

Comparison of Numerical Formulations for Two-phase Flow in Porous Media

B. Ataie-Ashtiani · D. Raeesi-Ardekani

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Abstract Numerical approximation based on different forms of the governing partial differential equation can lead to significantly different results for two-phase flow in porous media. Selecting the proper primary variables is a critical step in efficiently modeling the highly nonlinear problem of multiphase subsurface flow. A comparison of various forms of numerical approximations for two-phase flow equations is performed in this work. Three forms of equations including the pressure-based, mixed pressure–saturation and modified pressure–saturation are examined. Each of these three highly nonlinear formulations is approximated using finite difference method and is linearized using both Picard and Newton–Raphson linearization approaches. Model simulations for several test cases demonstrate that pressure based form provides better results compared to the pressure–saturation approach in terms of CPU_time and the number of iterations. The modification of pressure–saturation approach improves accuracy of the results. Also it is shown that the Newton–Raphson linearization approach performed better in comparison to the Picard iteration

linearization approach with the exception for in the pressure–saturation form.

Keywords Two-phase flow · Numerical model · Primary variables · Newton–Raphson · Picard

1 Introduction

Even with the continual progress made in both computational algorithms and computer hardware, numerical simulation of multiphase subsurface flow remains a challenging task. Flow of two or three-phase fluids in the subsurface results in a highly nonlinear, difficult problem and in general extensive computational resources are needed. In the past few decades, modeling multiphase flow through porous media has received increasing attention because of its importance in the areas of underground natural resource recovery, waste storage, soil physics, and environmental remediation (Wu and Forsyth 2001).

Despite of the significant progress since the late 1950s (Peaceman and Rachford 1955), modeling the coupled processes of multiphase fluid flow in a heterogeneous porous medium remains a conceptual and mathematical challenge (Ataie-Ashtiani et al. 2001, 2002). The difficulty stems from the nature of the inherent nonlinearity and poorly determined

B. Ataie-Ashtiani (✉) · D. Raeesi-Ardekani
Department of Civil Engineering, Sharif University
of Technology, P.O. Box 11365-9313, Tehran, Iran
e-mail: ataie@sharif.edu

D. Raeesi-Ardekani
e-mail: raeesi_damoon@alum.sharif.edu

constitutive relations for multiphase flow, as well as the computational requirements for a field application.

In recent years soil and groundwater contamination by nonaqueous phase liquids (NAPL), such as contaminants from oil and gasoline leakage, or other organic chemicals, has received increasing attention. The NAPL-related environmental concern has motivated research activities in developing and applying multiphase flow and transport models for assessing NAPL contamination and the associated clean up operations. These liquids are generally hazardous, demanding costly and time-consuming precautions to be taken when performing controlled laboratory experiments. However, there are rare studies based on the experimental simulation of spreading of NAPL (Pantazidou et al. 2000; Ataie-Ashtiani et al. 2003). Numerical modeling can be used as an effective tool in the design of such experiments and can be used to perform sensitivity and uncertainty analyses which would otherwise be difficult to carry out (Kueper and Frind 1991a, b).

As a result, many numerical models and computational algorithms have been developed and improved for solving multiphase fluid flow and organic-chemical transport problems in the vadose zone, porous, and fractured media (Abriola and Pinder 1985a, b; Faust 1985; Osborne and Sykes 1986; Forsyth 1988; Kaluarachchi and Parker 1989, Shodja and Feldkamp 1993; Kueper and Frind 1991a, b; Abriola and Rathfelder 1993, Forsyth et al. 1995). Numerical modeling approaches have become standard techniques in investigating subsurface NAPL contamination and implementing remediation measures.

In general, the numerical techniques used for modeling multiphase subsurface flow consist of (1) spatial discretization of mass conservation equations using finite-difference or finite-element schemes; (2) fully implicit time discretization; (3) iterative approaches, such as the Newton iteration, to solve nonlinear, discrete algebraic equations (Kees and Miller 2002).

The previous studies of modeling multiphase flow through porous media (Forsyth et al. 1998) have identified that choice of the primary variables for a Newton iteration has a significant impact on computational performance of a multiphase model. However, little investigation has been carried out regarding the general strategy and selection of

primary variables in modeling multiphase flow and transport processes (Wu and Forsyth 2001).

This paper presents a one dimensional finite difference model using the pressure-based (PP) formulation, a mixed pressure–saturation (PS) formulation and pressure–saturation modified (PSM) formulation. Each of these three highly nonlinear formulations is linearized using both Picard and Newton–Raphson linearization approaches. To the authors' knowledge a comprehensive study, comparing the performance of the combination of all of these methods have not been reported. As various forms of formulations and coding can be applied, we are providing the details of our numerical formulations in this work.

The objectives of this work are (1) to outline a set of formulations for two-phase flow problems; (2) to present a comparative analysis and general recommendations for selecting primary variables in simulating two phase flow; (3) to conduct a series of comparative studies of Picard and Newton–Raphson iteration schemes, and (4) to provide a numerical code that includes all forms of formulations and all different form of boundary conditions for two phase flow.

