SWI6 - A Sharp Interface Saltwater Intrusion Packge for MODFLOW 6

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Abstract

This document describes a sharp interface saltwater intrusion package for MODFLOW 6. The package is developed as an API to MODFLOW 6, The model is develoed for the case of steady-state freshwater flow, transient freshwater flow, and transient freshwater and saltwater flow. This document discusses the formulation of the equations and their finite-volume numerical expansion using a quasi-Newton simultaneous solution approach.

1 Governing Partial Differential Equations for Modeling 2D sharp interface saltwater intrusion

Figure 1 shows a conceptual model of a sharp interface between freshwater and saltwater occurring in an unconfined aquifer.

Using vertical integration in an aquifer, 2-dimensional freshwater and a saltwater volume balance equations can be developed. Defining ζ as the elevation of the saltwater-freshwater interface, the thicknesses of the freshwater b_f and saltwater b_s zones for a confined/unconfined system are given as (see Figure 1):

$$b^f = Z_T - \zeta \text{ if } h^f \geq Z_T \text{ or } h^f - \zeta \text{ if } h^f < Z_T \text{ or } 0 \text{ if } h^f < \zeta \tag{1}$$

and

$$b^s = \zeta - Z_B \text{ if } \zeta < Z_T \text{ or } Z_T - Z_B \text{ if } \zeta \geq Z_T \text{ or } 0 \text{ if } \zeta \leq Z_B \tag{2}$$

where Z_T and Z_B are the top and bottom of the aquifer, respectively. If the aquifer is unconfined then Z_T is equal to the freshwater head, h^f. The interface position can be calculated from the fresh and saltwater heads using the fresh and saltwater densities and the following equation also known as the Dupuit Assumption:

$$\zeta = \frac{1}{v}(\frac{\rho_s}{\rho_f}h^s - h^f) \tag{3}$$

where

$$v = \frac{\rho_s - \rho_f}{\rho_f} \tag{4}$$

The governing volume balance equations for freshwater and saltwater for a confined / unconfined aquifer system are, respectively:

$$(b^f S_s^f + S_y^f)\frac{\partial h^f}{\partial t} - \theta\frac{\partial \zeta}{\partial t} = \nabla \cdot (\tilde{K^f} b^f \nabla h^f) + \dot{W}_f \tag{5}$$

and

$$(b^s S_s^s + S_y^{s*})\frac{\partial h^s}{\partial t} - \theta\frac{\partial \zeta}{\partial t} = \nabla \cdot (\tilde{K^s} b^s \nabla h^s) + \dot{W}_s \tag{6}$$

Where the superscript f denotes the freshwater zone, and the superscript s denotes the saltwater zone. $h^f = P/\rho_f g + z$, $h^s = P/\rho_s g + z$, $\tilde{K}$ is the hydraulic conductivity, θ is the porosity, S_s is the confined aquifer specific storage, S_y is the specific yield, and $\dot{W}$ is the volumetric source/sink

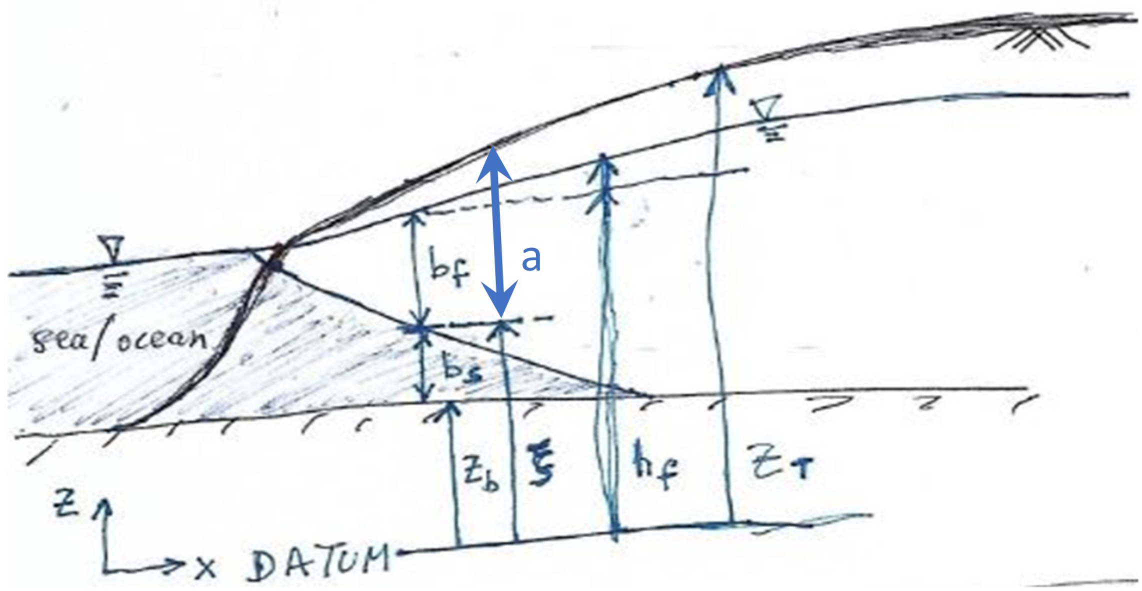

Figure 1: Conceptual model of a sharp interface between freshwater and saltwater in an unconfined aquifer.

term (a volumetric flux in 2D: volume per area per time). This source/sink term accounts for head-dependent leakage of fresh or saltwater from an overlying aquifer, using Darcy's law with a leakance term (similar to a leaky aquifer model). The source/sink term also accounts for wells, recharge, groundwater interaction with surface-water bodies, etc.

