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Implementation of the Fully Implicit Expanded Mixed Finite Element Method for Air-Water Flow in Porous Media

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Abstract

This paper describes a methodology for treating the fully implicit expanded mixed finite element method for modeling the air-water model in porous media. The problem is posed over an aquifer domain with varying topography due to the geological layering. We present an expanded mixed finite element method that can efficiently handled these difficulties. The approximating spaces are defined on a computational grid to the aquifer domain. Quadrature rules are introduced to transform the mixed method into a cell-centered finite difference method for the pressure. Rectangular computational elements give a 19 points stencil in 3 dimensions. We give the the model equations, the initialization algorithm, the discretization method, and the Jacobian formation.

Keywords: air-water model, implicit, finite element, finite differences, expanded mixed method

1 Introduction

The mixed finite element method was developed by Raviart and Thomas [1, 3, 5], and we restrict our attention to their lowest-order method. It was first used for subsurface problems by Douglas, Ewing, and Wheeler [6], though Russell and Wheeler [9] pointed out that the often used cell-centered finite difference method on rectangular grids [7] for problems with diagonal tensor coefficients is actually a mixed method with appropriate quadrature rules applied to the integrals. We generalize the approach of Russell and Wheeler to define our numerical methods for the full case of tensor coefficients.The problem with mixed method is that they can be difficult to implement directly. We

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consider an expanded mixed finite element for Darcy flow with tensor absolute permeability. The schemes are cell-centered finite difference approximations of a mixed finite element method; thus, they are easy to implement, have only one unknown per element, and are locally conservative.
Let Ω be a domain in $\mathbb{R}^3$ with boundary $\Gamma = \partial\Omega$, and let Γ^D, Γ^N be the portions of the boundary where the Dirichlet and Neumann conditions are specified respectively. We assume that $\Gamma = \Gamma^D \cup \Gamma^N$. We use relatively standard cell centered finite difference notation. Let the domain grid points be denoted by

$$\left(x_{i+1/2}, y_{j+1/2}, z_{k+1/2}\right), i = 0, ..., N_x; j = 0, ..., N_y; k = 0, ..., N_z. \tag{1}$$

and define the midpoints

$$x_i = \frac{1}{2}\left(x_{i+1/2} + x_{i-1/2}\right), i = 1, ..., N_x, \tag{2}$$

$$y_j = \frac{1}{2}\left(y_{j+1/2} + y_{j-1/2}\right), j = 1, ..., N_y, \tag{3}$$

$$z_k = \frac{1}{2}\left(z_{k+1/2} + z_{k-1/2}\right), k = 1, ..., N_z. \tag{4}$$

The outline of the paper is as follows: In section 2, we briefly describe the physical model. In section 3, we define the expanded mixed finite element discretizations. Backward Euler is used for the time discretization, giving a fully implicit method. Application of these methods results in a system of nonlinear discrete equations which must be solved at each time step. This nonlinear system is solved with Newton's method and an optional backtracking globalization technique with dynamic forcing term selection.

2 Model Formulation

The two-phase flow system is formulated as a continuity, or mass balance, equation, Darcy's Law modified for multi-phase flow, equation of state relationships describing the density of each fluid, capillary pressure relationships between two fluid interfaces, and a saturation relationship. The air-water model equations are the same as the two-phase model, where the non-wetting phase phase, i.e., air, is assumed to be compressible and the wetting phase, i.e., water, is assumed to be slightly compressible.
The mass balance equation for each of the α fluid phases is given by

$$\phi \frac{\partial\left(S_\alpha \rho_\alpha\right)}{\partial t} + div\mathbf{u}_\alpha = f_\alpha, \tag{5}$$

where ϕ is the porosity, S_α is the saturation of the α phase, ρ_α is the density of the α phase, and f_α is a source term.
Darcy's law for multi-phase flow is used to define the mass flux $\mathbf{u}_\alpha$ as

$$\mathbf{u}_\alpha = -\rho_\alpha K \frac{k_\alpha}{\mu_\alpha} \left(gradP_\alpha - \rho_\alpha G gradZ \right). \tag{6}$$

Here, K is the permeability tensor, k_α is the relative permeability, μ_α is the viscosity, P_α is the pressure of the α phase, G is gravity, and $Z = Z(x)$ is the depth of the reservoir. We will also use phase mobility $\lambda_\alpha = \rho_\alpha \frac{k_\alpha}{\mu_\alpha}$ and phase potential defined by

$$grad\Psi_\alpha = gradP_\alpha - \rho_\alpha G gradZ \tag{7}$$

so that the Darcy equation may be rewritten as

$$\mathbf{u}_\alpha = -K\lambda_\alpha grad\Psi_\alpha. \tag{8}$$

For the expanded mixed finite element method we consider a different formulation of Darcy's equation (8), by introducing the variable

$$\widetilde{\mathbf{u}}_\alpha = -grad\Psi_\alpha, \tag{9}$$

thus the Darcy equation rewrite as

$$\mathbf{u}_\alpha = K\lambda_\alpha \widetilde{\mathbf{u}}_\alpha. \tag{10}$$

The system is closed using the saturation and capillary pressure relationships. The saturation relationship is given as

$$S_w + S_a = 1. \tag{11}$$

Capillary pressure is the difference in pressure across the interface between the non-wetting (air) and wetting (water) phase fluids. This is a known function of saturation, so we have that

$$P_c\left(S_w\right) = P_a - P_w. \tag{12}$$

The water phase is assumed to be slightly compressible, so that his density is given by

$$\rho_w = \rho_{w,ref} \exp(\beta_w (P_w - P_{w,ref})), \tag{13}$$

where β_w is the compressibility constant for water and $\rho_{w,ref}$ is a reference water density, and $P_{w,ref}$ is a reference water pressure. The density for the air phase is given by the real gas law as

$$\rho_a = \frac{P_a M}{C(P_a) RT}, \tag{14}$$

where M is the molecular weight, R is the gas constant, T is the temperature, and $C(P_a)$, the compressibility factor, is a function of air pressure.
In general, the boundary conditions may be imposed on primary unknowns of the nonlinear system or on some other unknowns. Application may dictate what conditions are natural or useful. In particular, it may be more natural to impose conditions on Ψ_α than on P_α but we will consider the Dirichlet and Neumann conditions imposed on pressures and fluxes respectively

$$\begin{cases} P_\alpha = P_{\alpha,D} \text{ on } \Gamma^D, \\ \mathbf{u}_\alpha.\mathbf{n} = g_{\alpha,N} \text{ on } \Gamma^N, \end{cases} \tag{15}$$

where $\mathbf{n}$ is an outward pointing, unit, normal vector to Ω.
Finally, the initial condition of the reservoir needs to be defined. This can be done using an assumption of hydrostatic equilibrium or using *ad-hoc* values of primary unknowns. Here we will assume that the values of all phase pressures and saturations are known at the time zero.

