

the U.S. Geological Survey Water Availability and Use Science Program

MODFLOW 6 – Supplemental Technical Information

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Cover. Binary computer code illustration.

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Chapter 1. Introduction

This document is a technical reference document that describes the motivation and implementation of functionality added to MODFLOW 6 since the initial release ([Hughes and others, 2017](#); [Langevin and others, 2017](#)) and not documented in separate U.S. Geological Survey publications, for example [Provost and others \(2017\)](#). Examples have been included for the MODFLOW 6 components summarized in table 1–1.

Table 1–1. MODFLOW 6 enhancements.

MODFLOW 6 enhancements	Chapter	Initial MODFLOW 6 version	Latest update – MODFLOW 6 version
Specific Discharge	2	6.0.2	6.1.0
DRN Package	3	6.1.1	–
Discharge Scaling			
MAW Package			
Connection Flow Correction	4	6.1.1	–
STO Package Specific Storage Revision	5	6.1.3	–
TVK and TVS Capabilities for NPF	6	6.3.0	–
Generalized Coupling of Numerical Models	7	6.3.0	–
VSC Package	8	6.4.0	–

Chapter 2. Specific Discharge

A MODFLOW 6 flow simulation calculates the flow of water across all interfaces between cells. The flow reported for a given cell-cell interface is the component of the flow vector normal to the interface. The normal component of the specific discharge (L/T), or Darcy velocity, which we shorten here to "velocity," is obtained by dividing the normal component of flow by the interface area. The velocity vector at the center of a cell can then be estimated by interpolating component information from all the interfaces of the cell.

The velocity interpolation scheme presented here is an adaptation and simplification of the gradient interpolation scheme used in the XT3D capability of MODFLOW 6 ([Provost and others, 2017](#)). In XT3D, the three-dimensional head-gradient vector is estimated at a point on the interface between two cells using gradient-component information from the connections between each of those two cells and its neighboring cells. In this velocity interpolation scheme, the three-dimensional velocity vector is estimated at the center of a cell using velocity-component information from the cell-cell interfaces of the cell. (The scheme does not currently include velocity-component information from "external" faces of a cell but could be modified to do so.) The assembly of component information and the weighting scheme in the velocity interpolation are similar to those in the XT3D gradient interpolation: the greatest weight is given to component information from points that are closest to the cell center and whose directions are most closely aligned with the desired velocity component. In XT3D, gradient components are initially estimated in a coordinate system aligned with the connection between two cells, whereas in the velocity interpolation the components are estimated directly in (x, y, z) model coordinates. This simplifies the notation somewhat and, more importantly, allows the z component to be treated separately from the x and y components using information only from the horizontal interfaces of the cell (those along the top or bottom of the cell), which are the only interfaces that provide z -component information.

Estimating the z Component of Velocity (Specific Discharge)

The z component of velocity (L/T) at the cell center, v^z , is estimated by calculating a weighted average of the z components of velocity at the horizontal interfaces of the cell:

$$v^z = \sum_{k=1}^{N_H} \phi_k^z v_k^z, \quad (2-1)$$

where the summation is over the horizontal interfaces of the cell, which are locally indexed by $k = 1, \dots, N_H$, v_k^z is the z component of velocity (L/T) at horizontal interface k , and ϕ_k^z is the weight (unitless) assigned to v_k^z . (Weights are discussed in detail in the "[Weights](#)" section below.)

Estimating the x and y Components of Velocity (Specific Discharge)

The development in this section closely parallels the development in equations 9 through 16 in [Provost and others \(2017\)](#). The present development has been adapted specifically for interpolation of the velocity vector at a cell center in (x, y, z) model coordinates and is simplified by the separate treatment of the z component described in the previous section.

The vertical interfaces of a cell (those along the "sides" of the cell), which are locally indexed by $i = 1, \dots, N_V$, provide normal-component information that is used to estimate the x and y components of the velocity at the cell center. By definition, v_i^n , the normal component of velocity (L/T) at vertical interface i , is related to the three-dimensional velocity vector by

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$$\mathbf{n}_i^T \mathbf{v}_i = v_i^n, \quad (2-2)$$

where superscript “T” indicates the transpose, and the left-hand side of equation 2–2 is the scalar product (or “dot product”) of \mathbf{n}_i , the unit vector (unitless) normal to interface i , and \mathbf{v}_i , the velocity vector (L/T) at interface i . Expanding equation 2–2 in terms of vector components gives

$$n_i^x v_i^x + n_i^y v_i^y + n_i^z v_i^z = v_i^n. \quad (2-3)$$

where n_i^x , n_i^y , and n_i^z are, respectively, the x , y , and z components of \mathbf{n}_i , and v_i^x , v_i^y , and v_i^z are, respectively, the x , y , and z components of \mathbf{v}_i . Recognizing that $n_i^z = 0$ for a vertical interface and solving equation 2–3 for the x component of velocity gives

$$v_i^x = (v_i^n - n_i^y v_i^y) / n_i^x. \quad (2-4)$$

The expression for v_i^x in equation 2–4 is based on information solely from vertical interface i . However, the y component, v_i^y , which appears on the right-hand side of equation 2–4, is unknown and cannot be deduced based on information from interface i alone. Therefore, it is assumed that the y component of velocity (L/T) at the cell center, v^y , which is also unknown at this point but will eventually be estimated, may be substituted into equation 2–4 as an approximation to v_i^y . The x component of velocity (L/T) at the cell center, v^x , is then estimated by calculating a weighted average of the x components of velocity at all the vertical interfaces:

$$v^x = \sum_{i=1}^{N_V} \phi_i^x v_i^x = \sum_{i=1}^{N_V} \frac{\phi_i^x v_i^n}{n_i^x} - \left(\sum_{i=1}^{N_V} \frac{\phi_i^x n_i^y}{n_i^x} \right) v^y, \quad (2-5)$$

where ϕ_i^x is the weight (unitless) assigned to v_i^x . Analogous consideration of the y component of velocity (L/T) at the cell center, v^y , produces the weighted average

$$v^y = \sum_{i=1}^{N_V} \phi_i^y v_i^y = \sum_{i=1}^{N_V} \frac{\phi_i^y v_i^n}{n_i^y} - \left(\sum_{i=1}^{N_V} \frac{\phi_i^y n_i^x}{n_i^y} \right) v^x, \quad (2-6)$$

where ϕ_i^y is the weight (unitless) assigned to v_i^y . (Weights are discussed in detail in the “Weights” section below.) There are now two equations, 2–5 and 2–6, that can be solved for the two unknowns, v^x and v^y , to give

$$v^x = \frac{1}{1 - A^{xy} A^{yx}} \sum_{i=1}^{N_V} (B_i^x - A^{xy} B_i^y) v_i^n \quad (2-7)$$

$$v^y = \frac{1}{1 - A^{xy} A^{yx}} \sum_{i=1}^{N_V} (B_i^y - A^{yx} B_i^x) v_i^n, \quad (2-8)$$

where

$$A^{xy} = \sum_{i=1}^{N_V} B_i^x n_i^y \quad (2-9)$$

$$A^{yx} = \sum_{i=1}^{N_V} B_i^y n_i^x, \quad (2-10)$$

and

$$B_i^x = \frac{\phi_i^x}{n_i^x} \quad (2-11)$$

$$B_i^y = \frac{\phi_i^y}{n_i^y}. \quad (2-12)$$

Equations 2-7 and 2-8, with the coefficients given by equations 2-9 through 2-12, are the expressions used to estimate the x and y components of the velocity vector at the cell center based on normal-component information at the vertical interfaces of the cell.

Weights

For estimation of the z component of velocity as a weighted average, we define a set of weights (unitless) based on the shortest distance (L), D_k , from the cell center to each horizontal interface k as follows:

$$\omega_k^z = 1 - \frac{D_k}{\sum_{m=1}^{N_H} D_m}. \quad (2-13)$$

Interfaces that are closest to the cell center receive the greatest weights. Before incorporating the weights into equation 2-1, we normalize them so they sum to 1:

$$\phi_k^z = \frac{\omega_k^z}{N_H - 1} = \frac{1}{N_H - 1} \left(1 - \frac{D_k}{\sum_{m=1}^{N_H} D_m} \right). \quad (2-14)$$

For estimation of the x and y components of velocity, we define a set of weights (unitless) that take into account not only distance from the cell center, but also how closely the normal-component information at each vertical interface aligns with the velocity component (x or y) being expressed as a weighted average. For the x component of velocity the weights are

$$\omega_i^x = \left[1 - \frac{D_i |n_i^x|}{\sum_{l=1}^{N_V} D_l |n_l^x|} \right] |n_i^x| = \left[\frac{\sum_{l=1}^{N_V} D_l |n_l^x| - D_i |n_i^x|}{\sum_{l=1}^{N_V} D_l |n_l^x|} \right] |n_i^x|, \quad (2-15)$$

and for the y component of velocity the weights are

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$$\omega_i^y = \left[1 - \frac{D_i |n_i^y|}{\sum_{l=1}^{N_V} D_l |n_l^y|} \right] |n_i^y| = \left[\frac{\sum_{l=1}^{N_V} D_l |n_l^y| - D_i |n_i^y|}{\sum_{l=1}^{N_V} D_l |n_l^y|} \right] |n_i^y|. \quad (2-16)$$

Interfaces that are closest to the cell center and align most closely with the component direction (x or y) for which they are being used receive the greatest weights. The corresponding normalized weights used in equations 2-11 and 2-12 are:

$$\phi_i^x = \frac{\omega_i^x |n_i^x|}{\sum_{l=1}^{N_V} \omega_l^x |n_l^x|} \quad (2-17)$$

and

$$\phi_i^y = \frac{\omega_i^y |n_i^y|}{\sum_{l=1}^{N_V} \omega_l^y |n_l^y|}, \quad (2-18)$$

respectively. Substitution of equations 2-15 and 2-16 into equations 2-17 and 2-18, followed by substitution of equations 2-17 and 2-18 into equations 2-11 and 2-12, and simplification results in the following expressions for the coefficients B_i^x and B_i^y :

$$B_i^x = \frac{\left[\sum_{l=1}^{N_V} D_l |n_l^x| - D_i |n_i^x| \right] |n_i^x| \operatorname{sign}(n_i^x)}{\sum_{j=1}^{N_V} \left[\sum_{l=1}^{N_V} D_l |n_l^x| - D_j |n_j^x| \right] |n_j^x| |n_j^x|} \quad (2-19)$$

and

$$B_i^y = \frac{\left[\sum_{l=1}^{N_V} D_l |n_l^y| - D_i |n_i^y| \right] |n_i^y| \operatorname{sign}(n_i^y)}{\sum_{j=1}^{N_V} \left[\sum_{l=1}^{N_V} D_l |n_l^y| - D_j |n_j^y| \right] |n_j^y| |n_j^y|}, \quad (2-20)$$

where $\operatorname{sign}(n)$ equals +1, 0, or -1 when n is positive, zero, or negative, respectively.

Chapter 3. Drain Package Discharge Scaling

In the original release of the MODFLOW 6 Drain (DRN) Package a drain is designed to simulate the effects of agricultural drains, springs, and other features that remove water from the aquifer at a rate proportional to the difference between the head in the aquifer and some fixed head or elevation, called the drain elevation, so long as the head in the aquifer is above that elevation. If, however, the aquifer head falls below the drain elevation, then the drain has no effect on the aquifer. The constant of proportionality is called the drain conductance. This chapter describes a new feature of the MODFLOW 6 DRN Package that allows the drain conductance to gradually increase from zero to the user-specified value as a function of the simulated groundwater head.

Theory

The standard drain equation in MODFLOW 6 is

$$Q_{out,nb} = \begin{cases} 0 & h_n \leq HDRN_{nb} \\ CDRN_{nb} (h_n - HDRN_{nb}) & h_n > HDRN_{nb} \end{cases}, \quad (3-1)$$

where $Q_{out,nb}$ is the flow from the aquifer to drain nb ($L^3 T^{-1}$), $CDRN_{nb}$ is the drain conductance ($L^2 T^{-1}$), $HDRN_{nb}$ is the drain elevation (L), and h_n is the head in the cell containing the drain (L). Equation 3-1 rewritten in terms of flow from the drain into aquifer ($L^3 T^{-1}$), $QDRN$, is

$$QDRN_{nb} = \begin{cases} CDRN_{nb} (HDRN_{nb} - h_n) & h_n > HDRN_{nb} \\ 0 & h_n \leq HDRN_{nb} \end{cases}. \quad (3-2)$$

The standard DRN Package has been modified to include the option to scale the drain conductance using either linear or cubic scaling. The modified form of the drain equation (eq. 3-2) with linear scaling is

$$QDRN_{nb} = F_{DRN_{nb}} CDRN_{nb} (ZDRN_{nb} - h_n), \quad (3-3)$$

where $ZDRN_{nb}$ is the elevation at which drainage discharge begins (L), and $F_{DRN_{nb}}$ is the linear scaling function (unitless), which accounts for how the conductance of the drain changes with changes in head. Conceptually, the drain conductance changes because the area through which flow occurs depends on the head. The area through which flow occurs increases as the head at the drain increases. The linear scaling function is defined as

$$F_{DRN_{nb}} = \begin{cases} 0 & \Delta h_{n,nb}^r \leq 0 \\ \Delta h_{n,nb}^r & 0 < \Delta h_{n,nb}^r < 1, \\ 1 & \Delta h_{n,nb}^r \geq 1 \end{cases}, \quad (3-4)$$

where $DDRN_{nb}$ is the drainage depth (L) and the relative drain head difference (L) is defined as

$$\Delta h_{n,nb}^r \equiv \frac{h_n - ZDRN_{nb}}{|DDRN_{nb}|}. \quad (3-5)$$

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The elevation at which drainage begins, $ZDRN_{nb}$ depends on whether the drainage depth, $DDRN_{nb}$, is positive or negative and is calculated as

$$ZDRN_{nb} = \begin{cases} HDRN_{nb} - |DDRN_{nb}| & DDRN_{nb} < 0, \\ HDRN_{nb} & DDRN_{nb} \geq 0 \end{cases} \quad (3-6)$$

If $DDRN_{nb}$ is positive, $ZDRN_{nb}$ is the drain elevation just as it is in the standard formulation. If $DDRN_{nb}$ is negative, $ZDRN_{nb}$ is the drain elevation plus the (negative) drainage depth. If $DDRN_{nb}$ is zero, the standard formulation is used. The linear scaling function ($F_{DRN_{nb}}$) is shown in figure 3–1.