The storage term of equation (5) can be expanded from geometric considerations and rearranged as:

$$(b^f S_s^f + S_y^f)\frac{\partial h^f}{\partial t} - \theta\frac{\partial \zeta}{\partial t} = (b^f S_s^f + S_y^f)\frac{\partial h^f}{\partial t} - \theta\frac{\partial (h^f - b^f)}{\partial t} = (b^f S_s^f - \theta + S_y^f)\frac{\partial h^f}{\partial t} + \theta\frac{\partial b^f}{\partial t} \tag{7}$$

If it is assumed that the specific yield equals the effective porosity (i.e., pore water replaced by a saltwater interface movement would be the same as that replaced by the air-water interface movement), then the terms $-\theta$ and S_y^f cancel out giving the storage term as.

$$(b^f S_s^f + S_y^f)\frac{\partial h^f}{\partial t} - \theta\frac{\partial \zeta}{\partial t} = b^f S_s^f\frac{\partial h^f}{\partial t} + \theta\frac{\partial b^f}{\partial t} \tag{8}$$

Inserting equation (8) into the freshwater flow equation (5) gives

$$b^f S_s^f\frac{\partial h^f}{\partial t} + \theta\frac{\partial b^f}{\partial t} = \nabla \cdot (\tilde{K^f} b^f \nabla h^f) + \dot{W}_f \tag{9}$$

If it is assumed that the specific yield equals the effective porosity (i.e., pore water replaced by a saltwater interface movement would be the same as that replaced by the air-water interface movement), then the storage term of equation (6) can be written as:

$$(b^s S_s^s)\frac{\partial h^s}{\partial t} + \theta\frac{\partial \zeta}{\partial t} = (b^s S_s^s)\frac{\partial h^s}{\partial t} + \theta\frac{\partial (b^s + Z_B)}{\partial t} = (b^s S_s^s)\frac{\partial h^s}{\partial t} + \theta\frac{\partial b^s}{\partial t} \tag{10}$$

Where $\zeta = b^s + Z_B$ and the last equality is because the bottom Z_B is invariant with time. When the saltwater head is at the interface elevation (no freshwater above it) then the saltwater interfaces with air and change in saltwater head is equal to the change in the interface elevation.

Inserting Equation (10) into the saltwater flow equation (6) gives:

$$(b^s S_s^s)\frac{\partial h^s}{\partial t} + \theta\frac{\partial b^s}{\partial t} == \nabla \cdot (\tilde{K^s} b^s \nabla h^s) + \dot{W}_s \tag{11}$$

The saltwater hydraulic conductivity term may be modified from the freshwater hydraulic conductivity term and the associated densities and viscosities as:

$$K_{nm}^s = K_{nm}^f \frac{\rho^s}{\mu^s}\frac{\mu^f}{\rho^f} \tag{12}$$

Where the the freshwater hydraulic conductivity values and the density and viscosity for freshwater and saltwater are input for each grid cell by the user.

Equations (3), (9), and (11) form three equations which can be solved for the three variables, h^f, h^s, and ζ, where equations (1) and (2) give the freshwater and saltwater thicknesses b^f and b^s. Also, equation (12) gives a saltwater hydraulic condictivity, given the freshwater hydraulic conductivity of the aquifer.

Instead of solving both saltwater and freshwater equations, a simplification can be made whereby it may be assumed that the saltwater attains instant equilibrium with its boundaries. For instance, it is assumed that the saltwater head is always at sea level. In that case, only the freshwater flow equation (9) needs to be solved where the freshwater thickness b^f is given by equation (1) and the interface elevation by the Dupuit assumption of equation (3).

2 Finite Volume Formulation for Sharp Interface Saltwater Intrusion

The approach selected for representing saltwater intrusion within the MODFLOW 6 framework is to solve the freshwater flow equation for the freshwater head, and the saltwater flow equation for saltwater head. The interface elevation, where required in these equations is calculated by the relationship between these heads and the reference fluid densities. A single freshwater flow equation may also be solved as an option, assuming that the saltwater is in instant equilibrium with the freshwater flow behavior.

2.1 Freshwater Flow Equation

The freshwater flow equation for a confined / unconfined aquifer system is shown in (9) where the left hand side of equation (9) represents the freshwater storage terms, and the right side of the equation represents the freshwater flow (and source) terms.