2 The Mathematical Model

2.1 Governing Equations

A two-phase flow system in a porous media is treated here with averaged properties of the fluid, even though each of the two phases may have contained several components. For simplicity, we consider the case of incompressible fluids and no sink and source. The general form of the two-fluid flow equations is described by the two-fluid, volume-averaged momentum (Darcy velocity) and continuity equations (Bear 1979):

$$q_\alpha = -\frac{kk_{r\alpha}}{\mu_\alpha}(\nabla P_\alpha - \rho_\alpha g \nabla z) \quad (1)$$

$$\frac{\partial(\phi \rho_\alpha S_\alpha)}{\partial t} + \nabla(\rho_\alpha q_\alpha) = 0 \quad (2)$$

where $\alpha = w, nw$ represent the fluid phases (w water, nw nonwetting phase), t is time [T], ϕ is the

dimensionless porosity, S_α is the degree of fluid saturation relative to the porosity ϕ (volumetric fluid content $\theta_\alpha = \phi S_\alpha$), P_α is α -fluid pressure [M/LT^2], ρ_α is the α -fluid density [M/L^3], z is the positive downward vertical direction, q_α is the flux density vector [L/T]; g is the gravitational acceleration vector, μ_α is viscosity [M/LT], $K_\alpha = k_{r\alpha}k$ is the effective permeability tensor [L^2], where k is the intrinsic permeability [L^2] and $k_{r\alpha} = k_{r\alpha}(S_\alpha)$ is the relative permeability.

The substitution of Eq. 1 into Eq. 2 yields the conventional form of the fluid phase mass balance equations for a two-phase flow system, as follows:

$$\frac{\partial(\phi\rho_\alpha S_\alpha)}{\partial t} + \nabla \cdot \left[-\frac{\rho_\alpha k_\alpha}{\mu_\alpha} (\nabla P_\alpha - \rho_\alpha g \nabla z) \right] = 0 \quad (3)$$

$\alpha = w, nw$

Assuming one-dimensional vertical flow and incompressible fluid, Eq. 3 can be rearranged as:

$$\frac{\partial(\phi S_\alpha)}{\partial t} = \frac{\partial}{\partial z} \left[\frac{k_{r\alpha}k}{\mu_\alpha} \left(\frac{\partial P_\alpha}{\partial z} - \rho_\alpha g \right) \right] \quad \alpha = w, nw \quad (4)$$

Auxiliary relations include:

1. Assuming that the porous media is non-deformable implies continuity of fluid saturations and pore volume.

$$S_w + S_{nw} = 1 \text{ or } \theta_w + \theta_{nw} = 1 \quad (5)$$

2. Capillary pressure–saturation relationships represent:

$$P_c = P_{nw} - P_w = f(S_e) \quad (6)$$

$$S_e = \frac{S_w - S_{rw}}{1 - S_{rw} - S_{rmw}} \quad (7)$$

P_c is the capillary pressure between the non-wetting (NAPL or air) and wetting phases (water), S_{rw} and S_{rmw} is the irreducible wetting and non-wetting saturation, S_e is the effective water saturation.

3. Relative permeability–saturation relationships,

$$k_{rx} = f(S_w) \quad (8)$$

$$k_{rmw} = f(S_w) \quad (9)$$

Assumptions in this two-phase immiscible flow formulation include negligible interphase mass transfer, and ignoring hysteresis and organic liquid entrapment, a unique functional relations for $P_c(S_w)$ and $k_{r\alpha}(S_w)$ is considered.

The mass balance equations for the phases wetting and non-wetting can be written in terms of pressure and transmissibility, or pressure head and hydraulic conductivity of fluids as given in Table 1. In Table 1 ρ_{ow} is density of water at standard pressure and temperature, K_α is the hydraulic conductivity of fluid, λ_α is transmissibility (or mobility) of fluid.

Parameter estimation requires the functional description of the capillary pressure–saturation, $P_c(S_w)$, and permeability functions, $k_{rw}(S_w)$, $k_{rmw}(S_w)$. The constitutive relationships considered below are listed in Table 2.

2.2 Temporal Discretization

There are many choices of numerical methods, with temporal discretization being a topic of great interest in the literature. In hydrologic applications the predominant approach has been to employ fully implicit time stepping and adopted by many authors (Abriola and Pinder 1985a, b; Abriola 1989; Faust 1985; Forsyth 1988). Implicit solvers provide solutions five to ten times faster than explicit solvers (Haverkamp et al. 1977; Abriola and Rathfelder

Table 1 Different formulation of two-phase flow based on definition of hydraulic conductivity and mobility