3 Implementation

We describe the initialization procedure and the model discretization and include a description of the implicit temporal integration with the corresponding Jacobian contribution.

3.1 Variational Formulation

We consider the spaces

$$(W, V) = \left(L^2(\Omega), H(div, \Omega)\right) \tag{16}$$

as well as the space $\Lambda \subset H^{\frac{1}{2}}(\Gamma)$ or $\Lambda \subset L^2(\Gamma)$. The first two spaces provide test functions and pressure P_α and velocity $\mathbf{u}_\alpha$ variables, respectively, while the latter is used to define boundary values.

Let $\widetilde{V} = \left(L^2(\Omega)\right)^3$ denote the space of $\widetilde{\mathbf{u}}_\alpha$ which have all components in $L^2(\Omega)$. Furthermore, let $(.,.)$ denote the $L^2(\Omega)$ inner product, scalar and vector, and $\langle .,. \rangle$ denote the $L^2(\Gamma)$ inner product.
Using the spaces $W, \widetilde{V}, V, \Lambda$, we obtain the weak form of equations (5), (9) and (10). First we multiply equation (5) by a test function $w \in W$ and integrate over Ω as follow:

$$(\phi \frac{\partial (S_\alpha \rho_\alpha)}{\partial t}, w) + (div \mathbf{u}_\alpha, w) = (f_\alpha, w), \forall w \in W, \forall \alpha. \tag{17}$$

The weak form of equations (9) and (10) follows analogously except that the gradient of potential needs to be removed using integration by parts. We multiply the equations (9),(10) and the inflow on Γ_N by the test functions $\mathbf{v} \in V$, $\widetilde{\mathbf{v}} \in \widetilde{V}$, and $\mu \in \Lambda|_{\Gamma_N}$ respectively. We have

$$(\mathbf{u}_\alpha, \widetilde{\mathbf{v}}) = (K \lambda_\alpha \widetilde{\mathbf{u}}_\alpha, \widetilde{\mathbf{v}}), \forall \widetilde{\mathbf{v}} \in \widetilde{V}, \forall \alpha, \tag{18}$$

$$(\widetilde{\mathbf{u}}_\alpha, \mathbf{v}) = (\Psi_\alpha, div \mathbf{v}) - \langle \Psi_{\alpha,D}, \mathbf{v}.\mathbf{n} \rangle_{\Gamma_D} - \langle L_\alpha, \mathbf{v}.\mathbf{n} \rangle_{\Gamma_N}, \forall \mathbf{v} \in V, \forall \alpha. \tag{19}$$

$$\langle \mathbf{u}_\alpha.\mathbf{n}, \mu \rangle_{\Gamma_N} = \langle g_{\alpha,N}, \mu \rangle_{\Gamma_N}, \forall \mu \in \Lambda|_{\Gamma_N}, \forall \alpha. \tag{20}$$

The treatment of different boundary conditions is apparent through the last term in the above equation. If only no-flow boundary conditions are imposed then the boundary term is zero since $\mathbf{v}.\mathbf{n} = 0$. otherwise, while values of Ψ_α are defined directly or indirectly on Γ^D, they are replaced in the integral over Γ^N by Lagrange multipliers from the space Λ. An additional equation which guarantees the equality of fluxes with the prescribed Neumann data is imposed using test functions from Λ.

3.2 Initialization

The reservoir is initialized using hydrostatic equilibrium conditions for water pressure P_w, air pressure P_a, and water saturation S_w. The equilibrium condition for each phase α is

$$gradP_\alpha - \rho_\alpha G gradZ = 0. \tag{21}$$

The density functions make this equation nonlinear; thus, the root is found using Newton's method. The discrete version of equation (13), in the x coordinate direction, is

$$P_{\alpha,i+1,jk} - P_{\alpha,ijk} - G\frac{\rho_{\alpha,ijk} - \rho_{\alpha,i+1,jk}}{2}\left(Z_{i+1,jk} - Z_{ijk}\right) = 0, \tag{22}$$

where we use cell averages to evaluate the density.
Using the density of the water phase, we can get an expression for $\rho_{w,i+1,jk}$ in term of $\rho_{w,ijk}$ by noting that

$$\begin{aligned}
\rho_{w,i+1,jk} &= \rho_{w,ref}\exp\left(\beta_w\left(P_{w,i+1,jk} - P_{w,ref}\right)\right) \\
&= \rho_{w,ref}\exp\left(\beta_w\left(P_{w,i+1,jk} - P_{w,ijk} + P_{w,ijk} - P_{w,ref}\right)\right) \\
&= \rho_{w,ijk}\exp\left(\beta_w\Delta P_w\right),
\end{aligned} \tag{23}$$

where $\Delta P_w = P_{w,i+1,jk} - P_{w,ijk}$.
We can then formulate the discrete equation and hence the Newton function (14), as a function of the charge in water pressure ΔP_w:

$$F\left(\Delta P_w\right) = \Delta P_w - \frac{G}{2}\rho_{w,ijk}\left(1 + \exp\left(\beta_w\Delta P_w\right)\right)\left(Z_{i+1,jk} - Z_{ijk}\right). \tag{24}$$

Thus the Jacobian for the Newton iteration is

$$F'\left(\Delta P_w\right) = 1 - \frac{G}{2}\beta_w\rho_{w,ijk}\exp\left(\beta_w\Delta P_w\right)\Delta Z, \tag{25}$$

where $\Delta Z = Z_{i+1,jk} - Z_{ijk}$.
We obtain the initial guess for the Newton iteration by assuming that

$$\rho_{w,i+1,jk} = \rho_{w,ijk} + \frac{\partial\rho_w}{\partial P_w}|_{P_{w,ijk}}\left(P^0_{w,i+1,jk} - P_{w,ijk}\right) \tag{26}$$

so that, using equation (22), we have

$$\left(P^0_{w,i+1,jk} - P_{w,ijk}\right) = \frac{G}{2}\Delta Z\left(\rho_{w,ijk} + \rho_{w,ijk} + \beta_w\rho_{w,ijk}\left(P^0_{w,i+1,jk} - P_{w,ijk}\right)\right). \tag{27}$$