Expanding the flow term on the right hand side of equation (9) in by the finite volume approach yields:

$$\nabla \cdot (\tilde{K^f} b^f \nabla h^f) = \Sigma_m C_{nm}^h f(h_m^f - h_n^f)) \tag{13}$$

where C_{nm}^f is the conductance term for freshwater flow between cells n and m.

The flow conductance term C_{nm}^f is written as:

$$C_{nm}^h = \frac{A_{nm}^f K_{nm}^f}{d_{nm}} = b^f \frac{L_{nm} K_{nm}^f}{d_{nm}} = S^f \frac{L_{nm} K_{nm}^f}{d_{nm}} b^{TOT} \tag{14}$$

where A_{nm}^f is the area of the face between elements n and m saturated with freshwater, which is equal to $b^f L_{mn}$ where L_{mn} is the horizontal width of the interface between n and m, and b_f is the freshwater thickness in the aquifer between cells n and m (the upstream value is used in MODFLOW 6). The last equality occurs from the definition of a freshwater saturation, as:

$$S^f = \frac{b^f}{b^{TOT}} \tag{15}$$

where b^{TOT} is the total thickness. Different approaches are available to compute the interblock saturation S^f. Use of upstream weighting will compute the value using the upstream freshwater thickness b^f and cell thickness b^{TOT}. The upstream cell is denoted in MODFLOW 6 as the cell with the higher freshwater head, between cells n and m.

It is noted that the flow term for freshwater represented by the last equality of equation (14) is similar to the flow term represented by MODFLOW 6 for groundwater flow, where the freshwater conductivity and saturation replace the associated groundwater flow terms (which use the entire saturated flow thickness from the cell bottom and not just the freshwater thickness above the saltwater/freshwater interface). The freshwater hydraulic conductivity term is the same as in MODFLOW 6 and is input for each grid cell by the user (with various intercell averaging schemes available in MODFLOW for getting the interface hydraulic conductivity between cells n and m).

Expanding the storage terms on the left hand side of equation (9) in by the finite volume approach yields:

$$b^f S_s^f \frac{\partial h^f}{\partial t} + \theta \frac{\partial b^f}{\partial t} = A_n b^f S_s^f \left(\frac{h_n^f - h_n^{f(t-1)}}{\Delta t}\right) + A_n \theta \left(\frac{b_n^f - b_n^{f(t-1)}}{\Delta t}\right)$$
$$= A_n S^f S_s^f \left(\frac{h_n^f - h_n^{f(t-1)}}{\Delta t}\right) b^{TOT} + A_n \theta \left(\frac{S_n^f - S_n^{f(t-1)}}{\Delta t}\right) b^{TOT} \quad (16)$$

where A_n is the horizontal area of cell n and the last equality results from using equation (15) in the finite volume expansion.

The finite volume expansion of the storage term of equation (16) is similar to that of the flow equation's storage term in MODFLOW 6, for confined and unconfined flow, but with freshwater saturation S_n^f instead of a saturated aquifer thickness S_n. Thus, as long as a freshwater thickness replaces saturated aquifer thickness in the MODFLOW 6 computations, the same MODFLOW 6 routines can be used to evaluate the storage term for the freshwater equation of a sharp interface saltwater intrusion flow model. This can be done through the API by replacing S_n (the saturated cell fraction of equation 4-5 of the MODFLOW 6 Groundwater Flow Model Documentation) by S_n^f which may be calculated as:

$$S_n^f = \frac{b_n^f}{b_n^{TOT}} = \frac{b_n^f}{b_n^\zeta} \frac{b_n^\zeta}{b_n^{TOT}} = S_n^\zeta \frac{b_n^\zeta}{b_n^{TOT}} \quad (17)$$

where b_n^ζ is the thickness of the cell above the interface ζ (denoted as "a" in Figure 1), and S_n^ζ can be obtained using the same functions as the saturated thickness term of MODFLOW 6 if the thickness is taken from the interface elevation ζ, instead of from the aquifer bottom (Z_B) (the saturated cell fraction of equation 4-5 of the MODFLOW 6 Groundwater Flow Model Documentation). Thus the continuous and smooth functions of MODFLOW 6 are used to compute the saturation term S_n^ζ (instead of using the second to last equality of equation (17) with the relationships of equation (1) which has discontinuous derivatives). The term b_n^ζ can be obtained as below

$$b_n^\zeta = Z_T - \zeta \text{ if } Z_B < \zeta < Z_T \text{ or } 0 \text{ if } \zeta > Z_T \text{ or } Z_T - Z_B \text{ if } \zeta < Z_B \quad (18)$$

Thus, the API passes ζ to the MODFLOW6 code to compute S_n^ζ which is then multiplied by the ratio of b_n^ζ (obtained from equation (18)) to b_n^{TOT} to give S_n^f as per equation (17). This S_n^f is passed to MODFLOW 6 through the API to fill the flow equation matrix for the freshwater flow model.

The unstructured grid flow equation of MODFLOW 6 solves the equation using the Newton Raphson approach with the hydraulic head as the primary variable. Thus, if the hydraulic head were replaced by freshwater head of equation (9) with associated replacements for thickness, storage, and specific yield, and with the assumption that the freshwater specific yield is equal to the effective porosity for movement of the fresh/saline interface, the equivalent freshwater equations to the MODFLOW 6 equations solve the freshwater flow equation with the freshwater head as the primary variable of solution.