References	Parameters	Formulation
Chen et al. (1999) Parker et al. (1987)	$h_\alpha = \frac{P_\alpha}{\rho_\alpha g}, \theta_\alpha$ $K_\alpha = \frac{k_\alpha \rho_\alpha g}{\mu_\alpha}$ $\alpha = w, nw$	$\frac{\partial(\theta_\alpha)}{\partial t} = \frac{\partial}{\partial z} \left[K_\alpha \left(\frac{\partial h_\alpha}{\partial z} - \frac{\rho_\alpha}{\rho_w} \right) \right]$
Abriola and Rathfelder (1993)	P_α, S_α $\lambda_\alpha = \frac{k_\alpha}{\mu_\alpha}, \gamma_\alpha = \rho_\alpha g$ $\alpha = w, nw$	$\frac{\partial(\phi S_\alpha)}{\partial t} = \frac{\partial}{\partial z} \left[\lambda_\alpha \left(\frac{\partial P_\alpha}{\partial z} - \gamma_\alpha \right) \right]$

Table 2 Two-fluid capillary pressure head and permeability models (Chen et al. 1999)

References	Parameters	Capillary pressure function	Permeability function
VGM (Van Genuchten–Mualem 1980–1976)	S_{rw}, S_{rmw} α, n	$S_e = 1/(1 + \alpha P_c ^n)^m$	$m = 1 - 1/n$ $k_{rw} = S_e^{0.5} [1 - (1 - S_e^{1/m})^m]^2$
BCM (Brooks and Corey–Mualem 1964–1976)	S_{rw}, S_{rmw} P_d, λ	$S_e = (P_c/P_d)^{-\lambda}$	$k_{rmw} = (1 - S_e)^{0.5} [1 - S_e^{1/m}]^{2m}$ $k_{rw} = S_e^{2/\lambda+3}$
Touma and Vauclin (1986)	θ_{rw}, h_c A_w, B_w, A_a, B_a	$\theta_e = 1/(1 + \alpha h_c ^n)^m$ $\theta_e = \frac{\theta_w - \theta_{wr}}{\theta_{ws} - \theta_{rw}}$	$k_{rmw} = (1 - S_e)^2 (1 - S_e^{2/\lambda+1})$ $k_{rw} = A_w \theta_w^{B_w}$
Parker et al. (1987)	S_{rw}, S_{rmw} P_d, n	$S_e = [1 + (P_c/P_d)^n]^{-m}$	$k_{rmw} = A_a / (A_a + h_c ^{B_a})$ $k_{rw} = S_e^{0.5} [1 - (1 - S_e^{1/m})^m]^2$ $k_{rmw} = (1 - S_e)^{0.5} [1 - S_e^{1/m}]^{2m}$

1993). The better performance of the implicit solvers occurs, despite the need for iterations to deal with nonlinearities (Binning and Celia 1999).

2.3 Nonlinear Solver

2.3.1 Treatment of Nonlinearities by Picard Methods

The Picard method is one of the commonly used schemes to solve a set of nonlinear ordinary differential equations by a suitable finite difference approximation. A distinct advantage of the Picard iteration scheme is its simplicity and lower computational effort per iteration than more sophisticated schemes (Kaluarachchi and Parker 1989).

2.3.2 Treatment of Nonlinearities by Newton–Raphson Methods

The Newton–Raphson method is often recommended for highly nonlinear problems for which the picard scheme may fail or provide slow convergence (Huyakorn and Pinder 1983). The Newton–Raphson

iteration is based upon the choice of the discrete spatial approximation. In general, each finite difference approximation has the form $R_j(X) = 0$, where X is the vector of discrete nodal unknowns (the pressure head or the saturation).

A Taylor series expansion which maintains only the zero and first order derivatives can be written as: $R_j(X^{n+1,m+1}) = R_j(X^{n+1,m}) - \frac{\partial R_j}{\partial X_i} \approx 0$.

3 Simultaneous Solution Formulations and Numerical Models Discretization

In the following section, the numerical approximations used in the program for integrating the three forms of two-fluid-phase equations are given. The numerical discretization of these three partial differential equations implementation by finite difference method and linearized using the Picard and Newton–Raphson iterative schemes leads to a nonlinear set of equations of the following two forms of pressure–saturation and pressure-based formulation, respectively. Table 3 lists these methods according to their abbreviations.

Table 3 Specification of symbols for six numerical formulations of two phase flow

Abbreviation	Primary variables and iteration schemes for numerical modeling
PSP	Pressure–Saturation formulation and Picard iteration
PSN	Pressure–Saturation formulation and Newton–Raphson iteration
PSMP	Pressure–Saturation Modified formulation and Picard iteration
PSMN	Pressure–Saturation Modified formulation and Newton–Raphson iteration
PPP	Pressure–Pressure formulation and Picard iteration
PPN	Pressure–Pressure formulation and Newton–Raphson iteration