Thus we have that

$$\Delta P_w^0 = \frac{G}{2}\Delta Z\left(2\rho_{w,ijk} + \beta_w \rho_{w,ijk}\Delta P_w^0\right) \tag{28}$$

which gives

$$\Delta P_w^0 = \frac{G\Delta Z\rho_{w,ijk}}{1 - \frac{G}{2}\beta_w \rho_{w,ijk}\Delta Z} \tag{29}$$

as an initial guess for the equilibrium Newton iteration.
The next initialization is the calculation of the equilibrium pressure for the air phase. We can not get an expression for $\rho_{a,i,jk} + \rho_{a,i+1,jk}$ in terms of a pressure change ΔP_a. Thus our Newton function for the air equilibrium is

$$F\left(P_{a,i+1,jk}\right) = P_{a,i+1,jk} - P_{a,ijk} - \frac{G}{2}\left(\rho_{a,i,jk} + \rho_{a,i+1,jk}\right)\left(C_{i+1,jk} - C_{ijk}\right), \tag{30}$$

including the expression for air density gives

$$F\left(P_{a,i+1,jk}\right) = P_{a,i+1,jk} - P_{a,ijk} - \frac{G}{2}\Delta Z\frac{M}{RT}\left(\frac{P_{a,ijk}}{C_{ijk}} + \frac{P_{a,i+1,jk}}{C_{i+1,jk}}\right) \tag{31}$$

where, as before, $\Delta Z = Z_{i+1,jk} - Z_{ijk}$ and $C_{ijk} = C\left(P_{a,ijk}\right)$. Thus the Jacobian is

$$F'\left(P_{a,i+1,jk}\right) = 1 - \frac{G}{2}\Delta Z\frac{M}{RT}\left(\frac{P_{a,i+1,jk}}{C_{i+1,jk}}\right)' \tag{32}$$

and

$$\left(\frac{P_{a,i+1,jk}}{C_{i+1,jk}}\right)' = \frac{C_{i+1,jk} - P_{a,i+1,jk}C'_{i+1,jk}}{C_{i+1,jk}^2}. \tag{33}$$

The initial guess for $P_{a,i+1,jk}$ is obtained similarly to the Newton guess for $P_{w,i+1,jk}$, where now

$$P_{a,i+1,jk}^0 - P_{a,ijk} = \frac{G}{2}\Delta Z\frac{M}{RT}\left(\frac{P_{a,ijk}}{C_{ijk}} + \left(\frac{P_{a,ijk}}{C_{ijk}}\right)'\left(P_{a,i+1,jk}^0 - P_{a,ijk}\right)\right) \tag{34}$$

so that

$$\left(1-\frac{G}{2}\Delta Z\frac{M}{RT}\left(\frac{P_{a,ijk}}{C_{ijk}}\right)'\right)P^0_{a,i+1,jk}= P_{a,ijk}+\frac{G}{2}\Delta Z\frac{M}{RT}\left(\frac{P_{a,ijk}}{C_{ijk}}-\left(\frac{P_{a,ijk}}{C_{ijk}}\right)'P_{a,ijk}\right). \quad (35)$$

Hence

$$\left(1-\frac{G}{2}\Delta Z\frac{M}{RT}\left(\frac{P_{a,ijk}}{C_{ijk}}\right)'\right)P^0_{a,i+1,jk}= \left(1-\frac{G}{2}\Delta Z\frac{M}{RT}\left(\frac{P_{a,ijk}}{C_{ijk}}\right)'\right)P_{a,ijk}+\frac{G}{2}\Delta Z\frac{M}{RT}\frac{P_{a,ijk}}{C_{ijk}} \quad (36)$$

and the initial guess for the air phase equilibrium is

$$P^0_{a,i+1,jk}=P_{a,ijk}+\frac{\frac{G}{2}\Delta Z\rho_{a,ijk}}{1-\frac{G}{2}\Delta Z\frac{M}{RT}\left(\frac{P_{a,ijk}}{C_{ijk}}\right)'}. \quad (37)$$

3.3 Spatial and Temporal Discretization

3.3.1 The lowest order Raviart-Thomas mixed spaces

The model equations are discretized through the use of a cell-centered finite difference scheme which is equivalent to the expanded mixed finite element method of Arbogast, Wheeler and Yotov [2] where the approximation spaces are lowest order Raviart-Thomas spaces $(W_h, V_h) \subset (W, V)$ on a parallelepiped grid. This follows the procedure described in [9] and outlined bellow.
Let $\Im_h$ denote a quasi-uniform triangulation of Ω with mesh size h and consisting of rectangular solids in three dimensions.
The Raviart-Thomas-Nedelec (RTN) [3, 4] approximating space of order k on a rectangular element $E \in \Im_h$ is,

$$V_k(E) = Q_{k+1,k,k}(E) \times Q_{k,k+1,k}(E) \times Q_{k,k,k+1}(E), \quad (38)$$

where $Q_{r,s,t}$ is the space of polynomials de degree r in the x direction, s in the y direction and t in the z direction. Raviart and Thomas developed these spaces for two dimensions, and Nedelec for three dimensions. The space W is approximated by,

$$W_k(E) = Q_k(E). \tag{39}$$

For the finite difference scheme, we consider the lowest order RTN space, i.e. $k = 0$, on parallelepipeds,

$$V_h(E) = \left\{ \left(\xi_1 x_1 + \gamma_1, \xi_2 x_2 + \gamma_2, \xi_3 x_3 + \gamma_3\right)^T : \xi_i, \gamma_i \in \mathbb{R} \right\}, \tag{40}$$

$$W_h(E) = \left\{ \xi : \xi \in \mathbb{R} \right\}. \tag{41}$$

We also define a hybrid space, $\Lambda_h \subset L^2(\Gamma)$, of Lagrange multipliers for the pressure restricted to Γ and corresponding to the above RTN spaces [1, 8]. So, on a face e, we have the edge space,

$$\Lambda_h(e) = \left\{ \xi : \xi \in \mathbb{R} \right\}. \tag{42}$$

Finally, let $\widetilde{V}_h \subset \widetilde{V}$ denote the piecewise discontinuous version of V_h; that is, the space such that $V_h \subseteq \widetilde{V}_h$ and $\widetilde{V}_h|_E = V_h|_E$ for all elements $E \in \Im_h$, but with no constraint that the space be in V.
The functions in W_h are piecewise constant on each cell; a test function $\omega_{ijk} \in W_h$ is a characteristic function of the cell E_{ijk}. On the other hand, functions $\mathbf{v} \in V_h$ are linear in one coordinate direction and constant in the others. We will frequently use the function $\mathbf{v} = \mathbf{v}_{i+1/2,jk}$ which is linear in x direction and constant in y, z directions whose support is $E_{ijk} \cup E_{i+1,jk}$, and which has nodal value $\mathbf{v}_{i+1/2,jk} = 1$. The scalar unknowns pressures P_α, and saturations S_α, as well as the densities ρ_α, are interpreted as members of W_h. The vector unknowns velocities $\mathbf{u}_\alpha$ and $\widetilde{\mathbf{u}}_\alpha$ are interpreted as members of V_h.