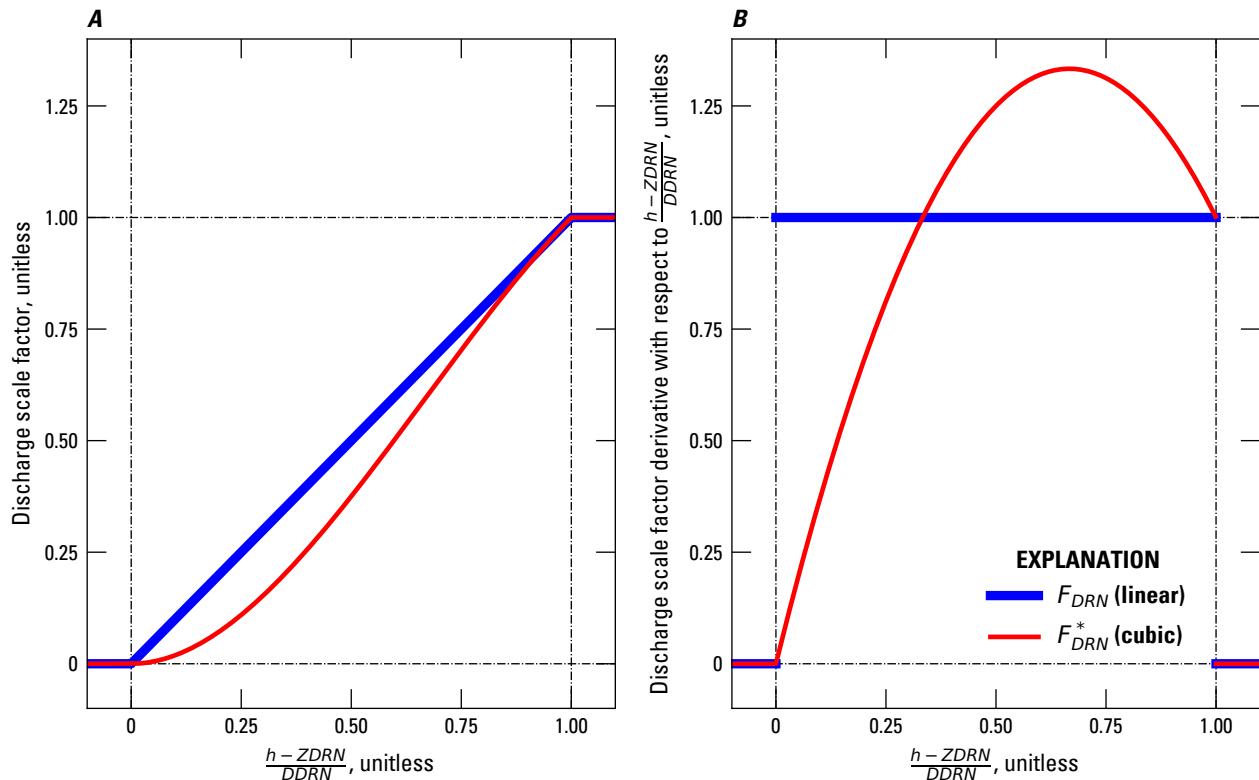


Figure 3–1. Graphs showing combined linear and cubic scaling functions for drain discharge and the derivatives of the linear and cubic scaling fraction functions. *A*, linear and cubic fraction functions and *B*, derivatives of the linear and cubic scaling functions with respect to the relative drain head difference ($\frac{h - ZDRN}{|DDRN|}$). The derivative of the linear and cubic scaling functions with respect to h is the product of the derivative with respect to $\frac{h - ZDRN}{|DDRN|}$ and $\frac{1}{|DDRN|}$.

The linear scaling function varies with head according to equations 3–4 and 3–5. Differentiation of equation 3–4 with respect to h_n , with application of the chain rule to account for the variation of $\Delta h_{n,nb}^r$ with respect to h_n in equation 3–5, gives

$$\frac{\partial F_{DRN_{nb}}}{\partial h_n} = \begin{cases} 0 & \Delta h_{n,nb}^r \leq 0 \\ \frac{1}{|DDRN_{nb}|} & 0 < \Delta h_{n,nb}^r < 1, \\ 1 & \Delta h_{n,nb}^r \geq 1 \end{cases} \quad (3-7)$$

which is discontinuous in the neighborhood of $h_n = ZDRN_{nb}$ and $h_n = ZDRN_{nb} - |DDRN_{nb}|$. The derivative of the linear scaled drain discharge (eq. 3-3) with respect to h_n is

$$\frac{\partial QDRN_{nb}}{\partial h_n} = -F_{DRN_{nb}} CDRN_{nb} + \frac{\partial F_{DRN_{nb}}}{\partial h_n} CDRN_{nb} (ZDRN_{nb} - h_n). \quad (3-8)$$

Substitution of equations 3-4 and 3-7 into equation 3-8 results in

$$\frac{\partial QDRN_{nb}}{\partial h_n} = \begin{cases} 0 & \Delta h_{n,nb}^r \leq 0 \\ -2 CDRN_{nb} \Delta h_{n,nb}^r & 0 < \Delta h_{n,nb}^r < 1, \\ -CDRN_{nb} & \Delta h_{n,nb}^r \geq 1 \end{cases} \quad (3-9)$$

which remains discontinuous in the vicinity of $ZDRN_{nb}$.

When the Newton-Raphson formulation is used, discontinuous derivatives can cause non-convergence in the neighborhood of the discontinuity (Kavetski and Kuczera, 2007). To ensure continuous drain discharge derivatives when the Newton-Raphson formulation is used, cubic smoothing of the linear relative drain head difference is used and equation 3-3 is modified to

$$QDRN_{nb}^* = F_{DRN_{nb}}^* CDRN_{nb} (ZDRN_{nb} - h_n), \quad (3-10)$$

where where $F_{DRN_{nb}}^*$ is the cubic scaling function. The cubic scaling function is defined as

$$F_{DRN_{nb}}^* = \begin{cases} 0 & \Delta h_{n,nb}^r \leq 0 \\ -(\Delta h_{n,nb}^r)^3 + 2(\Delta h_{n,nb}^r)^2 & 0 < \Delta h_{n,nb}^r < 1, \\ 1 & \Delta h_{n,nb}^r \geq 1 \end{cases} \quad (3-11)$$

which is continuous in the vicinity of $h_n = ZDRN_{nb}$ and $h_n = ZDRN_{nb} - |DDRN_{nb}|$ (fig. 3-1A). The derivative of equation 3-11 with respect to h_n is

$$\frac{\partial F_{DRN_{nb}}^*}{\partial h_n} = \begin{cases} 0 & \Delta h_{n,nb}^r \leq 0 \\ -\frac{3}{|DDRN_{nb}|} (\Delta h_{n,nb}^r)^2 + & \\ \frac{4}{|DDRN_{nb}|} \Delta h_{n,nb}^r & 0 < \Delta h_{n,nb}^r < 1, \\ 0 & \Delta h_{n,nb}^r \geq 1 \end{cases}, \quad (3-12)$$

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which is discontinuous in the vicinity of $h_n = ZDRN_{nb} - |DDRN_{nb}|$ (fig. 3–1B). The derivative of the cubic scaled drain discharge (eq. 3–10) with respect to h is

$$\frac{\partial QDRN_{nb}^*}{\partial h} = -F_{DRN_{nb}}^* CDRN_{nb} + \frac{\partial F_{DRN_{nb}}^*}{\partial h} CDRN_{nb} (ZDRN_{nb} - h_n). \quad (3-13)$$

Substitution of equations 3–11 and 3–12 into equation 3–13 results in

$$\frac{\partial QDRN_{nb}^*}{\partial h_n} = \begin{cases} 0 & \Delta h_{n,nb}^r \leq 0 \\ -CDRN_{nb} \left[-(\Delta h_{n,nb}^r)^3 + 2(\Delta h_{n,nb}^r)^2 \right] + \\ CDRN_{nb} \left[-\frac{3}{DDRN_{nb}} (\Delta h_{n,nb}^r)^2 + \right. \\ \left. \frac{4}{DDRN_{nb}} (\Delta h_{n,nb}^r) \right] (ZDRN_{nb} - h_n) & 0 < \Delta h_{n,nb}^r < 1 \\ -CDRN_{nb} & \Delta h_{n,nb}^r \geq 1 \end{cases}, \quad (3-14)$$

which is continuous in the vicinity of $h_n = ZDRN_{nb}$ and $h_n = ZDRN_{nb} - |DDRN_{nb}|$.

Example Drain Discharge Scaling Calculations

An example of the differences between the standard, linearly-scaled, and cubically-scaled drainage discharge are shown in figure 3–2. In this example the elevation that drainage discharge starts ($ZDRN$) is set at $\frac{DDRN}{2}$ below land surface elevation and drainage discharge is equal for all approaches at $ZDRN + DDRN$ (fig. 3–2A). In this conceptual problem, the groundwater head linearly increases from a value less than $ZDRN$ to greater than $ZDRN + DDRN$ during the simulation, which is presented as the head difference ($h - ZDRN$) divided by the drainage depth in figure 3–2B. The drainage discharge that results from the linear increase in groundwater head using the original-, linear-, and cubic-scaling increases with time as is shown in figure 3–2C and shows the continuous nature of the linear- and cubic scaled drainage discharge and that all three approaches result in the same drain discharge rate when the relative drain head difference is greater than or equal to one. Figure 3–2D shows that the cumulative drain discharge for the original drain formulation is 170 to 200 L^3 greater than the cubic- and linear-scaled drainage discharge, respectively.

Incorporation of the modified Drain (DRN) Package into the CVFD Groundwater Flow Equation

To prepare the CVFD equation for solution using the standard formulation, it is convenient to rearrange the discretized groundwater flow equation for a cell so that all terms containing heads at the end of the current time step are grouped on the left-hand side of the equation, and all terms that are independent of head at the end of the current time step are on the right-hand side of equation 6–1 in [Langevin and others \(2017\)](#). Refer to [Langevin and others \(2017\)](#) for additional information on how the groundwater flow equation is formulated in MODFLOW 6.