$$\begin{cases} A_{w_j}^{n+1,m} \delta S_{w_{j-1}}^{n+1,m+1} + B_{w_j}^{n+1,m} \delta P_{w_{j+1}}^{n+1,m+1} + C_{w_j}^{n+1,m} \delta S_{w_j}^{n+1,m+1} \\ + D_{w_j}^{n+1,m} \delta P_{w_j}^{n+1,m+1} + E_{w_j}^{n+1,m} \delta S_{w_{j+1}}^{n+1,m+1} + F_{w_j}^{n+1,m} \delta P_{w_{j+1}}^{n+1,m+1} = R_{w_j}^{n+1} \\ A_{nw_j}^{n+1,m} \delta S_{w_{j-1}}^{n+1,m+1} + B_{nw_j}^{n+1,m} \delta P_{w_{j+1}}^{n+1,m+1} + C_{nw_j}^{n+1,m} \delta S_{w_j}^{n+1,m+1} \\ + D_{nw_j}^{n+1,m} \delta P_{w_j}^{n+1,m+1} + E_{nw_j}^{n+1,m} \delta S_{w_{j+1}}^{n+1,m+1} + F_{nw_j}^{n+1,m} \delta P_{w_{j+1}}^{n+1,m+1} = R_{nw_j}^{n+1} \end{cases} \quad (10)$$

$$\begin{cases} A_{w_j}^{n+1,m} \delta P_{nw_{j-1}}^{n+1,m+1} + B_{w_j}^{n+1,m} \delta P_{w_{j+1}}^{n+1,m+1} + C_{w_j}^{n+1,m} \delta P_{nw_j}^{n+1,m+1} \\ + D_{w_j}^{n+1,m} \delta P_{w_j}^{n+1,m+1} + E_{w_j}^{n+1,m} \delta P_{nw_{j+1}}^{n+1,m+1} + F_{w_j}^{n+1,m} \delta P_{w_{j+1}}^{n+1,m+1} = R_{w_j}^{n+1} \\ A_{nw_j}^{n+1,m} \delta P_{nw_{j-1}}^{n+1,m+1} + B_{nw_j}^{n+1,m} \delta P_{w_{j+1}}^{n+1,m+1} + C_{nw_j}^{n+1,m} \delta P_{nw_j}^{n+1,m+1} \\ + D_{nw_j}^{n+1,m} \delta P_{w_j}^{n+1,m+1} + E_{nw_j}^{n+1,m} \delta P_{nw_{j+1}}^{n+1,m+1} + F_{nw_j}^{n+1,m} \delta P_{w_{j+1}}^{n+1,m+1} = R_{nw_j}^{n+1} \end{cases} \quad (11)$$

where $\delta S_w^{n+1,m+1} = S_w^{n+1,m+1} - S_w^{n+1,m}$ and $\delta P_\alpha^{n+1,m+1} = P_\alpha^{n+1,m+1} - P_\alpha^{n+1,m}$, $\alpha = w, nw$ are the iterative increment and A, B, C, D, E, F , and R are the coefficient that are derived based on the form of discretization method and are defined in the next section. The detail of derivation of six different schemes is provided in “Appendices A, B and C”. By solving Eqs. 10 or 11, the required corrections of the variables are found and pressures and saturations are updated. Iterations continue until iterative increments are sufficiently small. A maximum difference convergence criterion is used:

$$\begin{aligned} \max \frac{P_\alpha^{n+1,m+1} - P_\alpha^{n+1,m}}{P_\alpha^{n+1,m+1}} &\leq \epsilon_p, \\ \max \frac{S_w^{n+1,m+1} - S_w^{n+1,m}}{S_w^{n+1,m+1}} &\leq \epsilon_s \end{aligned} \quad (12)$$

3.1 Pressure–Saturation Formulations

It is possible to formulate the governing equations in terms of saturation and one of the phase pressures. Considering pressure and saturation of one phase as the primary variables is suitable for the problems

with phase disappearance. If the saturation in one of the phases is zero, the pressure in that phase is poorly defined and standard two-pressure formulation will not be able to handle this problem. The pressure–saturation formulation has been applied by Faust (1985), Kueper and Frind (1991a, b), Moridies and Reddell (1991), and Pruess (1987).

While other sets of primary variables are possible, we restrict ourselves to a $P_w - S_w$ formulation with the pressure of the wetting phase P_w and the saturation of the wetting phase S_w as unknowns. With the substitution $S_{nw} = 1 - S_w$ and $P_{nw} = P_c + P_w$, we obtain the coupled pressure–saturation formulation for incompressible two-phase flow equations:

$$\begin{aligned} f(P_w, S_w) &= \begin{cases} \frac{\phi}{\Delta t} \frac{\partial S_w}{\partial t} + \frac{\partial}{\partial z} \left[-\lambda_w \left(\frac{\partial P_w}{\partial z} - \rho_w g \right) \right] = 0 \\ -\frac{\phi}{\Delta t} \frac{\partial S_w}{\partial t} + \frac{\partial}{\partial z} \left[-\lambda_{nw} \left(\frac{\partial P_w}{\partial z} + \frac{\partial P_c}{\partial z} - \rho_{nw} g \right) \right] = 0 \end{cases} \end{aligned} \quad (13)$$