3.3.2 Quadrature Rule and Spatial Discretization

We will approximate the L^2 inner product with various quadrature rules, denoting these approximations by $(.,.)_R$, where $R = M, T$ and TM are application of the midpoint, trapezoidal and midpoint by trapezoidal rules, respectively.

Midpoint Rule (M) We explicit the three-dimensional midpoint rule for two scalar functions $f, g : \mathbb{R}^3 \to \mathbb{R}$ by

$$(f, g)_M = \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} \sum_{k=1}^{N_z} f_{ijk} g_{ijk} \Delta x_i \Delta y_j \Delta z_k. \tag{43}$$

where $\Delta s_l = s_{l+1/2} - s_{l-1/2}; s = x, y, z; l = i, j, k$.

Trapezoidal Rule (T) The three-dimensional trapezoidal rule for a scalar function $f : \mathbb{R}^3 \to \mathbb{R}$ is given by

$$T(f) = \sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z}\frac{1}{8}\left(\sum_{l=i-1/2}^{i+1/2}\sum_{m=j-1/2}^{j+1/2}\sum_{n=k-1/2}^{k+1/2} f_{lmn}\right)\Delta x_i \Delta y_j \Delta z_k. \tag{44}$$

The trapezoidal quadrature rule for two vectorial functions $\mathbf{v}, \mathbf{q} : \mathbb{R}^3 \to \mathbb{R}^3$ can be written as,

$$(\mathbf{v}, \mathbf{q})_T = T(v^x q^x + v^y q^y + v^z q^z). \tag{45}$$

By changing the order of index in the trapezoidal rule (44), we obtain the expression of (45) as,

$$(\mathbf{v}, \mathbf{q})_T = Q(v^x q^x) + Q(v^y q^y) + Q(v^z q^z), \tag{46}$$

where

$$\begin{aligned} Q(v^x q^x) \;=\; & \sum_{i=0}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z}\frac{1}{4}(v^x_{i+1/2,j-1/2,k-1/2} q^x_{i+1/2,j-1/2,k-1/2} \\ & + v^x_{i+1/2,j-1/2,k+1/2} q^x_{i+1/2,j-1/2,k+1/2} \\ & + v^x_{i+1/2,j+1/2,k-1/2} q^x_{i+1/2,j+1/2,k-1/2} \\ & + v^x_{i+1/2,j+1/2,k+1/2} q^x_{i+1/2,j+1/2,k+1/2})\Delta x_{i+1/2}\Delta y_j \Delta z_k, \end{aligned} \tag{47}$$

$$\begin{aligned} Q(v^y q^y) \;=\; & \sum_{i=1}^{N_x}\sum_{j=0}^{N_y}\sum_{k=1}^{N_z}\frac{1}{4}(v^y_{i-1/2,j+1/2,k-1/2} q^y_{i-1/2,j+1/2,k-1/2} \\ & + v^y_{i-1/2,j+1/2,k+1/2} q^y_{i-1/2,j+1/2,k+1/2} \\ & + v^y_{i+1/2,j+1/2,k-1/2} q^y_{i+1/2,j+1/2,k-1/2} \\ & + v^y_{i+1/2,j+1/2,k+1/2} q^y_{i+1/2,j+1/2,k+1/2})\Delta x_i \Delta y_{j+1/2} \Delta z_k, \end{aligned} \tag{48}$$

$$\begin{aligned} Q(v^z q^z) \;=\; & \sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=0}^{N_z}\frac{1}{4}(v^z_{i-1/2,j-1/2,k+1/2} q^z_{i-1/2,j-1/2,k+1/2} \\ & + v^z_{i-1/2,j+1/2,k+1/2} q^z_{i-1/2,j+1/2,k+1/2} \\ & + v^z_{i+1/2,j-1/2,k+1/2} q^z_{i+1/2,j-1/2,k+1/2} \\ & + v^z_{i+1/2,j+1/2,k+1/2} q^z_{i+1/2,j+1/2,k+1/2})\Delta x_i \Delta y_j \Delta z_{k+1/2}. \end{aligned} \tag{49}$$

Trapezoidal Midpoint Rule (TM) We explicit the trapezoidal midpoint quadrature rule for two vectorial functions $\mathbf{v}, \mathbf{q} : \mathbb{R}^3 \to \mathbb{R}^3$ by

$$(\mathbf{v}, \mathbf{q})_{TM} = (v^x, q^x)_{T\times M\times M} + (v^y, q^y)_{M\times T\times M} + (v^z, q^z)_{M\times M\times T}, \tag{50}$$

that is, for $d = x, y, z$, the dth integral on the right side uses the trapezoidal rule in the d coordinate direction and the midpoint in the other coordinate directions. Thus,

$$(v^x, q^x)_{T\times M\times M} = \sum_{i=0}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z} v^x_{i+1/2jk} q^x_{i+1/2jk} \Delta x_{i+1/2}\Delta y_j \Delta z_k, \tag{51}$$

$$(v^y, q^y)_{M\times T\times M} = \sum_{i=1}^{N_x}\sum_{j=0}^{N_y}\sum_{k=1}^{N_z} v^y_{ij+1/2k} q^y_{ij+1/2k} \Delta x_i \Delta y_{j+1/2}\Delta z_k, \tag{52}$$

$$(v^x, q^x)_{M\times M\times T} = \sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=0}^{N_z} v^z_{ijk+1/2} q^z_{ijk+1/2} \Delta x_i \Delta y_j \Delta z_{k+1/2}. \tag{53}$$

Expanded Mixed Finite Element Method The expanded mixed finite element method simultaneously approximates, $\Psi_\alpha, \widetilde{\mathbf{u}}_\alpha$ and $\mathbf{u}_\alpha$. This method with quadrature is given as follows. Find $\Psi_{\alpha,h} \in W_h, \widetilde{\mathbf{u}}_{\alpha,h} \in \widetilde{V}_h$, $\mathbf{u}_{\alpha,h} \in V_h$ and $L_{\alpha,h} \in \Lambda_h|_{\Gamma_N}$ satisfying

$$\begin{cases} (\phi\frac{\partial(S_\alpha\rho_\alpha)}{\partial t}, w)_M + (div\mathbf{u}_{\alpha,h}, w) = (f_\alpha, w), \forall w \in W_h, \forall\alpha, \\ (\widetilde{\mathbf{u}}_{\alpha,h}, \mathbf{v})_{TM} = (\Psi_{\alpha,h}, div\mathbf{v}) - \langle \Psi_{\alpha,D}, \mathbf{v}.\mathbf{n}\rangle_{\Gamma_D} - \langle L_{\alpha,h}, \mathbf{v}.\mathbf{n}\rangle_{\Gamma_N}, \forall \mathbf{v} \in V_h, \forall\alpha, \\ (\mathbf{u}_{\alpha,h}, \widetilde{\mathbf{v}})_{TM} = (K\lambda_\alpha\widetilde{\mathbf{u}}_{\alpha,h}, \widetilde{\mathbf{v}})_T, \forall\widetilde{\mathbf{v}} \in \widetilde{V}_h, \forall\alpha, \\ \langle \mathbf{u}_{\alpha,h}.\mathbf{n}, \mu\rangle_{\Gamma_N} = \langle g_{\alpha,N}, \mu\rangle_{\Gamma_N}, \forall\mu \in \Lambda_h^N, \forall\alpha. \end{cases} \tag{54}$$