2.2 Saltwater Flow Equation

The saltwater flow equation for a confined / unconfined aquifer system is shown in (11) where the left hand side of equation (11) represents the saltwater storage terms, and the right side of the equation represents the saltwater flow (and source) terms. A finite volume expansion of this equation is similar to the expansion for freshwater flow, but with reference to saltwater heads and thicknesses.

Expanding the flow term on the right hand side of equation (11) in by the finite volume approach yields:

$$\nabla \cdot (\tilde{K^s} b^s \nabla h^s) = \Sigma_m C^s_{nm}(h^s_m - h^s_n) \tag{19}$$

where C_{nm} is the conductance term for saltwater flow between cells n and m.

The flow conductance term C_{nm} is written as:

$$C^s_{nm} = \frac{A^s_{nm} K^s_{nm}}{d_{nm}} = b^s \frac{L_{nm} K^s_{nm}}{d_{nm}} = S^s \frac{L_{nm} K^s_{nm}}{d_{nm}} b^{TOT} \tag{20}$$

where A^s_{nm} is the area of the face between elements n and m filled by saltwater, which is equal to $b^s Lmn$ where L_{mn} is the horizontal width of the interface between n and m as defined earlier, and b_s is the saltwater thickness in the aquifer between cells n and m (the upstream value is used in MODFLOW 6). The last equality occurs from definition of a saltwater saturation as:

$$S^s = \frac{b^s}{b^{TOT}} \tag{21}$$

Different approaches are available to compute the interblock saturation S^s. Use of upstream weighting will compute the value using the upstream saltwater thickness b^s and cell thickness b^{TOT}. The upstream cell is denoted in MODFLOW 6 as the cell with the higher freshwater head, between cells n and m.

It is noted that the flow term for saltwater represented by the last equality of equation (20) is similar to the flow term represented by MODFLOW 6 for groundwater flow, where the saltwater conductivity and thickness replace the associated groundwater flow terms. The saltwater saturtion is the saltwater thickness in a grid-block from the bottom to the saltwater interface. The saltwater hydraulic conductivity is obtained from that of freshwater (entered by the user) by using equation (12).

Expanding the storage term on the left hand side of equation (11) by using a finite volume approach gives

$$\begin{aligned}(b^s S^s_s)\frac{\partial h^s}{\partial t} + \theta \frac{\partial b^s}{\partial t} &= A_n b^s S^s_s (\frac{h^s_n - h^{s(t-1)}_n}{\Delta t}) + A_n \theta (\frac{b^s_n - b^{s(t-1)}_n}{\Delta t}) \\ &= A_n b^s S^s_s (\frac{h^s_n - h^{s(t-1)}_n}{\Delta t}) + A_n \theta (\frac{S^s_n - S^{s(t-1)}_n}{\Delta t}) b^{TOT}\end{aligned} \tag{22}$$

where the last equality results from using equation (21) in the finite volume expansion.

The finite volume expansion of the storage term of equation (22) is similar to that of the flow equation's storage term in MODFLOW 6, for confined and unconfined flow, but with saltwater saturation S^s_n instead of a saturated aquifer thickness S_n. Thus, as long as a saltwater thickness replaces saturated aquifer thickness in the MODFLOW 6 computations, the same MODFLOW 6 routines can be used to evaluate the storage term for the saltwater equation of a sharp interface saltwater intrusion flow model. This can be done through the API by replacing S_n by S^s_n which may be calculated as:

$$S^s_n = \frac{b^s_n}{b^{TOT}_n} \tag{23}$$

The term S^s_n can be obtained using the continoous and smooth functions of MODFLOW 6 instead of using the last equality of equation (2). This can be done through the API by replacing the hydraulic head of MODFLOW with ζ in the smooth function for computing saturations (the saturated cell fraction of equation 4-5 of the MODFLOW 6 Groundwater Flow Model Documentation). This S^s_n can then be used by MODFLOW 6 for expressing the saltwater thickness.

The unstructured grid flow equation of MODFLOW 6 solves the groundwater flow equation using the Newton Raphson approach with the hydraulic head as the primary variable. Thus, if the hydraulic head were replaced by saltwater head of equation (11) with associated replacements for thickness, storage, and specific yield, and with the assumption that the saltwater specific yield is equal to the effective porosity for movement of the fresh/saline interface, the MODFLOW 6 equations solve the saltwater flow equation with the saltwater head as the primary variable of solution.

2.3 Solution Approaches

The sharp interface model is expressed by the freshwater flow equation and the saltwater flow equation. An assunption can be made whereby saltwater is assumed to always be at instant equilibrium, similar to the Richards' equation for unsaturated flow where the air phase flow equation is considered to be at instant equilibrium. This approach has several advantages that include solving only one equation instead of two at each node, and also for obtaining initial conditions (predevelopment conditions) where a saltwater wedge underlies a freshwater body.