The finite difference method employed in this model is:

$$\begin{cases} \phi \frac{S_{w_j}^{n+1} - S_{w_j}^n}{\Delta t} - \frac{\lambda_{w_{j+\frac{1}{2}}}^{n+1} \frac{P_{w_{j+1}}^{n+1} - P_{w_j}^{n+1}}{\Delta z} - \lambda_{w_{j-\frac{1}{2}}}^{n+1} \frac{P_{w_j}^{n+1} - P_{w_{j-1}}^{n+1}}{\Delta z}}{\Delta z} + \rho_w g \frac{\lambda_{w_{j+\frac{1}{2}}}^{n+1} - \lambda_{w_{j-\frac{1}{2}}}^{n+1}}{\Delta z} = 0 \\ -\phi \frac{S_{w_j}^{n+1} - S_{w_j}^n}{\Delta t} - \frac{\lambda_{nw_{j+\frac{1}{2}}}^{n+1} \frac{P_{w_{j+1}}^{n+1} - P_{w_j}^{n+1}}{\Delta z} - \lambda_{nw_{j-\frac{1}{2}}}^{n+1} \frac{P_{w_j}^{n+1} - P_{w_{j-1}}^{n+1}}{\Delta z}}{\Delta z} \\ + \frac{\lambda_{nw_{j+\frac{1}{2}}}^{n+1} \frac{P_{c_{j+1}}^{n+1} - P_{c_j}^{n+1}}{\Delta z} - \lambda_{nw_{j-\frac{1}{2}}}^{n+1} \frac{P_{c_j}^{n+1} - P_{c_{j-1}}^{n+1}}{\Delta z}}{\Delta z} + \rho_{nw} g \frac{\lambda_{nw_{j+\frac{1}{2}}}^{n+1} - \lambda_{nw_{j-\frac{1}{2}}}^{n+1}}{\Delta z} = 0 \end{cases} \quad (14)$$

where Δt is the backward difference operator in time and Δz is the uniform spacing of block j in the discretized space domain. The interblock transmissibility terms can be evaluated as the arithmetic mean, the harmonic mean, the geometric mean and the upstream method.

To denote iteration level the index ‘ m ’ is used, and terms dated at time level ‘ $n + 1$ ’ are double indexed such that ‘ $n + 1, m$ ’ indicates evaluations at the last known iteration solution, and ‘ $n + 1, m + 1$ ’ indicates the unknown quantity for which a solution is desired. Using this notation, the linearized form of the Eq. 14 is:

approach has been adopted by a number of authors including: Pinder and Abriola (1986), who employed a finite difference approximation of the governing equations to describe non-aqueous phase liquid flow in the saturated zone; Sleep and Sykes (1989), and Kaluarachchi and Parker (1989), who used a finite-element solver with a Newton–Raphson scheme to linearize the equations; Celia and Binning (1992), who employed a finite element discretization with fully implicit time stepping and Picard iteration to solve the air and water flow equations.

The pressure–pressure formulation recasts the phase mass balance Eq. 13 in terms of the selected

$$\left\{ \begin{aligned} f_w(S_w^{n+1}, P_w^{n+1})^{m+1} &= \varphi \frac{S_w^{n+1,m+1} - S_w^n}{\Delta t} - \frac{\lambda_{w,j+\frac{1}{2}}^{n+1,m} \frac{P_w^{n+1,m+1} - P_w^{n+1,m+1}}{\Delta z} - \lambda_{w,j-\frac{1}{2}}^{n+1,m} \frac{P_w^{n+1,m+1} - P_w^{n+1,m+1}}{\Delta z}}{\Delta z} \\ &+ \rho_w g \frac{\lambda_{w,j+\frac{1}{2}}^{n+1,m} - \lambda_{w,j-\frac{1}{2}}^{n+1,m}}{\Delta z} = 0 \\ f_{nw}(S_w^{n+1}, P_w^{n+1})^{m+1} &= -\varphi \frac{S_w^{n+1,m+1} - S_w^n}{\Delta t} - \frac{\lambda_{nw,j+\frac{1}{2}}^{n+1,m} \frac{P_w^{n+1,m+1} - P_w^{n+1,m+1}}{\Delta z} - \lambda_{nw,j-\frac{1}{2}}^{n+1,m} \frac{P_w^{n+1,m+1} - P_w^{n+1,m+1}}{\Delta z}}{\Delta z} \\ &+ \frac{\lambda_{nw,j+\frac{1}{2}}^{n+1,m} \frac{P_{c,j+1}^{n+1,m} - P_{c,j}^{n+1,m}}{\Delta z} - \lambda_{nw,j-\frac{1}{2}}^{n+1,m} \frac{P_{c,j}^{n+1,m} - P_{c,j-1}^{n+1,m}}{\Delta z}}{\Delta z} + \rho_{nw} g \frac{\lambda_{nw,j+\frac{1}{2}}^{n+1,m} - \lambda_{nw,j-\frac{1}{2}}^{n+1,m}}{\Delta z} = 0 \end{aligned} \right. \quad (15)$$