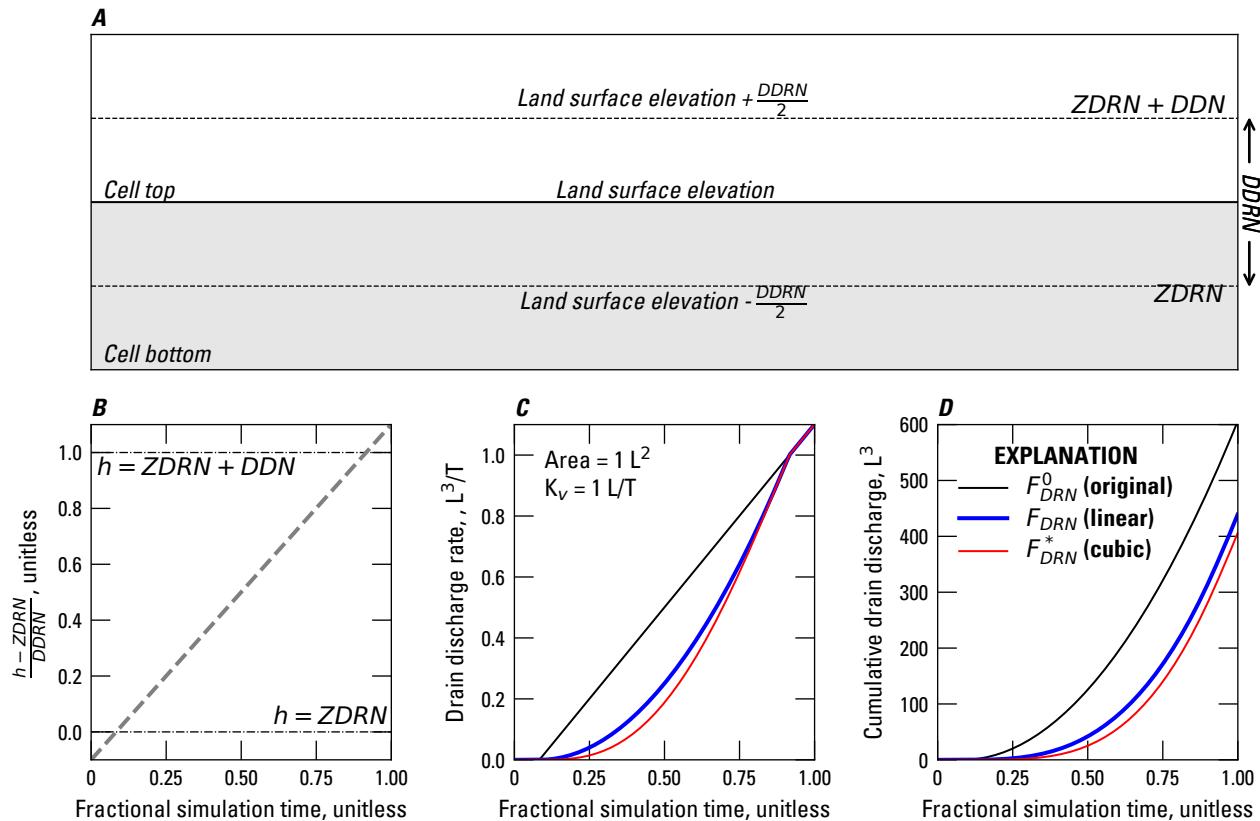


Figure 3–2. Graphs showing a conceptual model cell using scaled drain discharge and the relation between the groundwater level and drain discharge. *A*, Conceptual model cell containing a drain cell where drainage discharge starts $\frac{DDRN}{2}$ below land surface and is equal $\frac{DDRN}{2}$ above land surface for all drain scaling approaches. *B*, conceptual linear groundwater level increases, which are presented as a relative drain head difference, with fractional simulation time. *C*, calculated original, linear, and cubic scaled drainage discharge rates resulting from conceptual groundwater level increases, and *D*, calculated original, linear, and cubic scaled drainage cumulative discharge resulting from conceptual groundwater level increases.

Standard Formulation

According to the sign convention in MODFLOW 6, $QDRN_{nb}$ in the groundwater flow equation is defined as a head-dependent flow out of cell n , and corresponding terms must be added to the left and right sides of equation 6–1 in Langevin and others (2017) for each cell containing a drain. This is accomplished in the modified Drain Package by adding the head-dependent term and the known term in equation 3–3 to the left- and right-side of equation 6–1 in Langevin and others (2017). The contribution of the modified drain equations to the left-hand side and right-hand sides of the groundwater flow equation are

$$\begin{aligned} A_{n,n} &\leftarrow A_{n,n} - F_{DRN_{nb}} CDRN_{nb} \\ b_n &\leftarrow b_n - F_{DRN_{nb}} CDRN_{nb} ZDRN_{nb}, \end{aligned} \quad (3-15)$$

where $A_{n,n}$ is the diagonal of the coefficient matrix for cell n and b_n is the right-hand side of the groundwater flow equation for cell n . In the case where drainage discharge is not scaled, $F_{DRN_{nb}}$ is zero when h_n is less than or equal to $HDRN_{nb}$ and one when h_n is greater than $HDRN_{nb}$, which results in identical behavior as the original drain package formulation.

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Newton-Raphson Formulation

The modified Newton-Raphson form of equation 3–10 solved in terms of h instead of Δh and incorporated into the Newton-Raphson form of the groundwater flow equation (Langevin and others, 2017, eq. 2–26) is

$$\frac{\partial QDRN_{nb}^*}{\partial h_n} h_n^k = -QDRN_{nb}^* + \frac{\partial QDRN_{nb}^*}{\partial h_n} h_n^{k-1}, \quad (3-16)$$

where h_n^k is the head at the end of the current non-linear (picard) iteration and h_n^{k-1} is the head at the start of the current non-linear iteration. Substitution of equations 3–10 and 3–13 into equation 3–16 results in

$$\begin{aligned} A_{n,n} &\leftarrow A_{n,n} - F_{DRN_{nb}}^* CDRN_{nb} + \frac{\partial F_{DRN_{nb}}^*}{\partial h} CDRN_{nb} (ZDRN_{nb} - h_n) \\ b_n &\leftarrow b_n - F_{DRN_{nb}}^* CDRN_{nb} (ZDRN_{nb} - h_n^{k-1}) \\ &+ \left[-F_{DRN_{nb}}^* CDRN_{nb} + \frac{\partial F_{DRN_{nb}}^*}{\partial h} CDRN_{nb} (ZDRN_{nb} - h_n) \right] h_n^{k-1}. \end{aligned} \quad (3-17)$$

Simplifying the right-hand side contribution in equation 3–17 results in

$$b_n \leftarrow b_n - F_{DRN_{nb}}^* CDRN_{nb} ZDRN_{nb} + \left[\frac{\partial F_{DRN_{nb}}^*}{\partial h} CDRN_{nb} (ZDRN_{nb} - h_n) \right] h_n^{k-1}. \quad (3-18)$$

The $F_{DRN_{nb}}^* CDRN_{nb}$ term in equation 3–17 and the $F_{DRN_{nb}}^* CDRN_{nb} ZDRN_{nb}$ term in equation 3–18 are subtracted from the diagonal of the coefficient matrix and the right-hand side of the groundwater-flow equation, respectively, during the standard formulation step for the drain package. The Newton-Raphson formulation for the modified drain package is completed by augmenting the coefficient matrix with the derivative term in equation 3–17 and adding the second term in equation 3–18 (the product of a derivative term and the head at the start of the current iteration) to the right-hand side of the groundwater-flow equation.

Use of Drain Discharge Scaling

A few examples of how the modified drain package can be used to simulate drainage discharge consistent with other MODFLOW 6 packages are given below.

The original drain package formulation with a specified drainage depth value

Specifying $DDRN$ to be 0 results in a drain that behaves the same as the original DRN Package (eq. 3–1). Using a combination of $DDRN$ values set to zero and non-zero values will result in drains with 0 values behaving like the original drain package and others using the scaled drainage discharge approach.

Groundwater seepage from the Unsaturated Zone Flow Package

The drain package can be used as an alternative to the groundwater seepage option in the Unsaturated Zone Flow (UZF) Package. Specifying a positive $DDRN$ value and $HDRN_{nb}$ to be $\frac{DDRN}{2}$ below the single values specified with the standard DRN Package approach (for example, setting $DDRN$ to be at land surface) results in a formulation that is equivalent to the groundwater seepage option available in the UZF Package in

MODFLOW 6 ([Langevin and others, 2017](#)). To be consistent with the UZF package, the drain conductance should be calculated as

$$CDRN_{nb} = \frac{K_{v_{nb}} A_n}{DDRN_{nb}}, \quad (3-19)$$

where $K_{v_{nb}}$ is vertical hydraulic conductivity (LT^{-1}) and A_n is the horizontal area of cell n (L^2).

Chapter 4. Multi-Aquifer Well Package Connection Flow Correction

Special considerations are required for flow to convertible cells that can dry and rewet. When flow is between two cells that are wet, the head difference between them creates the driving force for flow. When the downstream cell is dry, however, a reference elevation can be used instead of the downstream head to express flow between the nodes. The “perched” option in the Node Property Flow (NPF) Package can be used to correct downward flow to a partially saturated cell.

The “flow correction” option in the Multi-Aquifer Well (MAW) Package implements the same correction as the NPF package “perched” option and corrects the flow between a multi-aquifer well connection and a GWF cell. The approach used in the MAW Package is identical to the “flow-to-dry-cell” option available in MODFLOW-USG ([Panday and others, 2013](#)).

Multi-Aquifer Well Flow Correction

When the “flow correction” option is enabled, flow to a well from a GWF cell based on equation 7–50 in [Langevin and others \(2017\)](#) is

$$Q_{MAW,MAW,n} = \begin{cases} S_{MAW,n} C_{MAW,n}^0 (h_n - e_{MAW,n}) & HMAW_i < e_{MAW,n}, \\ S_{MAW,n} C_{MAW,n}^0 (h_n - HMAW_i) & HMAW_i \geq e_{MAW,n}, \end{cases} \quad (4-1)$$

where $S_{MAW,n}$ is the well screen saturation (unitless), $C_{MAW,n}^0$ is the saturated well conductance ($L^2 T^{-1}$), h_n is the head in cell n (L), $e_{MAW,n}$ is the reference elevation for the well connection (L), and $HMAW_i$ is the head in well i (L). The reference elevation for the well connection is defined to be

$$e_{MAW,n} = \begin{cases} BOT_n & BOT_n > BOT_{MAW,n}, \\ BOT_{MAW,n} & BOT_{MAW,n} > BOT_n, \end{cases} \quad (4-2)$$

where BOT_n is the bottom of cell n (L) and $BOT_{MAW,n}$ is the bottom of the well screen for the connection of well i to cell n (L). For the case where the head in cell n is less than $e_{MAW,n}$, flow from a well to a GWF cell is

$$Q_{MAW,MAW,n} = \begin{cases} S_{MAW,n} C_{MAW,n}^0 (e_{MAW,n} - HMAW_i) & h_n < e_{MAW,n}, \\ S_{MAW,n} C_{MAW,n}^0 (h_n - HMAW_i) & h_n \geq e_{MAW,n}. \end{cases} \quad (4-3)$$

Incorporation of the Flow Correction into the CVFD Groundwater Flow Equation

Multi-aquifer well flow terms are incorporated into the CVFD flow equation ([Langevin and others, 2017](#), eq. 6–1) based on whether the standard or Newton-Raphson formulation is being used. The details of how the multi-aquifer well flow correction terms are incorporated into the CVFD flow equation is described below.

Standard Formulation

The terms in the standard flow equation for all groundwater cells connected to a multi-aquifer well i based on ([Langevin and others, 2017](#), eq. 7–55) is

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$$\sum_{n \in MAW_i} S_{MAW,n} C_{MAW,n}^0 (h_n - HMAW_i) = 0. \quad (4-4)$$

To implement the flow correction, equation 4–1 is modified to

$$QMAW_{MAW,n} = S_{MAW,n} C_{MAW,n}^0 (h_n - HMAW_i) + S_{MAW,n} C_{MAW,n}^0 (HMAW_i - \bar{h}_{MAW,n}), \quad (4-5)$$

where $\bar{h}_{MAW,n}$ is a function that transitions between the head at the downstream node, $HMAW_i$ in this case, and reference elevation $e_{MAW,n}$. The downstream head transition function used to correct the multi-aquifer flow for a connection is calculated as

$$\bar{h}_{MAW,n} = \begin{cases} e_{MAW,n} & h_{ds} < e_{MAW,n}, \\ h_{ds} & h_{ds} \geq e_{MAW,n} \end{cases}, \quad (4-6)$$

where h_{ds} is head in the downstream node (L), which is the minimum of $HMAW_i$ and h_n . The relation between the downstream head and $\bar{h}_{MAW,n}$ is shown in figure 4–1.

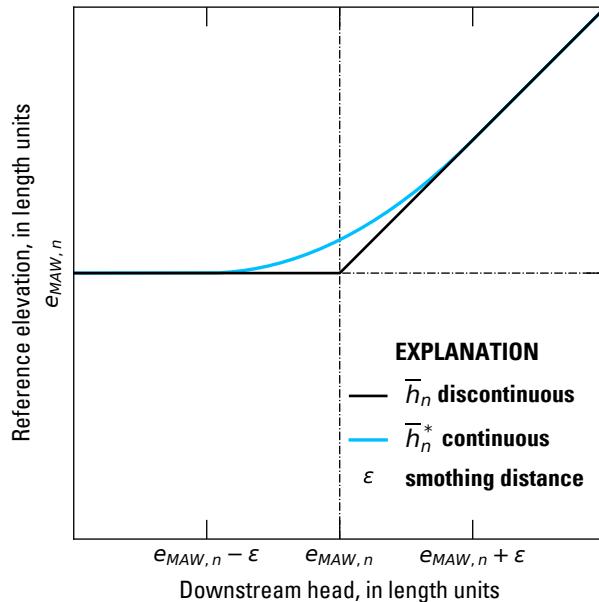


Figure 4–1. Graph showing the discontinuous (eq. 4–6) and continuous (eq. 4–9) downstream head transition function used to correct the multi-aquifer flow for a connection as it transitions from saturated to partially saturated conditions. The interval over which the smoothing occurs, ϵ , is also shown.