The system reduces to finite difference scheme for the hydraulic head approximations at each of the cell centers. To see this, consider first mass balance equation and let $w = w_{ijk} \in W_h$ to be the basis function,

$$w_{ijk} = \begin{cases} 1, \ \textit{in cell } E_{ijk}, \\ 0, \ \textit{otherwise.} \end{cases} \tag{55}$$

Then we obtain an equation of three terms; an accumulation term $\mathbf{A}_{\alpha,ijk}$, a transport term $\mathbf{T}_{\alpha,ijk}$, and source term $\mathbf{W}_{\alpha,ijk}$

$$\mathbf{A}_{\alpha,ijk} + \mathbf{T}_{\alpha,ijk} + \mathbf{W}_{\alpha,ijk} = 0, \forall \alpha. \tag{56}$$

The accumulation term is given as

$$\mathbf{A}_{\alpha,ijk} = \phi_{ijk}\Delta x_i \Delta y_j \Delta z_k \frac{\partial \left(S_\alpha \rho_\alpha\right)}{\partial t} = \Phi_{ijk} \frac{\partial \left(S_\alpha \rho_\alpha\right)}{\partial t}, \tag{57}$$

where $\Phi_{ijk} = \phi_{ijk}\Delta x_i \Delta y_j \Delta z_k$ is the pore volume of the cell. Note that if porosity is not changing as a function of time or pressure, then the pore volume is constant.
The transport term is given as

$$\mathbf{T}_{\alpha,ijk} = \left(div \mathbf{u}_\alpha, w_{ijk}\right) = \int_{E_{ijk}} div \mathbf{u}_\alpha dx. \tag{58}$$

For transport term we use the divergence theorem to obtain

$$\mathbf{T}_{\alpha,ijk} = \mathbf{T}^x_{\alpha,ijk} + \mathbf{T}^y_{\alpha,ijk} + \mathbf{T}^z_{\alpha,ijk}, \tag{59}$$

where $\mathbf{T}^x_{\alpha,ijk}$ is the transport term in the x direction

$$\begin{aligned} \mathbf{T}^x_{\alpha,ijk} &= \int_{\partial E_{i+1/2,jk}} \mathbf{u}_{\alpha,i+1/2,jk}.\mathbf{n} d\sigma + \int_{\partial E_{i-1/2,jk}} \mathbf{u}_{\alpha,i-1/2,jk}.\mathbf{n} d\sigma \\ &= \left(u^x_{\alpha,i+1/2,jk} - u^x_{\alpha,i-1/2,jk}\right) \Delta y_j \Delta z_k, \end{aligned} \tag{60}$$

The terms $\mathbf{T}^y_{\alpha,ijk}$ and $\mathbf{T}^z_{\alpha,ijk}$, in the y, z direction respectively, are computed similarly. Thus we have

$$\mathbf{T}^y_{\alpha,ijk} = \left(u^y_{\alpha,i,j+1/2,k} - u^y_{\alpha,i,j-1/2,k}\right) \Delta x_i \Delta z_k, \tag{61}$$

$$\mathbf{T}^z_{\alpha,ijk} = \left(u^z_{\alpha,ij,k+1/2} - u^z_{\alpha,ij,k-1/2}\right) \Delta x_i \Delta y_j. \tag{62}$$

The source term is given as

$$\mathbf{W}_{\alpha,ijk} = -\left(f_\alpha, w_{ijk}\right) = -f_{\alpha,ijk}\Delta x_i \Delta y_j \Delta z_k. \tag{63}$$

The second equation of the system (54) gives $\widetilde{\mathbf{u}}_{\alpha,h}$ in term of $\Psi_{\alpha,h}$; in particular, choosing $\mathbf{v} = \mathbf{v}_{i+1/2,jk} = \left(v^x_{i+1/2,jk}, v^y_{i+1/2,jk}, v^z_{i+1/2,jk}\right)$, where $\mathbf{v}_{i+1/2,jk}$ is the basis function associated with node $\left(x_{i+1/2}, y_j, z_k\right)$ over the *support* $(\mathbf{v}_{i+1/2,jk}) = E_{ijk} \cup E_{i+1,jk}$,

$$v^x_{i+1/2,jk} = \begin{cases} \frac{x - x_{i-1/2}}{\Delta x_i}, \ for\ (x,y,z) \in E_{ijk}, \\ \frac{x_{i+3/2} - x}{\Delta x_{i+1}}, \ for\ (x,y,z) \in E_{i+1,jk}, \\ 0, \ otherwise, \end{cases} \tag{64}$$

$$v^y_{i+1/2,jk} = v^z_{i+1/2,jk} = 0. \tag{65}$$

We evaluate the integral $\left(\widetilde{\mathbf{u}}_{\alpha,h}, \mathbf{v}_{i+1/2,jk}\right)_{TM}$ by using the trapezoidal midpoint quadrature rule (TM) and we have

$$\left(\widetilde{\mathbf{u}}_{\alpha,h}, \mathbf{v}_{i+1/2,jk}\right)_{TM} = \widetilde{u}^x_{\alpha,i+1/2,j,k} \Delta x_{i+1/2} \Delta y_j \Delta z_k. \tag{66}$$

The density ρ_α is a function of pressure P_α which is approximated by piecewise constant $P_{\alpha,h}$ and therefore over the *support* $(\mathbf{v}_{i+1/2,jk})$ the density values ρ_α as defined as

$$\rho_\alpha\left(P_{\alpha,h}\right) = \begin{cases} \rho_\alpha\left(P_{\alpha,ijk}\right) \ in\ E_{ijk}, \\ \rho_\alpha\left(P_{\alpha,i+1,jk}\right) \ in\ E_{i+1,jk}. \end{cases} \tag{67}$$