3.2 Pressure–Saturation-modified Formulation

Many formulations substitute $\frac{dP_c}{dS_w} \text{grad} S_w$ for $\text{grad} P_c$ (Morgan et al. 1984). The resulting system of equations differs from Eq. 13 with respect to the second equation which is then

$$-\varphi \frac{\partial S_w}{\partial t} = \frac{\partial}{\partial z} \left[\lambda_{nw} \left(\frac{\partial P_w}{\partial z} + \frac{dP_c}{dS_w} \frac{\partial S_w}{\partial z} - \gamma_{nw} \right) \right] \quad (16)$$

3.3 Pressure–Pressure Formulations

The pressure–pressure formulation has been widely used in the hydrologic literature approach. In this approach the governing equations are written in terms of the pressures in each of the two phases through a straightforward substitution of Darcy’s equation into the mass balance equations for each phase. This

primary dependent variables, fluid pressures. With defining the α -fluid capillary capacity coefficient and expanding the accumulation derivatives in terms of capillary pressure, Eq. 13 can be rearranged as:

$$\left\{ \begin{aligned} \varphi c_w \left(\frac{\partial P_{nw}}{\partial t} - \frac{\partial P_w}{\partial t} \right) &= \frac{\partial}{\partial z} \left[\lambda_w \left(\frac{\partial P_w}{\partial z} - \gamma_\alpha \right) \right] \\ -\varphi c_w \left(\frac{\partial P_{nw}}{\partial t} - \frac{\partial P_w}{\partial t} \right) &= \frac{\partial}{\partial z} \left[\lambda_{nw} \left(\frac{\partial P_{nw}}{\partial z} - \gamma_{nw} \right) \right] \end{aligned} \right. \quad (17)$$

The coefficients for the six methods of numerical formulations are summarized in Table 4.

4 Boundary Conditions

The governing equations are commonly subject to two types of boundary conditions. The first type or

Table 4 The coefficients for six methods of numerical formulations

PSN	PSMP	PSMN	PPP	PPN
$\frac{d\lambda_w}{dS_w}, \frac{d\lambda_{nw}}{dS_w}$	$\frac{dP_c}{dS_w}$	$\frac{d\lambda_w}{dS_w}, \frac{d\lambda_{nw}}{dS_w}, \frac{dP_c}{dS_w}, \frac{d^2P_c}{dS_w^2}$	$\frac{dS_w}{dP_c}$	$\frac{d\lambda_w}{dP_c}, \frac{d\lambda_{nw}}{dP_c}, \frac{dS_w}{dP_c}, \frac{d^2S_w}{dP_c^2}$
$\frac{dP_c}{dP_w} = -1 \frac{dP_c}{dP_{mv}} = 1$				

Dirichlet, type boundary condition along the inflow or outflow, is of the form

$$S_\alpha = f_1 \text{ or } P_\alpha = f_2 \quad t > 0 \quad \alpha = w, nw \quad (18)$$

where f_1, f_2 is a prescribed value or function of the dependent variables saturation or pressure along the boundary. The second type or Neumann type boundary condition requires that

$$q_\alpha = f_3 \quad t > 0 \quad \alpha = w, nw \quad (19)$$

To complete the mathematical formulation, an initial condition must also be given for each dependent variable:

$$S_\alpha = S_\alpha^0, P_\alpha = P_\alpha^0 \quad t = 0 \quad \alpha = w, nw \quad (20)$$

where S_α^0, P_α^0 is a prescribed value of the dependent variable saturation and pressure. The formulation presented in this study requires that the top boundary Conditions (18) and (19) be described in terms of various parameters specified in the Table 5.

By considering the similarity of some types of boundary conditions, five different boundary conditions can be considered.

Table 5 Nine types of boundary condition for two phase flow simulation

Types	S_w^{top}	S_{nw}^{top}	P_w^{top}	P_{nw}^{top}	q_w^{top}	q_{nw}^{top}	q_r^{top}
1	X			X			
2		X	X				
3	X					X	
4		X			X		
5	X						X
6			X	X			
7			X			X	
8				X	X		
9					X	X	

$$\begin{cases} \varphi \frac{\partial S_w}{\partial t} = -\frac{\partial q_w}{\partial z} = -\frac{q_{w\frac{3}{2}} - q_w^{\text{top}}}{\Delta z} \\ \varphi \frac{\partial S_{nw}}{\partial t} = -\frac{\partial q_{nw}}{\partial z} = -\frac{q_{nw\frac{3}{2}} - q_{nw}^{\text{top}}}{\Delta z} \end{cases} \quad (21a, b)$$

$$\begin{cases} q_w^{\text{top}} = -\lambda_{w\frac{1}{2}}^{n+1} \frac{P_w^{n+1} - \lambda_w^{\text{top}, n+1}}{\Delta z} + \rho_w g \lambda_{w\frac{1}{2}}^{n+1} \\ q_{nw}^{\text{top}} = -\lambda_{nw\frac{1}{2}}^{n+1} \frac{P_w^{n+1} + P_{c1}^{n+1} - P_{nw}^{\text{top}, n+1}}{\Delta z} + \rho_{nw} g \lambda_{nw\frac{1}{2}}^{n+1} \end{cases} \quad (22a, b)$$