3 Newton Raphson Solution to the Sharp Interface Saltwater Intrusion Equations

The sharp interface saltwater intrusion problem is expressed by the freshwater flow equation (9) and the saltwater flow equation (11). These equations are similar to the equations for groundwater flow in MODFLOW 6 with the respective heads replaced by the hydraulic head, and the respective phase thicknesses replaced by saturated aquifer thickness. Also, the solution can be simplified by solving just one equation for freshwater flow. Therefore, the primary variables of solution are the freshwater flow head h^f, and the saltwater flow head h^s (when saltwater flow equation is also solved).

3.1 Newton Raphson Expansion of the Freshwater Flow Equation

The finite volume discretized form of the freshwater flow equation (9) is obtained by substituting equation (16) for the storage term and (13) and (14) for the flow term into equation (9) and rearranging as:

$$F^f = A_n S^f S_s^f (\frac{h_n^f - h_n^{f(t-1)}}{\Delta t}) b^{TOT} + A_n \theta (\frac{S_n^f - S_n^{f(t-1)}}{\Delta t}) b^{TOT} \\ - \Sigma_m (S^f C_{nm}^{f(o)}) f(h_m^f - h_n^f) = Q_{STO(n)}^f - \Sigma_m Q_{nm}^f = 0 \quad (24)$$

whered F^f is the freshwater flow equation, $Q_{STO(n)}^f$ is the change in storage term (composed of the compressible storage term $Q_{SS(n)}^f$ plus the drainable storage term $Q_{SY(n)}^f$), and $Q_{n,m}$ is the flow term between node n and adnacent node m and $C_{nm}^{f(o)}$ is the constant portion of the freshwater conductance term between cells n and m expressed as:

$$C_{nm}^{f(o)} = \frac{L_{nm} K_{nm}^f}{d_{nm}} b^{TOT} \quad (25)$$

A Newton Raphson expansion of this equation with respect to freshwater head is given as:

$$\frac{\partial F^f}{\partial h^f} \Delta h^f = -F^f \quad (26)$$

As shown by Niswonger and others (2011) and Panday and others (2013), equation (26) can be rearranged to give

$$(\frac{\partial F^f}{\partial h^f})^{(k-1)} h^{f(k)} = -F^{f(k-1)} + (\frac{\partial F^f}{\partial h^f})^{(k-1)} h^{f(k-1)} \quad (27)$$

Equation (27) is the same form of the Newton Raphson equation solved by MODFLOW 6. The Newton expansion can be applied separately to the flow term $Q_{n,m}$ and to the storage term $Q_{STO(n)}$.

3.2 Newton Expansion of the Flow Term of the Freshwater Flow Equation

Applying the Newton expansion to the flow term in a similar manner as done in equations 4-33 through 4-41 of the MODFLOW 6 document gives

$$
\left[-S^f C_{nm}^{f(o)} + \frac{\partial S^f}{\partial h_n} C_{nm}^{f(o)} (h_m^{f(k-1)} - h_n^{f(k-1)})\right] h_n^{f(k)} + \left[S^f C_{nm}^{f(o)} + \frac{\partial S^f}{\partial h_m} C_{nm}^{f(o)} (h_m^{f(k-1)} - h_n^{f(k-1)})\right]] h_m^{f(k)} = \left[\frac{\partial S^f}{\partial h_n} C_{nm}^{f(o)} (h_m^{f(k-1)} - h_n^{f(k-1)})\right]] h_n^{f(k-1)} + \left[\frac{\partial S^f}{\partial h_n^f} C_{nm}^{f(o)} (h_m^{f(k-1)} - h_n^{f(k-1)})\right]] h_m^{f(k-1)} \quad (28)
$$

This equation is similar to equatin 4-41 of the MODFLOW 6 Groundwater Flow Model documentation. The terms $S^f C_{nm}^{f(o)}$ in equation (28) are subtracted from the upstream diagonal and added to the appropriate off-diagonal terms of the coefficient matrix during the Picard formulation, respectively. The derivative terms on the left hand side and the terms on the right hand side of equation (28) are added to the coefficient matrix and right hand side vector as the Newton terms.

3.3 Newton Expansion of the Storage Terms of the Freshwater Flow Equation

The compressible storage term of the freshwater flow equation (24) can be expanded by the Newton method in a similar manner as was done for the MODFLOW 6 compressible storage equation (equation 5-4) of the MODFLOW 6 Groundwater Flow Model documentation. Using a similar approach to equations 5-6 through 5-9 of the MODFLOW 6 Groundwater Flow Model document the compressible storage term can be expressed for the freshwater flow equation as:

$$
\left(-\frac{A_n S_s^f S^{f(k-1)}}{t - t_{old}} - \frac{A_n S_s^f}{t - t_{old}} \frac{\partial S^{f(k-1)}}{\partial h_n^f} h_n^{f(k-1)}\right) h_n^{f(k)} = - \frac{A_n S_s^f S^{f(t_{old})}}{t - t_{old}} HOLD_n - \left(\frac{A_n S_s^f}{t - t_{old}} \frac{\partial S^{f(k-1)}}{\partial h_n^f}\right) h_n^{f(k-1)} \quad (29)
$$

The first term on the left hand side and the first term on the right hand side of equation (29) are assembled into the diagonal matrix location and the right-hand side vector respectively during Picard assembly in MODFLOW 6. The second term on the left hand side and the first term on the right hand side of equation (29) are assembled into the diagonal matrix location and the right-hand side vector respectively during assembly of the Newton terms.