Similarly, when h_n is the downstream node equation 4–3 is modified to

$$QMAW_{MAW,n} = S_{MAW,n} C_{MAW,n}^0 (h_n - HMAW_i) + S_{MAW,n} C_{MAW,n}^0 (\bar{h}_{MAW,n} - h_n), \quad (4-7)$$

The first term on the right hand side of equations 4-5 and 4-7 ($S_{MAW,n}C_{MAW,n}^0$) are added to the coefficient matrix used to solve the coupled groundwater and multi-aquifer well flow equations as part of the standard MAW package formulation (Langevin and others, 2017, eq. 7-55). The flow correction is made by subtracting the second term on the right hand side of equations 4-5 and 4-7 from the right had side of equation 6-1 in Langevin and others (2017). In the case where $HMAW_i$ and h_n are both greater than $e_{MAW,n}$, the second term on the right hand side of equations 4-5 and 4-7 is equal to zero, which results in a equation identical to equation 4-4 for a single connection.

Newton-Raphson Formulation

The modified Newton-Raphson form of equation 4-4 solved for a single connection in terms of h instead of Δh and incorporated into the Newton-Raphson form of the groundwater flow equation (Langevin and others, 2017, eq. 2-26) is

$$\frac{\partial QMAW_{MAW,n}}{\partial HMAW_i} HMAW_i^k + \frac{\partial QMAW_{MAW,n}}{\partial h_n} h_n^k = -QMAW_{MAW,n} + \frac{\partial QMAW_{MAW,n}}{\partial HMAW_i} HMAW_i^{k-1} + \frac{\partial QMAW_{MAW,n}}{\partial h_n} h_n^{k-1}, \quad (4-8)$$

where $HMAW_i^k$ and h_n^k are the heads at the end of the current non-linear (picard) iteration and $HMAW_i^{k-1}$ and h_n^{k-1} are the head at the start of the current non-linear iteration.

When the Newton-Raphson formulation is used, discontinuous derivatives can cause non-convergence in the neighborhood of the discontinuity (Kavetski and Kuczera, 2007). As a result, the discontinuous well screen saturation ($S_{MAW,n}$) in equations 4-5 and 4-7 is replaced by a quadratically smoothed well screen saturation ($S_{MAW,n}^*$ – eq. 4-5 in Langevin and others (2017)). The discontinuous downstream head transition function ($\bar{h}_{MAW,n}$, eq. 4-6) in equations 4-5 and 4-7 is also replaced by

$$\bar{h}_{MAW,n}^* = \begin{cases} e_{MAW,n} & h_{ds} - e_{MAW,n} < -\epsilon \\ \frac{(h_{ds} - e_{MAW,n})^2}{4\epsilon} + \frac{(h_{ds} - e_{MAW,n})}{2} + \frac{\epsilon}{4} + e_{MAW,n} & -\epsilon < h_{ds} - e_{MAW,n} < +\epsilon \\ h_{ds} & h_{ds} - e_{MAW,n} \geq +\epsilon \end{cases} \quad (4-9)$$

where ϵ is the interval over which the head transition function is smoothed. The relation between the downstream head and $\bar{h}_{MAW,n}^*$ is shown in figure 4-1. Simplification of equations 4-5 and 4-7 results in

$$QMAW_{MAW,n} = S_{MAW,n}^* C_{MAW,n}^0 (h_n - \bar{h}_{MAW,n}^*) \quad (4-10)$$

and

$$QMAW_{MAW,n} = S_{MAW,n}^* C_{MAW,n}^0 (\bar{h}_{MAW,n}^* - HMAW_i) \quad (4-11)$$

when $HMAW_i$ and h_n are the downstream heads, respectively. The derivatives of equation 4-10 with respect to h_n and $HMAW_i$ are

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$$\frac{\partial Q_{MAW}}{\partial HMAW_i} = -S_{MAW,n}^* C_{MAW,n}^0 \frac{\partial \bar{h}_{MAW,n}^*}{\partial HMAW_i} \quad (4-12)$$

and

$$\frac{\partial Q_{MAW}}{\partial h_n} = S_{MAW,n}^* C_{MAW,n}^0 + \frac{\partial S_{MAW,n}^*}{\partial h_n} C_{MAW,n}^0 (h_n - \bar{h}_{MAW,n}^*), \quad (4-13)$$

respectively. The derivatives of equation 4-11 with respect to h_n and $HMAW_i$ are

$$\frac{\partial Q_{MAW}}{\partial HMAW_i} = -S_{MAW,n}^* C_{MAW,n}^0 + \frac{\partial S_{MAW,n}^*}{\partial HMAW_i} C_{MAW,n}^0 (\bar{h}_{MAW,n}^* - HMAW_i) \quad (4-14)$$

and

$$\frac{\partial Q_{MAW}}{\partial h_n} = S_{MAW,n}^* C_{MAW,n}^0 \frac{\partial \bar{h}_{MAW,n}^*}{\partial h_n}. \quad (4-15)$$

The derivative of $\bar{h}_{MAW,n}^*$ with respect to the downstream head is

$$\frac{\partial \bar{h}_{MAW,n}^*}{\partial h_{ds}} = \begin{cases} 0 & h_{ds} - e_{MAW,n} < -\epsilon \\ \frac{h_{ds} - e_{MAW,n}}{2\epsilon} + \frac{1}{2} & -\epsilon < h_{ds} - e_{MAW,n} < +\epsilon \\ 1 & h_{ds} - e_{MAW,n} \geq +\epsilon \end{cases} \quad (4-16)$$

Newton-Raphson formulation when $HMAW_i$ is the Downstream Head

The Newton-Raphson form of the equation 4-5, when $HMAW_i$ is the downstream head, is formulated by substituting equations 4-10, 4-12, and 4-13 into equation 4-8, which results in

$$\begin{aligned} & \left[-S_{MAW,n}^* C_{MAW,n}^0 \frac{\partial \bar{h}_{MAW,n}^*}{\partial HMAW_i} \right] HMAW_i^k + \\ & \left[S_{MAW,n}^* C_{MAW,n}^0 + \frac{\partial S_{MAW,n}^*}{\partial h_n} C_{MAW,n}^0 (h_n^{k-1} - \bar{h}_{MAW,n}^{k-1}) \right] h_n^k = \\ & -S_{MAW,n}^* C_{MAW,n}^0 (h_n^{k-1} - \bar{h}_{MAW,n}^{k-1}) + \\ & \left[-S_{MAW,n}^* C_{MAW,n}^0 \frac{\partial \bar{h}_{MAW,n}^*}{\partial HMAW_i} \right] HMAW_i^{k-1} + \\ & \left[S_{MAW,n}^* C_{MAW,n}^0 + \frac{\partial S_{MAW,n}^*}{\partial h_n} C_{MAW,n}^0 (h_n^{k-1} - \bar{h}_{MAW,n}^{k-1}) \right] h_n^{k-1}. \end{aligned} \quad (4-17)$$

Simplifying equation 4-17 results in

$$\begin{aligned}
 & \left[-S_{MAW,n}^* C_{MAW,n}^0 \frac{\partial \bar{h}_{MAW,n}^*}{\partial HMAW_i} \right] HMAW_i^k + \\
 & \left[S_{MAW,n}^* C_{MAW,n}^0 + \frac{\partial S_{MAW,n}^*}{\partial h_n} C_{MAW,n}^0 (h_n^{k-1} - \bar{h}_{MAW,n}^{*k-1}) \right] h_n^k = \\
 & S_{MAW,n}^* C_{MAW,n}^0 \bar{h}_{MAW,n}^{*k-1} + \left[-S_{MAW,n}^* C_{MAW,n}^0 \frac{\partial \bar{h}_{MAW,n}^*}{\partial HMAW_i} \right] HMAW_i^{k-1} + \\
 & \left[\frac{\partial S_{MAW,n}^*}{\partial h_n} C_{MAW,n}^0 (h_n^{k-1} - \bar{h}_{MAW,n}^{*k-1}) \right] h_n^{k-1}.
 \end{aligned} \tag{4-18}$$

To complete the Newton-Raphson formulation the terms added to the coefficient matrix and right-hand side during the standard formulation step (eq. 4-5) are modified by adding

$$S_{MAW,n}^* C_{MAW,n}^0 \left(1 - \frac{\partial \bar{h}_{MAW,n}^*}{\partial HMAW_i} \right) \tag{4-19}$$

to the diagonal position in the row for multi-aquifer well i , adding

$$\frac{\partial S_{MAW,n}^*}{\partial h_n} C_{MAW,n}^0 (h_n - \bar{h}_{MAW,n}^*) \tag{4-20}$$

to the off-diagonal position for GWF cell n in the row for multi-aquifer well i , and adding

$$S_{MAW,n}^* C_{MAW,n}^0 \left(1 - \frac{\partial \bar{h}_{MAW,n}^*}{\partial HMAW_i} \right) HMAW_i^{k-1} + \frac{\partial S_{MAW,n}^*}{\partial h_n} C_{MAW,n}^0 (h_n - \bar{h}_{MAW,n}^*) h_n^{k-1} \tag{4-21}$$

to the right-hand side in the row for multi-aquifer well i . The $\left(1 - \frac{\partial \bar{h}_{MAW,n}^*}{\partial HMAW_i} \right)$ term in equation 4-19 removes the $-S_{MAW,n}^* C_{MAW,n}^0$ term added during standard formulation step and correctly adds the $-S_{MAW,n}^* C_{MAW,n}^0 \frac{\partial \bar{h}_{MAW,n}^*}{\partial HMAW_i}$ term. The row for the connected groundwater cell (row n) is also modified by subtracting equations 4-19, 4-20, and 4-21 from the off-diagonal (column corresponding to multi-aquifer well i), diagonal, and right-hand side, respectively.

Newton-Raphson formulation when h_n is the Downstream Head

The Newton-Raphson form of the equation 4-7, when h_n is the downstream head, is formulated by substituting equations 4-11, 4-14, and 4-15 into equation 4-8, which results in

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$$\begin{aligned}
& \left[-S_{MAW,n}^* C_{MAW,n}^0 + \frac{\partial S_{MAW,n}^*}{\partial HMAW_i} C_{MAW,n}^0 (\bar{h}_{MAW,n}^{*k-1} - HMAW_i^{k-1}) \right] HMAW_i^k + \\
& \left[S_{MAW,n}^* C_{MAW,n}^0 \frac{\partial \bar{h}_{MAW,n}^*}{\partial h_n} \right] h_n^k = -S_{MAW,n}^* C_{MAW,n}^0 (\bar{h}_{MAW,n}^{*k-1} - HMAW_i^{k-1}) + \\
& \left[-S_{MAW,n}^* C_{MAW,n}^0 + \frac{\partial S_{MAW,n}^*}{\partial HMAW_i} C_{MAW,n}^0 (\bar{h}_{MAW,n}^{*k-1} - HMAW_i^{k-1}) \right] HMAW_i^{k-1} + \\
& \left[S_{MAW,n}^* C_{MAW,n}^0 \frac{\partial \bar{h}_{MAW,n}^*}{\partial h_n} \right] h_n^{k-1}.
\end{aligned} \tag{4-22}$$

Simplifying equation 4-22 results in

$$\begin{aligned}
& \left[-S_{MAW,n}^* C_{MAW,n}^0 + \frac{\partial S_{MAW,n}^*}{\partial HMAW_i} C_{MAW,n}^0 (\bar{h}_{MAW,n}^{*k-1} - HMAW_i^{k-1}) \right] HMAW_i^k + \\
& \left[S_{MAW,n}^* C_{MAW,n}^0 \frac{\partial \bar{h}_{MAW,n}^*}{\partial h_n} \right] h_n^k = -S_{MAW,n}^* C_{MAW,n}^0 \bar{h}_{MAW,n}^{*k-1} + \\
& \left[\frac{\partial S_{MAW,n}^*}{\partial HMAW_i} C_{MAW,n}^0 (\bar{h}_{MAW,n}^{*k-1} - HMAW_i^{k-1}) \right] HMAW_i^{k-1} + \\
& \left[S_{MAW,n}^* C_{MAW,n}^0 \frac{\partial \bar{h}_{MAW,n}^*}{\partial h_n} \right] h_n^{k-1}.
\end{aligned} \tag{4-23}$$

To complete the Newton-Raphson formulation the terms added to the coefficient matrix and right-hand side during the standard formulation step (eq. 4-7) are modified by adding

$$\frac{\partial S_{MAW,n}^*}{\partial HMAW_i} C_{MAW,n}^0 (\bar{h}_{MAW,n}^{*k-1} - HMAW_i^{k-1}) \tag{4-24}$$

to the diagonal position in the row for multi-aquifer well i , adding

$$S_{MAW,n}^* C_{MAW,n}^0 \left(\frac{\partial \bar{h}_{MAW,n}^*}{\partial h_n} - 1 \right) \tag{4-25}$$

to the off-diagonal position for GWF cell n in the row for multi-aquifer well i , and adding

$$\frac{\partial S_{MAW,n}^*}{\partial HMAW_i} C_{MAW,n}^0 (\bar{h}_{MAW,n}^{*k-1} - HMAW_i^{k-1}) HMAW_i^{k-1} + S_{MAW,n}^* C_{MAW,n}^0 \left(\frac{\partial \bar{h}_{MAW,n}^*}{\partial h_n} - 1 \right) h_n^{k-1} \tag{4-26}$$

to the right-hand side in the row for multi-aquifer well i . The $\left(\frac{\partial \bar{h}_{MAW,n}^*}{\partial h_n} - 1 \right)$ term in equation 4-25 removes the $S_{MAW,n}^* C_{MAW,n}^0$ term added during standard formulation step and correctly adds the

$S_{MAW,n}^* C_{MAW,n}^0 \frac{\partial \bar{h}_{MAW,n}^*}{\partial h_n}$ term. The row for the connected groundwater cell (row n) is also modified by subtracting equations 4-24, 4-25, and 4-26 from the off-diagonal (column corresponding to multi-aquifer well i), diagonal, and right-hand side, respectively.