$$\begin{cases} f_{w_1}(S_w^{n+1}, P_w^{n+1})^m = \varphi \frac{S_{w_1}^{n+1} - S_{w_1}^n}{\Delta t} \\ -\frac{\lambda_{w\frac{3}{2}}^{n+1} \frac{P_w^{n+1} - P_w^{n+1}}{\Delta z}}{\Delta z} + \rho_w g \frac{\lambda_{w\frac{3}{2}}^{n+1}}{\Delta z} - \frac{q_w^{\text{top}}}{\Delta z} = 0 \\ f_{nw_1}(S_w^{n+1}, P_w^{n+1})^m = -\varphi \frac{S_{w_1}^{n+1} - S_{w_1}^n}{\Delta t} \\ -\frac{\lambda_{nw\frac{3}{2}}^{n+1} \frac{P_w^{n+1} - P_w^{n+1}}{\Delta z} + \lambda_{nw\frac{3}{2}}^{n+1} \frac{P_{c2}^{n+1} - P_{c1}^{n+1}}{\Delta z}}{\Delta z} \\ + \rho_{nw} g \frac{\lambda_{nw\frac{3}{2}}^{n+1}}{\Delta z} - \frac{q_{nw}^{\text{top}}}{\Delta z} = 0 \end{cases} \quad (23a, b)$$

Using iterative increment equations it is possible to put Eq. 23a,b in the form of Eq. 10 where:

$$C_{w_1}^{n+1, m} = \frac{\varphi}{\Delta t}; \quad F_{w_1}^{n+1, m} = -\frac{\lambda_{w\frac{3}{2}}^{n+1, m}}{\Delta z^2} \quad (24a, b)$$

$$R_{w_1}^{n+1, m} = -f_{w_1}(S_w^{n+1}, P_w^{n+1})^m \quad (24c)$$

$$C_{nw_1}^{n+1, m} = -\frac{\varphi}{\Delta t}; \quad F_{nw_1}^{n+1, m} = -\frac{\lambda_{nw\frac{3}{2}}^{n+1, m}}{\Delta z^2} \quad (25a, b)$$

$$R_{nw_1}^{n+1, m} = -f_{nw_1}(S_w^{n+1}, P_w^{n+1})^m \quad (25c)$$

Depending on boundary condition the coefficients of $D_{w_1}^{n+1, m}, D_{nw_1}^{n+1, m}, f_{w_1}^{n+1, m}, f_{nw_1}^{n+1, m}$ are defined based on the following flowchart and the other coefficients of Eq. 10 are zero (Figs. 1, 2).

5 Time Step Control

Stability, accuracy and computational efficiency considerations require that a dynamic time stepping control be included in the simulator. The value of a given time step is based on how much the solution has changed over the last time step. In the present model the time steps increases if the iterations are less than a specific value, and decreases if the