The drainable storage term of the freshtwater flow equation (24) can be expanded by the Newton method in a similar manner as was done for the MODFLOW 6 drainable storage equation (equation 5-10) of the MODFLOW 6 Groundwater Flow Model documentation. Using a similar approach to equations 5-14 through 5-18 of the MODFLOW 6 Groundwater Flow Model document the drainable storage term can be expressed for the freshwater flow equation as:

$$
\left(\frac{A_n \theta b^{TOT}}{t - t_{old}} \frac{\partial S_n^f}{\partial h_n^{f(k)}}\right) h_n^{f(k)} = - \left(\frac{A_n \theta b^{TOT}}{t - t_{old}} S_n^{f(t_{old})} + \frac{A_n \theta b^{TOT}}{t - t_{old}} S_n^{f(k-1)}\right) - \left(\frac{A_n \theta b^{TOT}}{t - t_{old}} \frac{\partial S_n^f}{\partial h_n^{f(k)}}\right) h_n^{f(k-1)} \quad (30)
$$

The coefficient term on the left hand side of equation (30) is assembled into the diagonal matrix location and the term on the right hand side of equation (30) is assembled into the right-hand side vector in MODFLOW 6.

3.4 Newton Raphson Expansion of the Saltwater Flow Equation

The finite volume discretized form of the Saltwater flow equation (11) is obtained by substituting equation (22) for the storage term and (19) and (20) for the flow term into equation (11) and rearranging as:

$$F^s = A_n S^s S^s_s(\frac{h^s_n - h^{s(t-1)}_n}{\Delta t})b^{TOT} + A_n\theta(\frac{S^s_n - S^{s(t-1)}_n}{\Delta t})b^{TOT} \\ - \Sigma_m(S^s C^{s(o)}_{nm})f(h^s_m - h^s_n) = Q^s_{STO(n)} - \Sigma_m Q^s_{nm} = 0 \quad (31)$$

whered F^s is the saltwater flow equation, $Q^s_{STO(n)}$ is the change in storage term (composed of the compressible storage term $Q^s_{SS(n)}$ plus the drainable storage term $Q^s_{SY(n)}$), and $Q^s_{n,m}$ is the flow term between node n and adnacent node m and $C^{s(o)}_{nm}$ is the constant portion of the saltwater conductance term between cells n and m expressed as:

$$C^{s(o)}_{nm} = \frac{L_{nm}K^s_{nm}}{d_{nm}}b^{TOT} \quad (32)$$

A Newton Raphson expansion of this equation with respect to saltwater head is given as:

$$\frac{\partial F^s}{\partial h^s}\Delta h^s = -F^s \quad (33)$$

As shown by Niswonger and others (2011) and Panday and others (2013), equation (26) can be rearranged to give

$$(\frac{\partial F^s}{\partial h^s})^{(k-1)}h^{s(k)} = -F^{s(k-1)} + (\frac{\partial F^s}{\partial h^s})^{(k-1)}h^{s(k-1)} \quad (34)$$

Equation (34) is the same form of the Newton Raphson equation solved by MODFLOW 6. The Newton expansion can be applied separately to the flow term $Q^s_{n,m}$ and to the storage term $Q^s_{STO(n)}$.

3.5 Newton Expansion of the Flow Term of the Saltwater Flow Equation

Applying the Newton expansion to the flow term in a similar manner as done in equations 4-33 through 4-41 of the MODFLOW 6 document gives

$$\left[-S^s C^{s(o)}_{nm} + \frac{\partial S^s}{\partial h_n}C^{s(o)}_{nm}(h^{s(k-1)}_m - h^{s(k-1)}_n)\right]h^{s(k)}_n + \\ \left[S^s C^{s(o)}_{nm} + \frac{\partial S^s}{\partial h_m}C^{s(o)}_{nm}(h^{s(k-1)}_m - h^{s(k-1)}_n)\right]]h^{s(k)}_m = \\ \left[\frac{\partial S^s}{\partial h_n}C^{s(o)}_{nm}(h^{s(k-1)}_m - h^{s(k-1)}_n)\right]]h^{s(k-1)}_n + \\ \left[\frac{\partial S^s}{\partial h^s_n}C^{s(o)}_{nm}(h^{s(k-1)}_m - h^{s(k-1)}_n)\right]]h^{s(k-1)}_m \quad (35)$$

This equation is similar to equatin 4-41 of the MODFLOW 6 Groundwater Flow Model documentation. The terms $S^f C^{f(o)}_{nm}$ in equation (35) are subtracted from the upstream diagonal and added to the appropriate off-diagonal terms of the coefficient matrix during the Picard formulation, respectively. The derivative terms on the left hand side and the terms on the right hand side of equation (35) are added to the coefficient matrix and right hand side vector as the Newton terms.