The discrete potential values $\Psi_{\alpha,h}$ can be defined as piecewise constants and over the *support* $(\mathbf{v}_{i+1/2,jk})$ they are given by

$$\Psi_{\alpha,h} = \begin{cases} P_{\alpha,ijk} - P_{\alpha,ref} - G \int\limits_{Z_{ref}}^{Z_{ijk}} \rho_\alpha dx \ in\ E_{ijk}, \\ P_{\alpha,i+1,jk} - P_{\alpha,ref} - G \int\limits_{Z_{ref}}^{Z_{i+1,jk}} \rho_\alpha dx \ in\ E_{i+1,jk}, \end{cases} \tag{68}$$

where Z_{ref}, P_{ref} are the reference depth and pressure at which potential is zero. Note that we can write the potential Ψ_α as,

$$\Psi_\alpha = P_\alpha - P_{\alpha,ref} - G \int\limits_{Z_{ref}}^{Z(x)} \rho_\alpha dx. \tag{69}$$

Now consider the following calculation

$$\begin{aligned}\left(\Psi_{\alpha,h}, div\mathbf{v}_{i+1/2,jk}\right) &= \left(P_{\alpha,h}, div\mathbf{v}_{i+1/2,jk}\right) - G(\int_{Z_{ref}}^{Z_{ijk}} \rho_\alpha dx, div\mathbf{v}_{i+1/2,jk})_{E_{ijk}} \\ &\quad - G(\int_{Z_{ref}}^{Z_{i+1,jk}} \rho_\alpha dx, div\mathbf{v}_{i+1/2,jk})_{E_{i+1,jk}} \\ &= \left(P_{\alpha,h}, div\mathbf{v}_{i+1/2,jk}\right) - G(\int_{Z_{ijk}}^{Z_{i+1,jk}} \rho_\alpha dx, \left|div\mathbf{v}_{i+1/2,jk}\right|)_{E_{ijk}\cup E_{i+1,jk}}. \quad (70)\end{aligned}$$

To evaluate the density integral we apply the trapezoidal rule to $\int_{Z_{ijk}}^{Z_{i+1,jk}} \rho_\alpha dx$ and we have

$$\left(\int_{Z_{ijk}}^{Z_{i+1,jk}} \rho_\alpha dx\right)_T = \frac{1}{2}\left(\rho_{\alpha,ijk} + \rho_{\alpha,i+1,jk}\right)\Delta Z. \quad (71)$$

Define $\rho_{\alpha,i+1/2,jk} = \frac{1}{2}\left(\rho_{\alpha,ijk} + \rho_{\alpha,i+1,jk}\right)$, which is the average value of ρ_α over the cells E_{ijk} and $E_{i+1,jk}$, the above calculation is then completed by

$$\left(\Psi_{\alpha,h}, div\mathbf{v}_{i+1/2,jk}\right) = \left(P_{\alpha,ijk} - P_{\alpha,i+1,jk}\right)\Delta y_j \Delta z_k - G\rho_{\alpha,i+1/2,jk}\Delta Z. \quad (72)$$

Thus the discrete schema of the second equation of (54) in the strict interior face, i.e., $\partial E_{i+1/2,jk} = E_{i+1,jk} \cap E_{ijk}$, can be written as,

$$\widetilde{u}^x_{\alpha,i+1/2,j,k}\Delta x_{i+1/2}\Delta y_j \Delta z_k = \left(P_{\alpha,ijk} - P_{\alpha,i+1,jk}\right)\Delta y_j \Delta z_k - G\rho_{\alpha,i+1/2,jk}\Delta Z. \quad (73)$$

Now we proceed to discuss the discretization of boundary terms. Since we assumed that the boundary conditions can be at most in one of Γ_D or Γ_N, we need to consider each of the cases separately. The integrals with $\widetilde{\mathbf{u}}_{\alpha,h}$ are computed using the trapezoidal rule in x and the midpoint rule in y, z directions, and we get
if $\left(x_{i+1/2}, y_j, z_k\right) \in \Gamma_D$:

$$\widetilde{u}^x_{\alpha,i+1/2,j,k}\left(\frac{1}{2}\Delta x_i\right)\Delta y_j\Delta z_k = \left(P_{\alpha,ijk} - P_{\alpha,D,i+1/2,jk}\right)\Delta y_j\Delta z_k - \frac{1}{2}G\rho_{\alpha,ijk}\Delta Z, \tag{74}$$

if $\left(x_{i+1/2}, y_j, z_k\right) \in \Gamma_N$:

$$\begin{cases} \widetilde{u}^x_{\alpha,i+1/2,j,k}\left(\frac{1}{2}\Delta x_i\right)\Delta y_j\Delta z_k = \left(P_{\alpha,ijk} - L_{\alpha,i+1/2,jk}\right)\Delta y_j\Delta z_k - \frac{1}{2}G\rho_{\alpha,ijk}\Delta Z, \\ \widetilde{u}^x_{\alpha,i+1/2,j,k}\Delta y_j\Delta z_k = g_{\alpha,N,i+1/2,jk}\Delta y_j\Delta z_k. \end{cases} \tag{75}$$

The discrete schema of the third equation of (54) need to account for the dependence of mobilities λ_α upon the pressures and saturations and for their possible degeneracy. The mobilities introduce a hyperbolic type nonlinearity which cannot be treated with symmetric differences.
First we evaluate $\left(\mathbf{u}_{\alpha,h}, \mathbf{v}_{i+1/2,jk}\right)_{TM}$ by using the quadrature rule (TM) and we have

$$\left(\mathbf{u}_{\alpha,h}, \mathbf{v}_{i+1/2,jk}\right)_{TM} = u^x_{\alpha,i+1/2,j,k}\Delta x_{i+1/2}\Delta y_j\Delta z_k. \tag{76}$$

Now we explicit the discrete schema of $\left(K\lambda_\alpha\widetilde{\mathbf{u}}_{\alpha,h}, \widetilde{\mathbf{v}}\right)_T$. We assume that the tensor K is symmetric and we have

$$K\widetilde{\mathbf{u}}_{\alpha,h} = \begin{bmatrix} K_{11}\widetilde{u}^x_{\alpha,h} + K_{12}\widetilde{u}^y_{\alpha,h} + K_{13}\widetilde{u}^z_{\alpha,h} \\ K_{12}\widetilde{u}^x_{\alpha,h} + K_{22}\widetilde{u}^y_{\alpha,h} + K_{23}\widetilde{u}^z_{\alpha,h} \\ K_{13}\widetilde{u}^x_{\alpha,h} + K_{23}\widetilde{u}^y_{\alpha,h} + K_{33}\widetilde{u}^z_{\alpha,h} \end{bmatrix} = \begin{bmatrix} \widetilde{U}^1_{\alpha,h} \\ \widetilde{U}^2_{\alpha,h} \\ \widetilde{U}^3_{\alpha,h} \end{bmatrix}. \tag{77}$$