Chapter 5. Storage Package Modifications

The MODFLOW 6 Storage (STO) Package simulates the contributions of specific storage and specific yield to the groundwater flow equations. Under confined conditions, in which the head above the top of the cell, storage changes are attributable solely to specific storage. Under unconfined conditions, in which the head is above the bottom but below the top of the cell, storage changes are attributable primarily to specific yield, but the contribution of specific storage is also taken into account.

In the original release of the MODFLOW 6 STO Package, the contribution of specific yield is formulated in terms of hydraulic head in a way that conserves water volume but renders the storage change under unconfined conditions dependent on the vertical datum relative to which heads and elevations are defined. Reexamination of the specific storage contribution in terms of pressure head leads to a revised formulation that eliminates the vertical datum dependence and still honors water conservation. This chapter describes the revised specific storage formulation used in the MODFLOW 6 STO Package.

Original Approach

The specific storage formulation used prior to MODFLOW 6 version 6.1.3 is

$$Q_{SS} = \frac{SC1}{\Delta t} \left(S_F^{t_{old}} h^{t_{old}} - S_F^t h^t \right), \quad (5-1)$$

where Q_{SS} is the volumetric flow rate from specific storage in the cell (L^3/T), $SC1$ is the primary storage coefficient (L^2), $\Delta t = t - t_{old}$ is the time step length (T), S_F is the fractional saturation of the cell for the previous (t_{old}) or current (t) time step (unitless), h is the head in the cell for the previous (t_{old}) or current (t) time step (L). The subscript that indicates the cell number has been omitted for clarity. The primary storage coefficient is calculated as

$$SC1 = S_s A \Delta z, \quad (5-2)$$

where S_s is the specific storage coefficient for the cell (L^{-1}), A is the horizontal area of the cell (L^2), and Δz is the cell thickness (L) defined by

$$\Delta z = TOP - BOT, \quad (5-3)$$

where TOP and BOT are the top and bottom elevations (L) of the cell, respectively. The cell saturation is related to the head in the cell by

$$S_F = \begin{cases} 1 & h > TOP \\ \frac{h - BOT}{\Delta z} & BOT < h \leq TOP \\ 0 & h \leq BOT \end{cases}. \quad (5-4)$$

When the Newton-Raphson formulation is used, the cell saturation in equation 5-4 is quadratically smoothed to provide a continuous derivative with respect to head (see [Langevin and others, 2017](#), Fig. 4-1 and Eq. 4-5).

The cell saturation was included in equation 5-1 to scale the primary storage coefficient in proportion to the saturated volume of water in the cell under water-table conditions. However, the formulation in equa-

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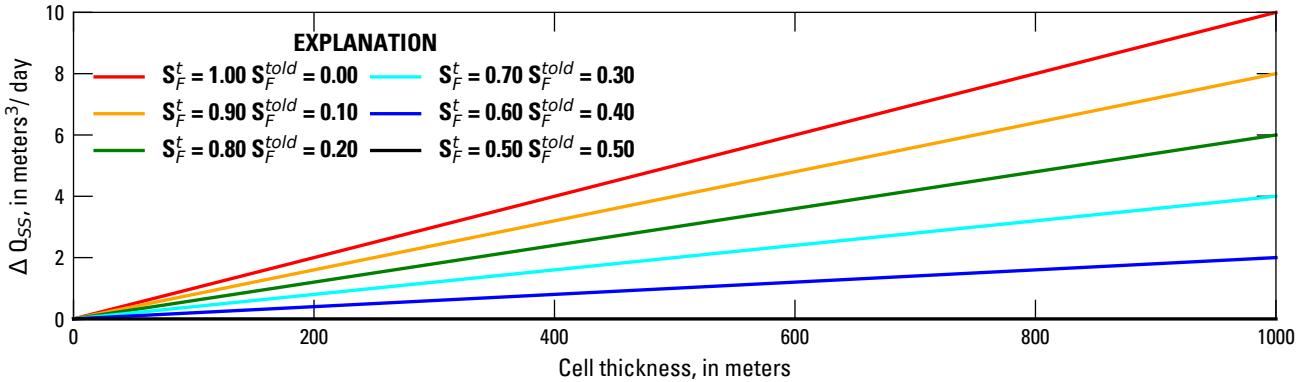


Figure 5–1. Graph showing changes in the flow from specific storage, Q_{SS} , that result from changing the vertical datum from 0 to 1,000 m. The change in Q_{SS} is plotted at a function of cell thickness, Δz , for various combinations of initial and final cell saturations, S_F^{told} and S_F^t . In this example, $S_s = 1 \times 10^{-5} \text{ m}^{-1}$, $A = 1 \text{ m}^2$, and $\Delta t = 1 \text{ d}$.

tion 5–1 causes the calculated value of Q_{SS} to depend on the vertical datum, or reference elevation, relative to which heads and elevations are defined. If the vertical datum is changed by an amount Δz_{ref} (L), all head values change by an amount $-\Delta z_{ref}$, and equation 5–1 becomes

$$Q_{SS} = \frac{SC1}{\Delta t} \left[S_F^{told} (h^{told} - \Delta z_{ref}) - S_F^t (h^t - \Delta z_{ref}) \right], \quad (5–5)$$

Comparison of equations 5–1 and 5–5 shows that changing the vertical datum by Δz_{ref} changes the calculated value of Q_{SS} by

$$\Delta Q_{SS} = \frac{SC1}{\Delta t} \left(S_F^{told} - S_F^t \right) \Delta z_{ref}, \quad (5–6)$$

Dependence of Q_{SS} on the vertical datum is not physically realistic and introduces error into the calculated value of Q_{SS} . To illustrate the magnitude of the error that can be introduced, equations 5–6 and 5–2 were used to calculate ΔQ_{SS} for a range of cell saturations at times t and t_{old} and cell thicknesses (fig. 5–1). For this example, a specific storage value of $1 \times 10^{-5} \text{ m}^{-1}$, a cell area of 1 m^2 , and a time step length of 1 d was used in all of the calculations. ΔQ_{SS} increases as the cell thickness increases or the difference in cell saturations at times t and t_{old} increases.

A related deficiency of equation 5–1 concerns when a cell is dry either at the beginning ($S_F^{told} = 0$) or the end ($S_F^t = 0$) of a time step, in which case the volumetric flow from specific storage equals

$$Q_{SS} = \begin{cases} \frac{SC1}{\Delta t} S_F^{told} h^{told} & S_F^t = 0 \\ -\frac{SC1}{\Delta t} S_F^t h^t & S_F^{told} = 0 \end{cases}. \quad (5–7)$$

Equation 5–7 can overestimate or underestimate the volumetric flow from specific storage, depending on the values of h^{told} and h^t , which in turn depend on the vertical datum. For example, in the case of a cell going dry ($S_F^{told} > 0$, $S_F^t = 0$), water flows from specific storage, which implies Q_{SS} is positive in sign. Because the cell is initially not dry, the initial cell head, h^{told} , is above the cell bottom elevation. However, depending on the vertical datum, it is possible that h^{told} is negative in sign (with the cell bottom elevation being even more neg-

ative). In that case, equation 5-7 calculates a negative value for Q_{SS} , which is opposite to what is expected on physical grounds.

Revised Formulation

To correct the deficiencies in the original specific storage formulation, the contribution of specific storage to the groundwater flow equation under water-table conditions is reexamined in terms of pressure head, which for a given elevation z is defined as

$$\psi = h - z. \quad (5-8)$$

The hydraulic head, h , associated with a MODFLOW cell is formally assigned to a point in the cell called the node, which under water-table conditions is at an elevation halfway between the cell bottom and the water table. The water-table elevation is, in turn, equal to the cell head, h . Thus, the value of the hydraulic head is the same at the node as it is at the water table, which is consistent with conceptualizing hydraulic head as being constant throughout the saturated portion of the cell. Extending this conceptualization to pressure head via equation 5-8 implies a linear variation of pressure head between a value of 0 at the water table and a value of $h - BOT$ at the cell bottom. The revised specific storage formulation is therefore based on linear variation of pressure head with elevation within a cell.

The volumetric water content, θ , at elevation z within a cell is related to pressure head by

$$\theta = \begin{cases} \theta_r & z > h \\ S_s\psi + S_y + \theta_r & z \leq h \end{cases}, \quad (5-9)$$

where θ_r is the specific retention (unitless) and S_y is the specific yield (unitless) in the cell. Integration of equation 5-9 from the bottom to the top of the cell gives the total volume of water stored in the cell:

$$V_S = A \int_{BOT}^{TOP} \theta dz = A \int_{BOT}^{z_{wt}^*} S_s\psi dz + A \int_{BOT}^{z_{wt}^*} S_y dz + A \int_{BOT}^{TOP} \theta_r dz, \quad (5-10)$$

where z_{wt}^* is the water-table elevation limited by the top elevation of the cell, given by

$$z_{wt}^* = BOT + \Delta z S_F. \quad (5-11)$$

Assuming θ_r , S_y , and S_s are uniform throughout the cell, substitution of equation 5-8 into equation 5-10 and evaluation of the integrals gives

$$V_S = S_s A \Delta z S_F (h - \bar{z}) + S_y A \Delta z S_F + \theta_r A \Delta z, \quad (5-12)$$

where \bar{z} is the node elevation (the vertical center of the saturated portion of the cell) given by

$$\bar{z} = \frac{1}{z_{wt}^* - BOT} \int_{BOT}^{z_{wt}^*} z dz = BOT + \frac{\Delta z}{2} S_F. \quad (5-13)$$

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The remainder of this chapter focuses on the contribution of specific storage (the first term on the right-hand side of equation 5–12) to the change in storage in a cell during a time step. The contribution of specific yield is calculated separately in MODFLOW 6 and remains unchanged by the revised approach described here. The volume of water in specific retention is assumed to be constant and therefore does not contribute to changes in storage.

Substitution of equations 5–2 and 5–13 into the first term on the right-hand side of equation 5–12 gives the volume of water in compressible storage in the cell,

$$V_{SS} = SC1 S_F \left(h - BOT - \frac{\Delta z}{2} S_F \right). \quad (5-14)$$

The revised volumetric flow rate from compressible storage is then

$$Q_{SS} = \frac{SC1}{\Delta t} \left[S_F^{t_{old}} \left(h^{t_{old}} - BOT - \frac{\Delta z}{2} S_F^{t_{old}} \right) - S_F^t \left(h^t - BOT - \frac{\Delta z}{2} S_F^t \right) \right]. \quad (5-15)$$

When a cell is fully saturated ($S_F = 1$) at times t and t_{old} , equation 5–15 simplifies to

$$Q_{SS} = \frac{SC1}{\Delta t} (h^{t_{old}} - h^t), \quad (5-16)$$

which is identical to the original specific storage formulation under confined conditions in MODFLOW 6 and the specific storage formulation under both confined and unconfined conditions in MODFLOW-2005 (Harbaugh, 2005).

The revised formulation in equation 5–15 is no longer dependent on the vertical datum because it involves cell saturations, S_F , and head differences of the form $h - BOT$, which do not change when the vertical datum changes. In the case of a cell being dry either at the beginning or the end of a time step, the volumetric flow from specific storage based on the revised formulation equals

$$Q_{SS} = \begin{cases} \frac{SC1}{\Delta t} S_F^{t_{old}} \left(h^{t_{old}} - BOT - \frac{\Delta z}{2} S_F^{t_{old}} \right) & S_F^t = 0 \\ -\frac{SC1}{\Delta t} S_F^t \left(h^t - BOT - \frac{\Delta z}{2} S_F^t \right) & S_F^{t_{old}} = 0 \end{cases}, \quad (5-17)$$

which is the revised-formulation counterpart of equation 5–7. It can be deduced from equation 5–4 that

$$h - BOT - \frac{\Delta z}{2} S_F > 0 \quad \text{if } h > BOT, \quad (5-18)$$

which implies that equation 5–17 calculates the correct sign for Q_{SS} when a cell goes dry or resaturates.

Incorporation of the Revised Specific Storage Formulation into the CVFD Groundwater Flow Equation

The approaches used to incorporate the contribution from specific storage into the linear matrix problem that represents the discretized groundwater flow equation are detailed below. When the standard formulation is used, the cell saturation defined in equation 5–4 is used without modification. To allow for a smooth transition

from dry (water level at or below the bottom of a cell) to fully saturated (water level at or above the top of the cell) conditions when the Newton formulation is used, quadratic smoothing is applied to the cell saturation over a small interval when the water level approaches the top or bottom of a cell, as described in Eq. 4–5 in [Langevin and others \(2017\)](#).

