the diagonal position of the **A** matrix for row  $n$  as

$$A_{n,n} \leftarrow A_{n,n} - V_{cell} S_w^{t+\Delta t} \zeta. \quad (9-4)$$

The last term on the right side of equation 9–3 is part of the term describing mass transfer between the mobile and immobile domains. This term is recast as a function of the mobile domain solute concentrations. In order to express  $C_{im}^{t+\Delta t}$  as a function of mobile domain solute concentrations and other known terms, an

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**Figure 9–1.** Diagram of a model cell with an immobile domain. 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 in the cell.

implicit finite-difference equation can be applied to equation 9–2, the balance equation for the immobile domain. The implicit finite-difference for the immobile domain is

$$\begin{aligned} & \frac{\theta_{im} V_{cell}}{\Delta t} S_w^{t+\Delta t} C_{im}^{t+\Delta t} - \frac{\theta_{im} V_{cell}}{\Delta t} S_w^t C_{im}^t \\ & + \frac{f_{im} \rho_b V_{cell}}{\Delta t} K_d S_w^{t+\Delta t} C_{im}^{t+\Delta t} - \frac{f_{im} \rho_b V_{cell}}{\Delta t} K_d S_w^t C_{im}^t = \\ & -\lambda_{1,im} \theta_{im} V_{cell} S_w^{t+\Delta t} C_{im}^{t+\Delta t} - \lambda_{2,im} f_{im} V_{cell} \rho_b K_d C_{im}^{t+\Delta t} \\ & - \gamma_{1,im} \theta_{im} V_{cell} S_w^{t+\Delta t} - \gamma_{2,im} f_{im} \rho_b V_{cell} \\ & + V_{cell} S_w^{t+\Delta t} \zeta C^{t+\Delta t} - V_{cell} S_w^{t+\Delta t} \zeta C_{im}^{t+\Delta t} \end{aligned} \quad (9-5)$$

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

$$\begin{aligned} C_{im}^{t+\Delta t} = & \frac{V_{cell} S_w^{t+\Delta t} \zeta}{F} C^{t+\Delta t} + \frac{\frac{\theta_{im} V_{cell}}{\Delta t} S_w^t + \frac{f_{im} \rho_b V_{cell}}{\Delta t} K_d S_w^t}{F} C^t \\ & - \frac{\gamma_{1,im} \theta_{im} V_{cell} S_w^{t+\Delta t}}{F} - \frac{\gamma_{2,im} f_{im} \rho_b V_{cell}}{F} \end{aligned} \quad (9-6)$$

where  $F$  is defined as

$$\begin{aligned} F = & \frac{\theta_{im} V_{cell}}{\Delta t} S_w^{t+\Delta t} + \frac{f_{im} \rho_b V_{cell}}{\Delta t} K_d S_w^{t+\Delta t} \\ & + \lambda_{1,im} \theta_{im} V_{cell} S_w^{t+\Delta t} + \lambda_{2,im} f_{im} V_{cell} \rho_b K_d + V_{cell} S_w^{t+\Delta t} \zeta \end{aligned} \quad (9-7)$$

This expression for  $C_{im}^{t+\Delta t}$  in equation 9-7 can be substituted into the last term on the right side of equation 9-3. By doing so, the **A** matrix and **b** right-hand side vector are further updated as

$$A_{n,n} \leftarrow A_{n,n} + \frac{(V_{cell}S_w^{t+\Delta t}\zeta)^2}{F}, \quad (9-8)$$

and

$$\begin{aligned} b_n \leftarrow b_n - \frac{V_{cell}S_w^{t+\Delta t}\zeta}{F} & \left[ \frac{\theta_{im}V_{cell}}{\Delta t} S_w^t + \frac{f_{im}\rho_b V_{cell}}{\Delta t} K_d S_w^t C^t \right. \\ & \left. - \gamma_{1,im} \theta_{im} V_{cell} S_w^{t+\Delta t} - \gamma_{2,im} f_{im} \rho_b V_{cell} \right]. \end{aligned} \quad (9-9)$$

## Chapter 10. Source Mass Loading

Solute mass not associated with a groundwater inflow or outflow can be specified directly by the user through the  $\dot{M}_n^{SRC}$  term. The program is flexible in that multiple source terms can be specified for a single cell as

$$\dot{M}_n^{SRC} = \sum_{isrc=1}^{nsrc} M_{n,isrc}^{SRC} \quad (10-1)$$

where  $nsrc$  is the number of source terms for cell  $n$ .

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