Using the quadrature rule (T) we obtain

$$\left(K\lambda_\alpha\widetilde{\mathbf{u}}_{\alpha,h}, \mathbf{v}_{i+1/2,jk}\right)_T = \frac{1}{8}(\lambda_\alpha)_{i+1/2,jk}\sum_{l=1}^{N_x}\sum_{m=1}^{N_y}\sum_{n=1}^{N_z}\Delta x_l\Delta y_m\Delta z_n \left[\sum_{r=l-1/2,l+1/2} S^\alpha_{r,m\pm1/2,n\pm1/2}\right], \tag{78}$$

with

$$\begin{aligned} S^{\alpha}_{r,m\pm1/2,n\pm1/2} &= \widetilde{U}^{1}_{\alpha,h}(x_r, y_{m-1/2}, z_{n-1/2})v^{x}_{i+1/2,j,k}(x_r, y_{m-1/2}, z_{n-1/2}) \\ &\quad +\widetilde{U}^{1}_{\alpha,h}(x_r, y_{m-1/2}, z_{n+1/2})v^{x}_{i+1/2,j,k}(x_r, y_{m-1/2}, z_{n+1/2}) \\ &\quad +\widetilde{U}^{1}_{\alpha,h}(x_r, y_{m+1/2}, z_{n-1/2})v^{x}_{i+1/2,j,k}(x_r, y_{m+1/2}, z_{n-1/2}) \\ &\quad +\widetilde{U}^{1}_{\alpha,h}(x_r, y_{m+1/2}, z_{n+1/2})v^{x}_{i+1/2,j,k}(x_r, y_{m+1/2}, z_{n+1/2}). \end{aligned}$$

So we have

$$(K\lambda_{\alpha}\widetilde{\mathbf{u}}_{\alpha,h}, \mathbf{v}_{i+1/2,jk})_T = (S^{\alpha}_{i+1/2,j\pm1/2,k\pm1/2})_{|_{E_{ijk}}} + (S^{\alpha}_{i+1/2,j\pm1/2,k\pm1/2})_{|_{E_{i+1,jk}}}, \tag{79}$$

with

$$\begin{aligned} (S^{\alpha}_{i+1/2,j\pm1/2,k\pm1/2})_{|_{E_{ijk}}} &= \frac{1}{8}(\lambda_{\alpha})_{i+1/2,jk}\Delta x_i \Delta y_j \Delta z_k \\ &\quad \{\widetilde{U}^{1}_{\alpha,h_{|E_{ijk}}}(x_{i+1/2}, y_{j-1/2}, z_{k-1/2}) + \widetilde{U}^{1}_{\alpha,h_{|E_{ijk}}}(x_{i+1/2}, y_{j-1/2}, z_{k+1/2}) \\ &\quad + \widetilde{U}^{1}_{\alpha,h_{|E_{ijk}}}(x_{i+1/2}, y_{j+1/2}, z_{k-1/2})\widetilde{U}^{1}_{\alpha,h_{|E_{ijk}}}(x_{i+1/2}, y_{j+1/2}, z_{k+1/2})\}, \end{aligned} \tag{80}$$

$$\begin{aligned} (S^{\alpha}_{i+1/2,j\pm1/2,k\pm1/2})_{|_{E_{i+1,jk}}} &= \frac{1}{8}(\lambda_{\alpha})_{i+1/2,jk}\Delta x_{i+1} \Delta y_j \Delta z_k \\ &\quad \{\widetilde{U}^{1}_{\alpha,h_{|E_{i+1jk}}}(x_{i+1/2}, y_{j-1/2}, z_{k-1/2}) + \widetilde{U}^{1}_{\alpha,h_{|E_{i+1jk}}}(x_{i+1/2}, y_{j-1/2}, z_{k+1/2}) \\ &\quad + \widetilde{U}^{1}_{\alpha,h_{|E_{i+1jk}}}(x_{i+1/2}, y_{j+1/2}, z_{k-1/2}) + \widetilde{U}^{1}_{\alpha,h_{|E_{i+1jk}}}(x_{i+1/2}, y_{j+1/2}, z_{k+1/2})\}. \end{aligned} \tag{81}$$

and

$$\begin{aligned} \widetilde{U}^{1}_{\alpha,h_{|E_{ijk}}}(x_{i+1/2}, y_{j\pm1/2}, z_{k\pm1/2}) &= K_{11,i+1/2,j\pm1/2,k\pm1/2}\widetilde{u}^{x}_{\alpha,i+1/2,jk} \\ &\quad + K_{12,i+1/2,j\pm1/2,k\pm1/2}\widetilde{u}^{y}_{\alpha,i,j\pm1/2,k} + K_{13,i+1/2,j\pm1/2,k\pm1/2}\widetilde{u}^{z}_{\alpha,ij,k\pm1/2}, \end{aligned} \tag{82}$$

$$\begin{aligned} \widetilde{U}^{1}_{\alpha,h_{|E_{i+1jk}}}(x_{i+1/2}, y_{j\pm1/2}, z_{k\pm1/2}) &= K_{11,i+1/2,j\pm1/2,k\pm1/2}\widetilde{u}^{x}_{\alpha,i+1/2,jk} \\ &\quad + K_{12,i+1/2,j\pm1/2,k\pm1/2}\widetilde{u}^{y}_{\alpha,i+1,j\pm1/2,k} + K_{13,i+1/2,j\pm1/2,k\pm1/2}\widetilde{u}^{z}_{\alpha,i+1,j,k\pm1/2}. \end{aligned} \tag{83}$$

We obtain the discrete schema of the third equation of (54) can be written as

$$u^x_{\alpha,i+1/2,j,k}\Delta x_{i+1/2} = \frac{1}{8}(\lambda_\alpha)_{i+1/2,jk}[(K_{11,i+1/2,j-1/2,k-1/2} + K_{11,i+1/2,j-1/2,k+1/2} + K_{11,i+1/2,j+1/2,k-1/2} + K_{11,i+1/2,j+1/2,k+1/2})(\Delta x_i \widetilde{u}^x_{\alpha,i+1/2,jk} + \Delta x_{i+1}\widetilde{u}^x_{\alpha,i+1/2,jk}) + (K_{12,i+1/2,j-1/2,k-1/2}+K_{12,i+1/2,j-1/2,k+1/2})(\Delta x_i \widetilde{u}^y_{\alpha,i,j-1/2,k}+\Delta x_{i+1}\widetilde{u}^y_{\alpha,i+1,j-1/2,k}) + (K_{12,i+1/2,j+1/2,k-1/2}+K_{12,i+1/2,j+1/2,k+1/2})(\Delta x_i \widetilde{u}^y_{\alpha,i,j+1/2,k}+\Delta x_{i+1}\widetilde{u}^y_{\alpha,i+1,j+1/2,k}) + (K_{13,i+1/2,j-1/2,k-1/2}+K_{13,i+1/2,j+1/2,k-1/2})(\Delta x_i \widetilde{u}^z_{\alpha,ij,k-1/2}+\Delta x_{i+1}\widetilde{u}^z_{\alpha,i+1,j,k-1/2}) + (K_{13,i+1/2,j-1/2,k+1/2}+K_{13,i+1/2,j+1/2,k+1/2})(\Delta x_i \widetilde{u}^z_{\alpha,i,j,k+1/2}+\Delta x_{i+1}\widetilde{u}^z_{\alpha,i+1,j,k+1/2})]. \tag{84}$$

For stability we use upwinding, which is also known as one-point upstream weighting. We define the discrete mobility as

$$\lambda_{\alpha,sjk} = \frac{1}{\mu_\alpha} k_\alpha\left(S_{w,sjk}\right)\rho_\alpha\left(P_{\alpha,sjk}\right), \tag{85}$$

with the s in sjk found by upwinding

$$s = \begin{cases} i & if\ P_{\alpha,ijk} \geq P_{\alpha,i+1,jk} \\ i+1 & if\ otherwise \end{cases} \tag{86}$$

Note that the velocities and mobilities are similarly defined for the y and z directions.