Standard Formulation

Adding the cell number subscript “ n ” to cellwise quantities in equation [5–15](#) and adding specific storage terms dependent on the current value of head and known terms to the left- and right-hand sides of the discretized groundwater flow equation ([Langevin and others, 2017](#), eq. 6–1), respectively, results in

$$\begin{aligned} A_{n,n} &\leftarrow A_{n,n} - \frac{SC1_n}{\Delta t} S_{F_n}^{k-1} \\ b_n &\leftarrow b_n - \frac{SC1_n}{\Delta t} \left[S_{F_n}^{t_{old}} \left(h_n^{t_{old}} - BOT_n - \frac{\Delta z_n}{2} S_{F_n}^{t_{old}} \right) + S_{F_n}^{k-1} \left(BOT_n + \frac{\Delta z_n}{2} S_{F_n}^{k-1} \right) \right], \end{aligned} \quad (5–19)$$

where $A_{n,n}$ is the diagonal of the coefficient matrix for cell n and b_n is the right-hand side of the groundwater flow equation for cell n . A variant of equation [5–19](#) that tries to take advantage of the fact that

$$h_n - BOT_n - \frac{\Delta z_n}{2} S_{F_n} = \frac{1}{2} (h_n - BOT_n) \quad (5–20)$$

under water-table conditions (head in the cell below the top of the cell) was also evaluated. However, the form presented in equation [5–19](#) was found to converge better for the test problems evaluated and to simplify the additional terms added to the left- and right-hand sides of the discretized groundwater equation to complete the Newton-Raphson formulation.

Newton-Raphson Formulation

Adding the cell number subscript “ n ” to cellwise quantities in equation [5–15](#) and rearranging the equation to facilitate differentiation with respect to the current value of head, h_n^t , results in

$$Q_{SS_n} = \frac{SC1_n}{\Delta t} \left[S_{F_n}^{*t_{old}} \left(h_n^{t_{old}} - BOT_n - \frac{\Delta z_n}{2} S_{F_n}^{t_{old}} \right) - S_{F_n}^{*t} (h_n^t - BOT_n) + \frac{\Delta z_n}{2} (S_{F_n}^{*t})^2 \right], \quad (5–21)$$

where S_F^* is the quadratically smoothed cell saturation (see [Langevin and others, 2017](#), Eq. 4–5). The derivative of equation [5–21](#) with respect to h_n^t is

$$\frac{\partial Q_{SS_n}}{\partial h_n} = -\frac{SC1_n}{\Delta t} S_{F_n}^{*t} - \frac{SC1_n}{\Delta t} \frac{\partial S_{F_n}^{*t}}{\partial h_n} (h_n^t - BOT_n) + \frac{SC1_n}{\Delta t} \Delta z_n S_{F_n}^{*t} \frac{\partial S_{F_n}^{*t}}{\partial h_n}, \quad (5–22)$$

where the superscript “ t ” has been omitted from h_n^t in the derivatives for clarity. The fully implicit form of the Newton-Raphson formulation for the contribution of specific storage in the cell in the form of equation 2–30 in [Langevin and others \(2017\)](#) is

$$\frac{\partial Q_{SS_n}}{\partial h_n} h_n^k = -Q_{SS_n} + \frac{\partial Q_{SS_n}}{\partial h_n} h_n^{k-1}. \quad (5–23)$$

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where the superscripts “ k ” and “ $k - 1$ ” indicate quantities evaluated on the current and previous outer iterations of the solution procedure, respectively. Replacement of h_n^t and $S_{F_n}^{*t}$ by their previous iterates, h_n^{k-1} and $S_{F_n}^{*k-1}$, in equations 5–21 and 5–22 and substitution of those equations into equation 5–23 results in

$$\begin{aligned} A_{n,n} &\leftarrow A_{n,n} + \left[-\frac{SC1_n}{\Delta t} S_{F_n}^{*k-1} - \frac{SC1_n}{\Delta t} \frac{\partial S_{F_n}^{*k-1}}{\partial h_n} \left(h_n^{k-1} - BOT_n \right) + \frac{SC1_n}{\Delta t} \Delta z_n S_{F_n}^{k-1} \frac{\partial S_{F_n}^{*k-1}}{\partial h_n} \right] \\ b_n &\leftarrow b_n - \frac{SC1_n}{\Delta t} \left[S_{F_n}^{*t_{old}} \left(h_n^{t_{old}} - BOT_n - \frac{\Delta z_n}{2} S_{F_n}^{*t_{old}} \right) + S_{F_n}^{*k-1} \left(BOT_n + \frac{\Delta z_n}{2} S_{F_n}^{*k-1} \right) \right] \\ &\quad + \left[-\frac{SC1_n}{\Delta t} \frac{\partial S_{F_n}^{*k-1}}{\partial h_n} \left(h_n^{k-1} - BOT_n \right) + \frac{SC1_n}{\Delta t} \Delta z_n S_{F_n}^{*k-1} \frac{\partial S_{F_n}^{*k-1}}{\partial h_n} \right] h_n^{k-1}. \end{aligned} \quad (5-24)$$

Comparison of equation 5–24 to equation 5–19 shows that many of the terms in the Newton-Raphson formulation were added as part of the standard formulation. The Newton-Raphson formulation is completed by adding the second and third terms on the right-hand side of equation 5–22 and the product of these terms and the current head to the terms already added to the diagonal of the coefficient matrix and right-hand side by the standard formulation, respectively.

Chapter 6. Time-Varying Hydraulic Conductivity and Storage

The MODFLOW 6 Time-Varying Hydraulic Conductivity (TVK) and Time-Varying Storage (TVS) packages allow hydraulic conductivity, specific storage and specific yield properties of model cells to be varied transiently throughout a simulation. This can be useful for modeling caved rock, void and spoil in mining applications, or for other physical changes to a system that can reasonably be represented by changing material properties.

Changes are made on a cell-by-cell basis in TVK and TVS package input files by specifying new values for elements of NPF package arrays K, K22 and K33, and STO package arrays SS and SY. New values may be applied at the start of each stress period, or alternatively interpolated via time series to determine new values at each time step. Changes are only made to those model cells explicitly specified in the TVK and TVS package input files; other cells retain their original NPF and STO values. Additionally, a change may be made to a cell's value for one property independently without affecting other property values at the same cell, e.g. SS may be changed for a cell without affecting SY, if desired.

Where a property value change is given by a time series, the value continues to change at each time step until the last entry in the time series is reached. Otherwise, once a cell property value has been changed, it remains at its new value until subsequently changed in the TVK or TVS files for a later period, or until the end of the simulation if no further changes are enacted.

By default, when the TVS package is used to change SS or SY values, the MODFLOW 6 storage formulation is modified to integrate these changes such that the head solution correctly reflects changes in pressure due to the corresponding increase or decrease in stored water volume. The modifications are described in the “[Storage Change Integration: Specific Storage](#)” and “[Storage Change Integration: Specific Yield](#)” sections below. If this functionality is not desired, storage change integration may be disabled by activating the DISABLE_STORAGE_CHANGE_INTEGRATION option in the TVS package input file.

Storage Change Integration: Specific Storage

Revisiting the derivation of the revised storage formulation in the [Storage Package Modifications chapter](#), changes in specific storage are introduced by first separating equation 5–14 into two separate equations:

$$V_{SS}^{t_{old}} = SC1^{t_{old}} S_F^{t_{old}} \left(h^{t_{old}} - BOT - \frac{\Delta z}{2} S_F^{t_{old}} \right), \quad (6-1)$$

giving the volume of water in compressible storage at time t_{old} , and

$$V_{SS}^t = SC1^t S_F^t \left(h^t - BOT - \frac{\Delta z}{2} S_F^t \right), \quad (6-2)$$

giving the volume of water in compressible storage at time t . The volumetric flow rate from compressible storage taking into account changes in specific storage is then

$$\begin{aligned} Q_{SS} &= \frac{V_{SS}^{t_{old}} - V_{SS}^t}{\Delta t} \\ &= \frac{SC1^{t_{old}}}{\Delta t} S_F^{t_{old}} \left(h^{t_{old}} - BOT - \frac{\Delta z}{2} S_F^{t_{old}} \right) - \frac{SC1^t}{\Delta t} S_F^t \left(h^t - BOT - \frac{\Delta z}{2} S_F^t \right). \end{aligned} \quad (6-3)$$

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Standard Formulation

Following the same process used to arrive at equation 5–19 in the [Storage Package Modifications chapter](#), equation 6–3 leads to the following additions to the left- and right-hand sides of the discretized groundwater flow equation:

$$\begin{aligned} A_{n,n} &\leftarrow A_{n,n} - \frac{SC1_n^t}{\Delta t} S_{F_n}^{k-1} \\ b_n &\leftarrow b_n - \frac{SC1_n^{t_{old}}}{\Delta t} S_{F_n}^{t_{old}} \left(h_n^{t_{old}} - BOT_n - \frac{\Delta z_n}{2} S_{F_n}^{t_{old}} \right) + \frac{SC1_n^t}{\Delta t} S_{F_n}^{k-1} \left(BOT_n + \frac{\Delta z_n}{2} S_{F_n}^{k-1} \right). \end{aligned} \quad (6-4)$$

In the absence of specific storage changes, i.e. for $SC1_n^{t_{old}} = SC1_n^t = SC1_n$, equation 6–4 simplifies to equation 5–19.

Newton-Raphson Formulation

Evaluating equation 6–3 cellwise with subscript “*n*” and applying quadratically smoothed cell saturations S_F^* results in

$$Q_{SS_n} = \frac{SC1_n^{t_{old}}}{\Delta t} S_{F_n}^{*t_{old}} \left(h_n^{t_{old}} - BOT_n - \frac{\Delta z_n}{2} S_{F_n}^{*t_{old}} \right) - \frac{SC1_n^t}{\Delta t} \left[S_{F_n}^{*t} (h_n^t - BOT_n) + \frac{\Delta z_n}{2} (S_{F_n}^{*t})^2 \right]. \quad (6-5)$$

Upon differentiation of equation 6–5 with respect to h_n^t , all terms involving $SC1_n^{t_{old}}$ disappear. The result is equivalent to equation 5–22 with $SC1_n = SC1_n^t$:

$$\frac{\partial Q_{SS_n}}{\partial h_n} = -\frac{SC1_n^t}{\Delta t} S_{F_n}^{*t} - \frac{SC1_n^t}{\Delta t} \frac{\partial S_{F_n}^{*t}}{\partial h_n} (h_n^t - BOT_n) + \frac{SC1_n^t}{\Delta t} \Delta z_n S_{F_n}^{*t} \frac{\partial S_{F_n}^{*t}}{\partial h_n}, \quad (6-6)$$

where the superscript “*t*” has been omitted from h_n^t in the derivatives for clarity. Replacement of h_n^t and $S_{F_n}^{*t}$ by their previous iterates, h_n^{k-1} and $S_{F_n}^{*k-1}$, in equations 6–5 and 6–6 and substitution of those equations into equation 5–23 yields the following contributions to $A_{n,n}$ and b_n :

$$\begin{aligned} A_{n,n} &\leftarrow A_{n,n} + \left[-\frac{SC1_n^t}{\Delta t} S_{F_n}^{*k-1} - \frac{SC1_n^t}{\Delta t} \frac{\partial S_{F_n}^{*k-1}}{\partial h_n} (h_n^{k-1} - BOT_n) + \frac{SC1_n^t}{\Delta t} \Delta z_n S_{F_n}^{*k-1} \frac{\partial S_{F_n}^{*k-1}}{\partial h_n} \right] \\ b_n &\leftarrow b_n - \frac{SC1_n^{t_{old}}}{\Delta t} S_{F_n}^{t_{old}} \left(h_n^{t_{old}} - BOT_n - \frac{\Delta z_n}{2} S_{F_n}^{t_{old}} \right) + \frac{SC1_n^t}{\Delta t} S_{F_n}^{*k-1} \left(BOT_n + \frac{\Delta z_n}{2} S_{F_n}^{*k-1} \right) \\ &\quad + \left[-\frac{SC1_n^t}{\Delta t} \frac{\partial S_{F_n}^{*k-1}}{\partial h_n} (h_n^{k-1} - BOT_n) + \frac{SC1_n^t}{\Delta t} \Delta z_n S_{F_n}^{*k-1} \frac{\partial S_{F_n}^{*k-1}}{\partial h_n} \right] h_n^{k-1}. \end{aligned} \quad (6-7)$$

In the absence of storage changes ($SC1_n^{t_{old}} = SC1_n^t = SC1_n$), equation 6–7 simplifies to equation 5–24.

Storage Change Integration: Specific Yield

For constant specific yield, MODFLOW 6 calculates the specific yield contribution to groundwater flow ([Langevin and others, 2017](#), eq. 5–10) as

$$Q_{Sy_n} = \frac{SC2_n \Delta z_n}{\Delta t} \left(S_{F_n}^{t_{old}} - S_{F_n}^t \right), \quad (6-8)$$

where Q_{Sy_n} is the volumetric flow rate from specific yield (L^3/T) and $SC2_n = Sy_n \cdot A_n$ is the secondary storage capacity for cell n with specific yield Sy_n and horizontal cell area A_n .