3.6 Newton Expansion of the Storage Terms of the Saltwater Flow Equation

The compressible storage term of the saltwater flow equation (31) can be expanded by the Newton method in a similar manner as was done for the MODFLOW 6 compressible storage equation (equation

5-4) of the MODFLOW 6 Groundwater Flow Model documentation. Using a similar approach to equations 5-6 through 5-9 of the MODFLOW 6 Groundwater Flow Model document the compressible storage term can be expressed for the freshwater flow equation as:

$$\left(-\frac{A_n S_s^s S^{s(k-1)}}{t-t_{old}} - \frac{A_n S_s^s}{t-t_{old}}\frac{\partial S^{s(k-1)}}{\partial h_n^s} h_n^{s(k-1)}\right) h_n^{s(k)} = \\ -\frac{A_n S_s^s S^{s(t_{old})}}{t-t_{old}} HOLD_n - \left(\frac{A_n S_s^s}{t-t_{old}}\frac{\partial S^{s(k-1)}}{\partial h_n^s}\right) h_n^{s(k-1)} \quad (36)$$

The first term on the left hand side and the first term on the right hand side of equation (36) are assembled into the diagonal matrix location and the right-hand side vector respectively during Picard assembly in MODFLOW 6. The second term on the left hand side and the first term on the right hand side of equation (36) are assembled into the diagonal matrix location and the right-hand side vector respectively during assembly of the Newton terms.

The drainable storage term of the freshwater flow equation (31) can be expanded by the Newton method in a similar manner as was done for the MODFLOW 6 drainable storage equation (equation 5-10) of the MODFLOW 6 Groundwater Flow Model documentation. Using a similar approach to equations 5-14 through 5-18 of the MODFLOW 6 Groundwater Flow Model document the drainable storage term can be expressed for the freshwater flow equation as:

$$\left(\frac{A_n \theta b^{TOT}}{t-t_{old}}\frac{\partial S_n^s}{\partial h_n^{s(k)}}\right) h_n^{s(k)} = \\ -\left(\frac{A_n \theta b^{TOT}}{t-t_{old}} S_n^{s(t_{old})} + \frac{A_n \theta b^{TOT}}{t-t_{old}} S_n^{s(k-1)}\right) - \left(\frac{A_n \theta b^{TOT}}{t-t_{old}}\frac{\partial S_n^s}{\partial h_n^{s(k)}}\right) h_n^{s(k-1)} \quad (37)$$

The coefficient term on the left hand side of equation (37) is assembled into the diagonal matrix location and the term on the right hand side of equation (37) is assembled into the right-hand side vector in MODFLOW 6.

3.7 Obtaining Cross-Storge Terms for Simultaneous Solution Approach

The simultaneous solution of a freshwater and saltwater flow model can accommodate a full Newton expansion of the storage term through the MODFLOW 6 exchange term which sets up a connection between the freshwater and saltwater model. Since the freshwater and saltwater flow models occupy the same space, each node of the freshwater flow model can have an exchange (a connection) term with each node of the saltwater flow model. This can be accommodated by performing a Newton expansion of the freshwater flow equation storage term with the freshwater head h^f as well as the saltwater head h^s. Also, the saltwater flow equation storage term can be expanded using Newton linearization using both the freshwater head h^f as well as the saltwater head h^s.

The unconfined storage term for freshwater flow in equation (24) is expressed as

$$Q^f_{Sy(n)} = A_n \theta b^{TOT} \frac{S_n^f - S_n^{f(t-1)}}{\Delta t} \quad (38)$$

Newton expansion of this term with respect to both freshwater and saltwater heads is

$$\frac{\partial Q^f_{Sy(n)}}{\partial h^f}\Delta h^f + \frac{\partial Q^f_{Sy(n)}}{\partial h^s}\Delta h^s = -Q^f_{Sy(n)} \quad (39)$$

Inserting equation (38) into (39) gives

$$A_n b^{TOT}\frac{\theta}{\Delta t}\frac{\partial S_n^f}{\partial h^f}\Delta h^f + A_n b^{TOT}\frac{\theta}{\Delta t}\frac{\partial S_n^f}{\partial h^s}\Delta h^s = -A_n b^{TOT}\frac{\theta}{\Delta t}(b_n^f - b_n^{f(t-1)}) \quad (40)$$

It is noted that the first term on the left-hand side, and the term on the right-hand side of equation (40) are already assembled in the freshwater flow equation's storage term Newton expansion with respect to the freshwater head. Thus, the cross term that needs to be filled in the exchange location of the freshwater equation in terms of the saltwater head variable is the second term on the left-hand side of equation (40) which can be expanded as

$$A_n b^{TOT} \frac{\theta}{\Delta t} \frac{\partial S_n^f}{\partial h^s} h^{s^{n+1}} = A_n b^{TOT} \frac{\theta}{\Delta t} \frac{\partial S_n^f}{\partial h^s} h^{s^n} \tag{41}$$

Where the coefficient on the left-hand side $A_n b^{TOT} \frac{\theta}{\Delta t} \frac{\partial S_n^f}{\partial h^s}$ is added to the cross-term connection of the coefficient matrix, and the term on the right-hand side is added to the right hand side of the freshwater flow equation.