3.3.3 Temporal Discretization and Nonlinear Equation Solver

Let $0 = t^0 < t^1 < ... < t^N = T$ be a given sequence of time steps, $\Delta t^n = t^n - t^{n-1}$, $\Delta t = \max_n \Delta t^n$, and for $S = S\left(.,t\right)$, let $S^n = S\left(.,t^n\right)$. The model is advanced in time using the backward Euler method for implicit temporal integration. The air-water model would be to use an IMPES (IMplicit Pressure, Explicit Saturation) scheme to advance in time.
The backward Euler method applied to our system gives

$$\phi\frac{S^{n+1}_\alpha\rho^{n+1}_\alpha - S^n_\alpha\rho^n_\alpha}{\Delta t^{n+1}} - div\mathbf{u}^{n+1}_\alpha = f^{n+1}_\alpha, \forall\alpha. \tag{87}$$

Thus at each time step we solve a nonlinear, residual problem given as

$$\mathbf{R}^{n+1}_{\alpha,ijk} = \mathbf{A}^{n+1}_{\alpha,ijk} + \mathbf{T}^{n+1}_{\alpha,ijk} + \mathbf{W}^{n+1}_{\alpha,ijk} = 0, \forall\alpha. \tag{88}$$

The Jacobian is formulated by differentiating each of these terms with respects to the primary unknowns water pressure P_w and water saturation S_w. In order to make calculations easier, the mobilities are normalized by the appropriate reference density when they are computed. Thus the Jacobian contributions from each of $\mathbf{A}, \mathbf{T}$, and $\mathbf{W}$ must be normalized.
These nonlinear equations are solved with a backtracking line search globalized inexact Newton's method 10. Algorithm 3.1 describes an inexact Newton method applied to the problem of finding a root to the nonlinear equation $F(\mathbf{x}) = 0$ where $\mathbf{J} = DF(\mathbf{x})$ is the Jacobian of F.

Algorithm 3.1 *1. Let* $\mathbf{x}^{(0)}$ *be the initial guess.*

2. For $k = 0, 1, 2, ...$ *until convergence, do*

(a) Choose $\eta^{(k)} \in [0, 1)$.

(b) Using some Krylov iterative method, compute a vector $\delta^{(k)}$ *satisfying* $\mathbf{J}^{(k)}\delta^{(k)} = -F^{(k)} + r^{(k)}$ *, with* $\frac{\|r^{(k)}\|}{\|F(\mathbf{x}^{(k)})\|} \leqslant \eta^{(k)}$.

(c) Set $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \xi^{(k)}\delta^{(k)}$.

The parameter η is chosen with a dynamic selection criteria, which reflects the agreement between F and its linear model at the previous iteration,

$$\eta^{(k)} = \frac{\left|\left\|F^{(k)}\right\| - \left\|F^{(k-1)} + \mathbf{J}^{(k-1)}\delta^{(k-1)}\right\|\right|}{\|F^{(k-1)}\|}. \tag{89}$$

The parameter ξ is chosen with a backtracking line-search globalization technique.

3.4 Jacobian Contribution

The transport contribution are evaluated at the half-points, separately each of the coordinate directions. Jacobian transport contributions are calculated for each of the water and air equations by taking derivatives, with respect to each of the primary unknowns, of the discretized flow equation

$$F_\alpha = \lambda_{\alpha,sjk}\left(P_{\alpha,ijk} - P_{\alpha,i+1,jk} - G\rho_{\alpha,i+1/2,jk}\left(Z_{i+1,jk} - Z_{ijk}\right)\right). \tag{90}$$

The mobility terms are upwinded, i.e., if $P_{\alpha,ijk} - P_{\alpha,i+1,jk} \geqslant 0$ then the mobility is evaluated at the ijk point; otherwise, it is evaluated at the $i-1, jk$ point. If the mobility is evaluated at the ijk point then the Jacobian contributions for the water equation with the respect to water pressure are

$$\frac{\partial F_w}{\partial P_{w,ijk}} = \frac{\partial \lambda_{w,ijk}}{\partial P_{w,ijk}} \left(P_{w,ijk} - P_{w,i+1,jk} - G\rho_{w,i+1/2,jk} \left(Z_{i+1,jk} - Z_{ijk} \right) \right) + \lambda_{w,ijk} \left(1 - \frac{G}{2} \beta_w \rho_{w,ijk} \left(Z_{i+1,jk} - Z_{ijk} \right) \right),$$

and

$$\frac{\partial F_w}{\partial P_{w,i+1jk}} = \lambda_{w,ijk} \left(-1 - \frac{G}{2} \beta_w \rho_{w,i+1,jk} \left(Z_{i+1,jk} - Z_{ijk} \right) \right). \tag{91}$$

The Jacobian transport contribution for the water equation with respect to water saturation is, for mobility upwinded at the ijk cell,

$$\frac{\partial F_w}{\partial S_{w,ijk}} = \frac{\partial \lambda_{w,ijk}}{\partial S_{w,ijk}} \left(P_{w,ijk} - P_{w,i+1,jk} - G\rho_{w,i+1/2,jk} \left(Z_{i+1,jk} - Z_{ijk} \right) \right), \tag{92}$$

and

$$\frac{\partial F_w}{\partial S_{w,i+1,jk}} = 0. \tag{93}$$

The transport contributions are calculated similarly for each of the y, z directions, depending on the location of the boundary. The mobilities are still upwinded as in the interior. When calculating the $x+$ contribution, the upwinding criterion is the difference in

$$P_{\alpha,i+1,jk} - P_{\alpha,ijk}, \tag{94}$$

whereas for $x-$ the criterion is

$$P_{\alpha,ijk} - P_{\alpha,i-1jk}. \tag{95}$$

The fluxes across the boundary are also computed and added to the total mass balance.

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