When specific yield changes transiently, the secondary storage capacity term is expressed in terms of its new value $SC2_n^t$ and its old value $SC2_n^{t_{old}}$, resulting in

$$Q_{Sy_n} = \frac{SC2_n^{t_{old}} \Delta z_n}{\Delta t} S_{F_n}^{t_{old}} - \frac{SC2_n^t \Delta z_n}{\Delta t} S_{F_n}^t. \quad (6-9)$$

Standard Formulation

Rearranging equation 6–9 for solution at the current iteration k in terms of h_n^k instead of saturation $S_{F_n}^t$ gives

$$Q_{Sy_n}^k = \frac{SC2_n^{t_{old}} \Delta z_n}{\Delta t} S_{F_n}^{t_{old}} - \frac{SC2_n^t \Delta z_n}{\Delta t} \frac{h_n^k - BOT_n}{\Delta z_n}, \quad (6-10)$$

which results in the following contributions to $A_{n,n}$ and b_n :

$$\begin{aligned} A_{n,n} &\leftarrow A_{n,n} - \frac{SC2_n^t}{\Delta t} \\ b_n &\leftarrow b_n - \frac{SC2_n^{t_{old}}}{\Delta t} \Delta z_n S_{F_n}^{t_{old}} - \frac{SC2_n^t}{\Delta t} BOT_n. \end{aligned} \quad (6-11)$$

As in the base formulation ([Langevin and others, 2017](#), Chapter 5), for cells where the head at the end of the time step is at or above the top of the cell, $S_{F_n}^t = 1$ and the specific yield contribution is known. In these cases, no terms are added to $A_{n,n}$ and the right-hand side contribution instead becomes

$$b_n \leftarrow b_n - \frac{SC2_n^{t_{old}}}{\Delta t} \Delta z_n S_{F_n}^{t_{old}} + \frac{SC2_n^t}{\Delta t} \Delta z_n. \quad (6-12)$$

Newton-Raphson Formulation

As all $SC2_n^{t_{old}}$ terms are eliminated by differentiation, the derivative of equation 6–9 at iteration k , and with quadratically smoothed cell saturations S_F^* applied, is equivalent to that of the base formulation ([Langevin and others, 2017](#), eq. 5–14) with $SC2_n = SC2_n^t$:

$$\frac{\partial Q_{Sy_n}}{\partial h_n} = - \frac{SC2_n^t \Delta z_n}{\Delta t} \frac{\partial S_{F_n}^{*k-1}}{\partial h_n}. \quad (6-13)$$

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The fully implicit Newton-Raphson formulation for specific yield storage contribution in cell n is

$$\frac{\partial Q_{Sy_n}}{\partial h_n} h_n^k = -Q_{Sy_n}^k + \frac{\partial Q_{Sy_n}}{\partial h_n} h_n^{k-1}. \quad (6-14)$$

Substitution of equations 6-9 and 6-13 into equation 6-14 results in the following general expression of the Newton-Raphson formulation for the contribution of specific yield storage to cell n :

$$\begin{aligned} \left[-\frac{SC2_n^t \Delta z_n}{\Delta t} \frac{\partial S_{F_n}^{*k-1}}{\partial h_n} \right] h_n^k &= - \left[\frac{SC2_n^{t_{old}} \Delta z_n}{\Delta t} S_{F_n}^{*t_{old}} - \frac{SC2_n^t \Delta z_n}{\Delta t} S_{F_n}^{*k-1} \right] \\ &\quad + \left[-\frac{SC2_n^t \Delta z_n}{\Delta t} \frac{\partial S_{F_n}^{*k-1}}{\partial h_n} \right] h_n^{k-1}, \end{aligned} \quad (6-15)$$

which yields the following contributions to $A_{n,n}$ and b_n :

$$\begin{aligned} A_{n,n} &\leftarrow A_{n,n} - \frac{SC2_n^t \Delta z_n}{\Delta t} \frac{\partial S_{F_n}^{*k-1}}{\partial h_n} \\ b_n &\leftarrow b_n - \frac{SC2_n^{t_{old}} \Delta z_n}{\Delta t} S_{F_n}^{*t_{old}} + \frac{SC2_n^t \Delta z_n}{\Delta t} S_{F_n}^{*k-1} - \frac{SC2_n^t \Delta z_n}{\Delta t} \frac{\partial S_{F_n}^{*k-1}}{\partial h_n} h_n^{k-1}. \end{aligned} \quad (6-16)$$

For cells where the head at the end of the time step is at or above the top of the cell, the derivative is zero. In these cases, no terms are added to $A_{n,n}$ and the right-hand side contribution reverts to the standard formulation in equation 6-12.

Chapter 7. Generalized Coupling of Numerical Models

The multi-model concept was introduced in MODFLOW 6 using GWF Model Exchange objects to support a tight coupling between any two groundwater flow models at the matrix level. This concept has proven to be successful and valued by the modeling community, but the implementation has had its drawbacks too. The information on the spatial discretization at the interface between models as it is available in the Model Exchange object is limited, designed to carry out the basic conductance calculation between connected cells but not sufficient for more advanced discretization schemes. For example, the XT3D option in the NPF package enables simulation of fully three-dimensional (3D) anisotropy by taking into account the full, three-dimensional conductivity tensor [Provost and others \(2017\)](#). In doing so, it requires data not only from any pair of cells between which a flow needs to be calculated but also from their neighboring cells. These data are not available in the Model Exchange object and the XT3D option could not be applied across the model interface, at least not without a significant restructuring of the code.

The extension of MODFLOW 6 with the transport model (GWT) comes with the need for a more generic coupling of sub-models too. Here the XT3D option is used in a similar fashion for the dispersion calculation, and the TVD (total variation diminishing) scheme in the advective transport calculation has a computational stencil (i.e. the group of cells required to determine the flux through a particular cell face) that requires information from neighboring cells as well. Finally, the GWF Model Exchange object merely replicates logic already present in the standard GWF packages, e.g. the standard NPF conductance calculation, the Newton-Raphson formulation, or the cell rewetting algorithm, and is not easily adapted when additions or modifications to those packages are made. We introduce a generalized method for coupling of Numerical Models that addresses these challenges and extends MODFLOW 6 with the capability to couple GWT models.

The generalized coupling uses the concept of an Interface Model and is described in more detail below. In essence, this Interface Model uses the object-oriented paradigm in MODFLOW 6 to mimic a regular GWF or GWT model by means of type extension. This way it can use the existing packages and their algorithms in those models to calculate coefficients for the matrix and right-hand-side vector in the Numerical Solution, a responsibility it takes over from the Model Exchange object on which it relies. Its grid is constructed around the interface defined by the Model Exchange with a sufficiently large extent to perform the calculations. Note that the Interface Model is never being solved and neither its configuration data nor its solution vector have any independent meaning: they are merely an image of those parts of the actual Numerical Models that contribute to the interface grid. As a matter of fact, and this is probably the most important point to make here, this generalized coupling with the Interface Model does not introduce any new model functionality. It even avoids the need for the alternative formulations currently present in the GWF Model Exchange. However, it does enable the user to apply the well-tested concepts of existing MODFLOW 6 packages not only on a model's interior domain, but also across the interface between connected models.

The Interface Model

Generalized coupling is based on the Interface Model to provide the coefficients for the linear system in Numerical Solution. In order to utilize the routines in the existing flow and transport packages to calculate these coefficients, the grid for the Interface Model is constructed from the individual model grids and the coupling information specified by the user and its package data is kept synchronized with the model data during each step of the simulation. Because the Model Exchange makes it possible to connect model grids of different type (DIS, DISV, and DISU), the resulting interface grid is always unstructured, i.e. of type DISU.

Connecting models such that the dynamics at the interface can be described properly by an Interface Model does impose a few conditions on the configuration. For more advanced functionality such as XT3D, it is required that the relative position of the model grids is specified. They should also share the cell faces over which they are connected, such that the resulting grid for the interface can be specified as a valid DISU dis-

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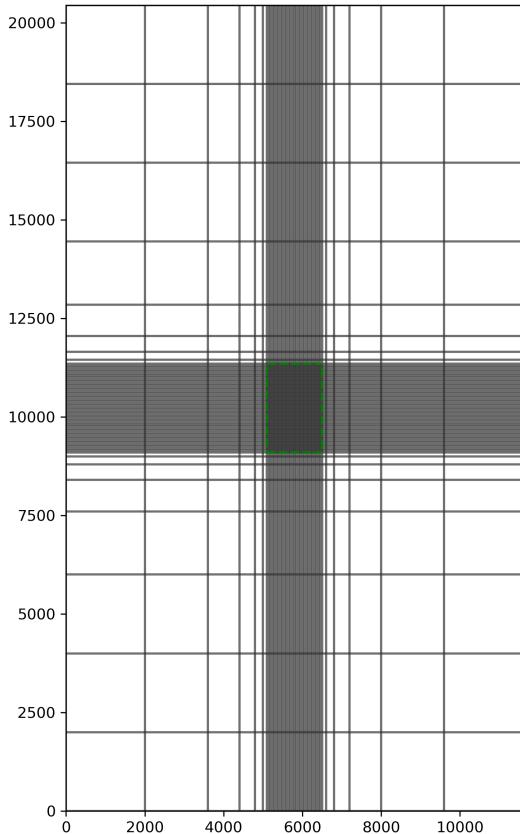


Figure 7–1. A plan view of the model grid for the simulation as defined in MT3DMS problem 10. The green dashed rectangle shows the location of the interface that is used for decomposing this case into a system of coupled GWF and GWT models.

cretization. Another consequence is that a certain compatibility is required with respect to the active processes and configuration in the individual models: enabling advection (ADV) or dispersion (DSP), for example, only in one of two connected models introduces ambiguity in how to construct the Interface Model for the transport process. Similar arguments hold when two groundwater models are connected and only one of them is configured with a buoyancy package (BUY). Such model setups are currently not supported.

To illustrate the concept of this new coupling, a well known, single-model case study (problem 10 in the MT3DMS manual [Zheng and Wang \(1999\)](#)) is implemented as a coupled system where the connection between the GWT models is handled by the Interface Model framework. This study is part of the official set of examples that comes with every MODFLOW 6 software release¹. The coefficients for the flow coupling in this case are calculated with the basic GWF Model Exchange module and the following discussion will focus on the GWT-GWT exchange. Figure 7–1 shows a plan view of the grid and the location of the interface between the submodels. Note that changing only the composition of the grid and leaving the model configuration the same, does not affect the outcome of the simulation² and therefore makes for a very suitable test case of this coupling.

Figure 7–2 shows a plan view of the grid that is reconstructed as part of the Interface Model for the inner GWT model. The red band with cells belong to the inner model's grid and the blue cells are part of the outer, coarser grid. Because two Interface Models are constructed for every Exchange, (one for each of the models

¹<https://modflow6-examples.readthedocs.io/en/master/>

²At the highest level of detail, the outcome does change because the numbering of the grid nodes is different in both scenarios leading to a reordered matrix system to be solved. As expected, these differences turn out to be well within the configured (IMS) solver tolerance.

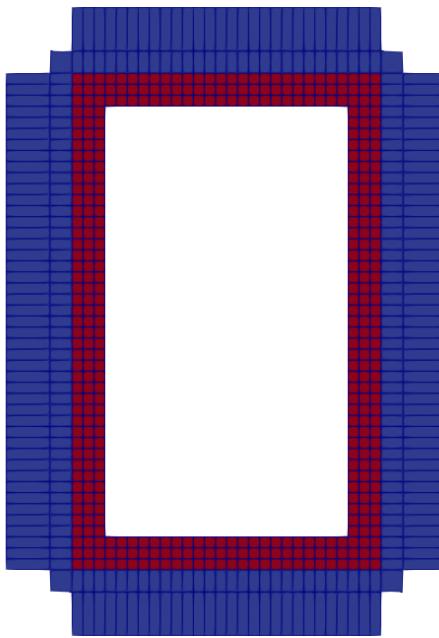


Figure 7–2. A top view of the grid for the Interface Model belonging to the inner GWT model in the example described in the text. The blue cells are located in the outer model’s grid, the red cells are internal. Note that deeper layers have an identical horizontal structure..

in it) a similar though not identical picture can be drawn for the outer GWT model. However, the extent of this grid is not necessarily equal on both sides of the exchange. The task of the Interface Model is twofold. First of all, it is designed to calculate the coefficients for the linear system for fluxes through the faces directly at the interface. Additionally, it can provide coefficients for those fluxes that would be affected by cells on the other side of the interface just as if the simulation would have been set up as a single model. It is the requirement to support the latter that causes the asymmetry. This becomes clearer when looking at Figure 7–3 which shows the XT3D computational stencils and how they determine what the required extent of the interface grid is. To determine the flux through a face at the model interface, the cells on either side and their immediate neighbors are sufficient (the circle). To correctly calculate the flux through cell faces not directly at the interface but influenced by the connection to another model, more additional levels of connectivity are required, depending on the exact size of the computation stencil (the diamond).