The unconfined storage term for saltwater flow equation (31) is expressed as

$$Q^s_{Sy(n)} = A_n \theta b^{TOT} \frac{S_n^s - S_n^{s(t-1)}}{\Delta t} \tag{42}$$

Newton expansion of this term with respect to both freshwater and saltwater heads is

$$\frac{\partial Q^s_{Sy(n)}}{\partial h^f} \Delta h^f + \frac{\partial Q^s_{Sy(n)}}{\partial h^s} \Delta h^s = -Q^s_{Sy(n)} \tag{43}$$

Inserting equation (42) into (43) gives

$$A_n b^{TOT} \frac{\theta}{\Delta t} \frac{\partial S_n^s}{\partial h^f} \Delta h^f + A_n b^{TOT} \frac{\theta}{\Delta t} \frac{\partial S_n^s}{\partial h^s} \Delta h^s = -A_n b^{TOT} \frac{\theta}{\Delta t} (S_n^s - S_n^{s(t-1)}) \tag{44}$$

It is noted that the first term on the left-hand side, and the term on the right-hand side of equation (44) are already assembled in the saltwater flow equation's storage term Newton expansion with respect to the saltwater head. Thus, the cross term that needs to be filled in the exchange location of the saltwater equation in terms of the freshwater head variable is the second term on the left-hand side of equation (44) which can be expanded as

$$A_n b^{TOT} \frac{\theta}{\Delta t} \frac{\partial S_n^s}{\partial h^s} h^{s^{n+1}} = A_n b^{TOT} \frac{\theta}{\Delta t} \frac{\partial S_n^s}{\partial h^s} h^{s^n} \tag{45}$$

Where the coefficient on the left-hand side $A_n b^{TOT} \frac{\theta}{\Delta t} \frac{\partial S_n^s}{\partial h^s}$ is added to the cross-term connection of the coefficient matrix, and the term on the right-hand side is added to the right hand side of the saltwater flow equation.

Note that when a cell has no saltwater (interface is at or below tbe bottom of the cell), the saltwater relative permeability term is zero and therefore saltwater cannot leave that cell further. Also when a cell has no freshwater (cell is dry or interface is at or above the top of the cell), the freshwater relative permeability is zero and freshwater cannot leave that cell further. Therefore, it is not necessary to flatten out or smooth the saltwater curve at the bottom. Similarly, it is not necessary to flatten or smooth the freshwater curve at the bottom. Also, since

4 References

Aharmouch A, B. Amaziane, M El Ossmani, and K Talali, A Fully Implicit Finite Volume Scheme for a Seawater Intrusion Problem in Coastal Aquifers, Water, MDPI, 12, 1639; doi:10.3390/w12061639

El–Amin M.F., J Kou, S Sun, A Salama, 2017. Adaptive time-splitting scheme for two-phase flow in heterogeneous porous media, Adv. Geo-Energy Res. Vol. 1, No. 3, p. 182-189, Ausasia Science and Technology Press.

Kou J., and S. Sun, 2004. On iterative IMPES formulation for two-phase flow with capillarity in heterogeneous porous media, International journal of numerical analysis and Modeling, Series B, Volume 1, Number 1, Pages 20–40

Huyakorn, P.S., Y.S. Wu, and N.S. Park, 1996. Multiphase approach to the numerical solution of a sharp interface saltwater intrusion problem, Water Resources Research, Vol. 32, No. 1, Pages 93-102, January 1996, DOI: 10.1029/95WR02919.

Bakker, M., and Schaars, F, 2005. The Sea Water Intrusion (SWI) Package Manual Part I. Theory, User Manual, and Examples. Version 1.2.

Bakker, M., and F. Schaars, J.D. Hughes, C.D. Langevin, and A.M. Dausman, 2013. Documentation of the seawater intrusion (SWI2) package for MODFLOW: U.S. Geological Survey Techniques and Methods, book 6, chap. A46, 47 p., http://pubs.usgs.gov/tm/6a46/.

Voss, C.I., 1984. AQUIFEM - A finite-element model for aquifers containing a seawater interface, U.S. Geological Survey Water-Resources Investigations Report 84 4263.

Bakker, M., and Schaars, F, 2013. Modeling Steady Sea Water Intrusion with Single-Density Groundwater Codes, Groundwater, Vol. 51, No. 1, pages 135–144, doi: 10.1111/j.1745-6584.2012.00955.x.

Sbai, M.A., A. Larabi, and F. DeSmedt, 1998. Modelling saltwater intrusion by a 3-D sharp interface finite element model, Transactions on Ecology and the Environment vol 17, © 1998 WIT Press, www.witpress.com, ISSN 1743-3541.