This case study is used to demonstrate the concept of the generalized coupling method with the Interface Model. It serves as an excellent test case because the outcome should be identical to the known results, at least within the configured tolerance of the Numerical Solution. However, from a modeling perspective it would make more sense to redesign the model grid of the problem. With the new capability to use the multi-model approach also for problems containing solute transport, there is no longer a need to refine the study area by using varying column and row width as was done in the original MT3DMS problem. Both the study area and the surrounding domain can be configured as coupled models with a regularly structured (DIS) grid. The granularity of the inner grid can be independently refined to improve the resolution of the results without the need to set up the entire problem based on an unstructured (DISU) grid.

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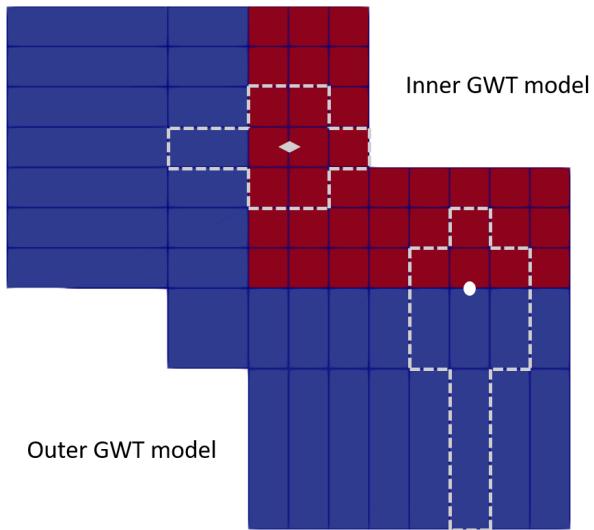


Figure 7–3. Top view when zoomed in to the South-West corner of the interface grid. The dashed line surrounds the grid cells participating in the calculation of the dispersive XT3D flux directly at the interface (the white circle) and through a face in the model's interior (the white diamond) which is nonetheless affected by the connection to the outer GWT model. The extension of the computational stencil in the vertical direction is omitted but straightforward..

Finally, such a setup would allow to apply the Interface Model in another powerful way. A refinement of the grid is known to produce inaccuracies at the interface, as discussed in the introduction of [Provost and others \(2017\)](#). This can be remedied by enabling the XT3D option in the GWF NPF package. The new coupling mechanism based on the Interface Model makes it now possible to enable this option *only* at the interface, which will mitigate the distorting effects of such a grid refinement on the calculated flow field and still avoids the computational overhead of calculating the XT3D terms on the entire domain.

Chapter 8. Accounting for Fluid Viscosity

The dynamic viscosity of a fluid is a function of fluid composition and temperature and typically has a weak dependence on pressure. In some applications, particularly those that involve large variations in temperature, viscosity can vary significantly in space and over time. Variations in viscosity, in turn, can affect groundwater flow by changing the hydraulic conductivity, which is inversely proportional to viscosity. In the original release of MODFLOW 6, variations in viscosity and their effects on hydraulic conductivity were not taken into account. The MODFLOW 6 Viscosity (VSC) Package allows viscosity to vary as a function of solute concentrations and fluid temperature and accounts for the effect of variable viscosity on hydraulic conductivity in the Node-Property Flow (NPF) Package and in stress packages that involve head-dependent groundwater flow. Temperature-dependent viscosity has been implemented in other groundwater modeling codes, including HST3D (Kipp, 1987), VS2DH (Healy and Ronan, 1996), SUTRA-MS (Hughes and Sanford, 2004), and SEAWAT Version 4 (Langevin and others, 2008). Like these other codes, the VSC Package does not account for the dependence of viscosity on pressure, which is negligible in most applications.

For cases in which the rate of groundwater flow is proportional to the head gradient in the direction of flow, as in an isotropic porous medium, the flow between two adjacent locations can be approximated using a one-dimensional form of Darcy's Law (Langevin and others, 2017, equation 4-15):

$$Q = C (h_1 - h_2), \quad (8-1)$$

where h_1 and h_2 are the hydraulic heads at locations 1 and 2, respectively, Q is the flow from location 1 to location 2, and C is a hydraulic conductance defined by (Langevin and others, 2017, equation 4-14):

$$C = \frac{KA}{L_{1,2}}, \quad (8-2)$$

where K is the hydraulic conductivity of the porous medium that connects the two locations, A is the cross-sectional area perpendicular to flow, and $L_{1,2}$ is the distance between two locations. A form of equation 8-1 is used in the MODFLOW 6 "conductance-based" formulation for flow between two adjacent model cells (Langevin and others, 2017). In that case, the conductance is based on an effective hydraulic conductivity between the two cells, the area of the cell-cell interface, and the distance between the cell centers. A form of equation 8-1 is also used in MODFLOW 6 stress packages in which the flow into or out of the model at a model boundary is head-dependent. For example, in the General-Head Boundary (GHB) Package, flow between an external source and a groundwater model cell is proportional to the difference between the head assigned to the external source and the simulated head in the cell, and the conductance is representative of the material between the external source and the cell center.

Because hydraulic conductivity is inversely proportional to viscosity, the conductivity K for a simulated fluid composition and temperature is related to the conductivity K_0 for some reference composition and temperature by

$$K = \frac{\mu_0}{\mu} K_0. \quad (8-3)$$

It follows from equation 8-2 that the conductance C for a simulated fluid composition and temperature is related to the conductance C_0 for the reference composition and temperature by

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$$C = \frac{\mu_0}{\mu} C_0, \quad (8-4)$$

where μ and μ_0 are the viscosities at the simulated and reference conditions, respectively. The VSC Package uses equations 8–3 and 8–4 to update hydraulic conductivities and conductances to account for changes in solute concentrations and temperature during a flow and transport simulation based on the Groundwater Flow (GWF) and Groundwater Transport (GWT) Models. The GWT Model is designed to simulate solute transport but can be used to simulate heat transport in some applications by appropriately scaling the input parameters to render the solute-transport equation mathematically equivalent to the heat-transport equation (Zheng, 2010). In such cases, the “solute concentration” calculated by a GWT-based heat-transport model can be identified in the VSC Package input file as representing temperature. Although the VSC Package allows viscosity to vary with solute concentration, variations in viscosity are typically most significant in heat-transport applications.

Dependence of Viscosity on Concentration and Temperature

The VSC Package calculates viscosity as a function of concentration and temperature using the following equation (Langevin and others, 2008, equation 17):

$$\mu = \mu_T(T) + \sum_{k=1}^{NS} \frac{\partial \mu}{\partial C^k} (C^k - C_0^k) \quad (8-5)$$

where NS is the number of chemical species (solutes) whose concentrations affect viscosity, C^k and C_0^k are the simulated and user-specified reference concentrations of species k , respectively, and $\partial \mu / \partial C^k$ is the user-specified rate at which viscosity changes linearly with the concentration of species k . (Symbols C^k and C_0^k are not to be confused with the symbols for conductance, C and C_0 , introduced earlier.) When all concentrations are equal to their reference values, the viscosity is equal to $\mu_T(T)$, which embodies the dependence of viscosity on temperature according to

$$\mu_T(T) = \begin{cases} \mu_0 + \frac{\partial \mu}{\partial T} (T - T_0) & \text{linear} \\ \mu_0 A_2^{\frac{A_3(T_0-T)}{(T+A_4)(T_0+A_4)}} & \text{nonlinear} \end{cases}. \quad (8-6)$$

where T and T_0 are the simulated and user-specified reference temperature, respectively, and μ_0 is the user-specified reference viscosity. The reference viscosity is commonly set to $0.001 \text{ kg m}^{-1} \text{ s}^{-1}$, which is representative of freshwater at a reference temperature of 20°C (Maidment, 1993, Table 11.1). When T equals T_0 , or if temperature is not designated by the user as affecting viscosity, $\mu_T(T)$ equals μ_0 . Equation 8–6 includes both linear and nonlinear variation of viscosity with temperature. Linear variation is the default, in which case $\partial \mu / \partial T$ is the user-specified rate at which viscosity changes linearly with temperature. Nonlinear variation is a user-selectable option, in which case the variation of viscosity from the reference value is determined by user-specified parameters A_2 , A_3 , and A_4 . The nonlinear option in equation 8–6 is mathematically equivalent to one of the options available in SEAWAT Version 4 (Guo and Langevin, 2002, equation 18) but is written in a form that explicitly sets $\mu_T(T)$ equal to μ_0 when T equals T_0 . Setting μ_0 , A_2 , A_3 , and A_4 to $0.001002 \text{ kg m}^{-1} \text{ s}^{-1}$, 10.0 , 248.37 , and 133.15 , respectively, and rounding the lead coefficient to one decimal place gives the temperature dependence of viscosity used in SUTRA (Voss, 1984) and SUTRA-MS (Hughes and

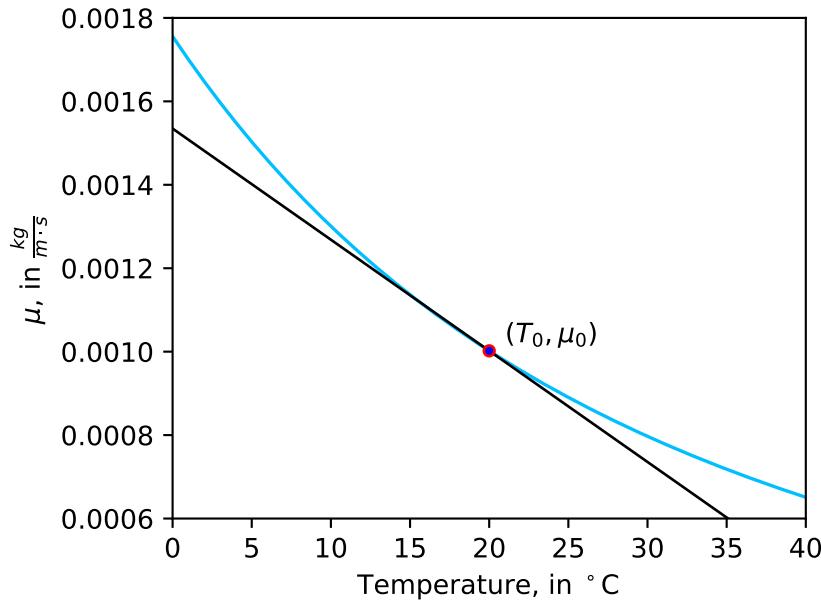


Figure 8-1. Nonlinear dependence of viscosity on temperature (blue curve) that is representative of freshwater over the temperature range 0 – 40°C, and a linear approximation (black curve) that has the same value (μ_0) and slope at the reference temperature (T_0). The blue curve is generated using 0.001002 kg m⁻¹ s⁻¹, 10.0, 248.37, and 133.15 for μ_0 , A_2 , A_3 , and A_4 , respectively.

Sanford, 2004). VS2DH (Healy and Ronan, 1996) also calculate the temperature dependence of viscosity using functions that are, respectively, mathematically equivalent to and a special case of equation 8-6.

Over the temperature range 0 – 40°C, the viscosity of freshwater varies between approximately 0.0007 and 0.00175 kg m⁻¹ s⁻¹, as indicated by the nonlinear (blue) curve in figure 8-1. The black line in figure 8-1 depicts a linear approximation that coincides with the nonlinear curve at the reference temperature and viscosity, $(T_0, \mu_0) = (20^\circ\text{C}, 0.001 \text{ kg m}^{-1} \text{ s}^{-1})$.

Accounting for Variable Viscosity in Flows Between Cells

The VSC Package uses concentrations and temperatures calculated for each cell by a GWT model on the previous time step or outer solution iteration to calculate viscosities for the current time step. These viscosities are used to adjust cell hydraulic conductivity values in the NPF Package using equation 8-3. The reference values of conductivity are the values specified by the user in the NPF Package and, optionally, the Time-Varying Conductivity (TVK) Package (Chapter 6 of this document). The conductivity adjustment is performed after the user-specified conductivities are read in but before conductivity values are passed to program units that use cell conductivities to formulate expressions for flow between cells, which include the “conductance-based” formulation for flow and the XT3D capability (Provost and others, 2017). If the VSC Package is not active, cell conductivities are not adjusted for variable viscosity, and the user-specified values are used.

Accounting for Variable Viscosity in Boundary Flows

The VSC Package uses concentrations and temperatures calculated for each cell by a GWT model on the previous time step or outer solution iteration in calculating viscosities for the current time step. These viscosities are used to adjust hydraulic conductances, using equation 8-4, in stress packages that involve head-

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dependent boundary flows, which include the River (RIV), General-Head Boundary (GHB), Drain (DRN), Streamflow Routing (SFR), Lake (LAK), and Multi-Aquifer Well (MAW) Packages ([Langevin and others, 2017](#)). For a boundary flow out of the model, the viscosity is based on the simulated concentration or temperature in the cell from which the boundary flow originates. For a boundary flow into the model, the viscosity is based on the concentration or temperature of the water entering the cell from the boundary. The reference values of conductance are the values normally set or calculated by the stress package based on user input. The conductance adjustment is performed after the stress package completes its normal conductance calculation but before the conductance value is used to formulate the expression for the boundary flow. If the VSC Package is not active, stress-package conductances are not adjusted for variable viscosity.

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