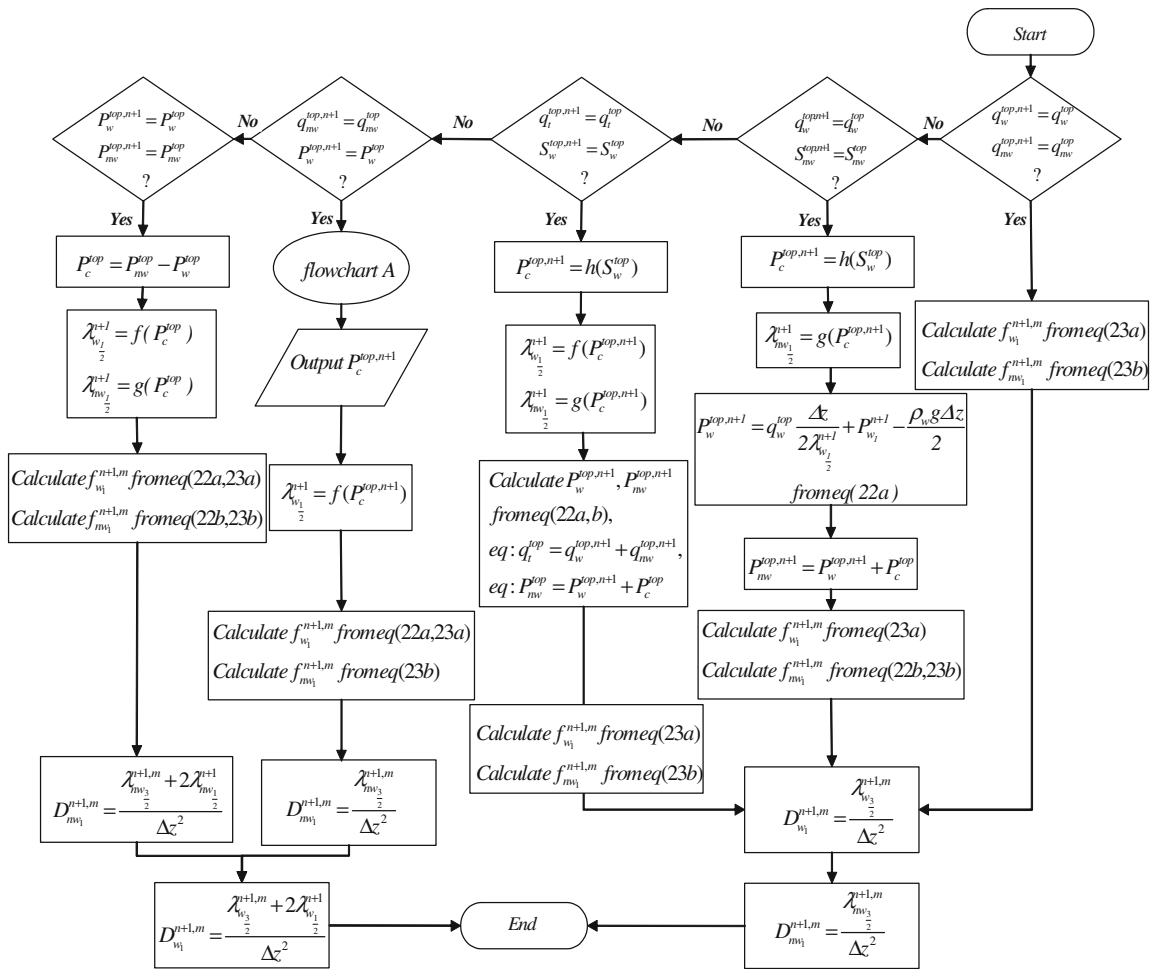


Fig. 1 Flow chart of solving boundary conditions, selecting pressure–saturation as primary variables

solution does not converge after a specific number of iterations.

6 Linear Equations System Solver

To solve linear Eqs. 10 and 11, matrix (a), Gauss elimination method was applied. Using this method, it can be observed that for the even and odd steps, the method should only be used for the elements defined in matrix (b) and matrix (c), respectively (Fig. 3).

7 Mass Balance Calculations

In recent years, the importance of using mass conservative numerical scheme has been recognized and implemented in the groundwater literature (e.g.

Celia et al. 1990; Huyakorn et al. 1994; Forsyth et al. 1995). It should be point out that a mass conservative solution may not guarantee the accuracy of the solution. Mass conservation is a necessary but not sufficient condition for convergence (Celia et al. 1990). A cumulative mass balance error was calculated using

$$\% \text{ cumulative error } (t) = 100 \left| 1.0 - \frac{M_\alpha^t - M_\alpha^0}{\sum_{\Delta t} q_\alpha^{\Delta t}} \right| \tag{26}$$

where M_α^t is the α -fluid mass storage at time t , M_α^0 is the initial mass storage at time zero, and $q_\alpha^{\Delta t}$ is the net α -fluid mass entering the computation domain during the time step Δt .

Figure 4 shows the logical flowchart of solving the two-phase flow model.

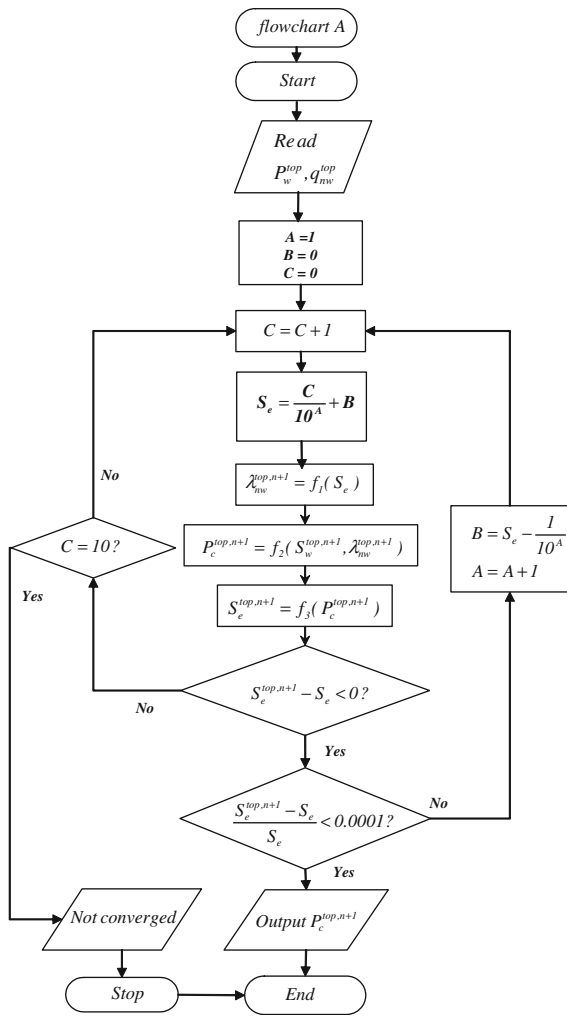
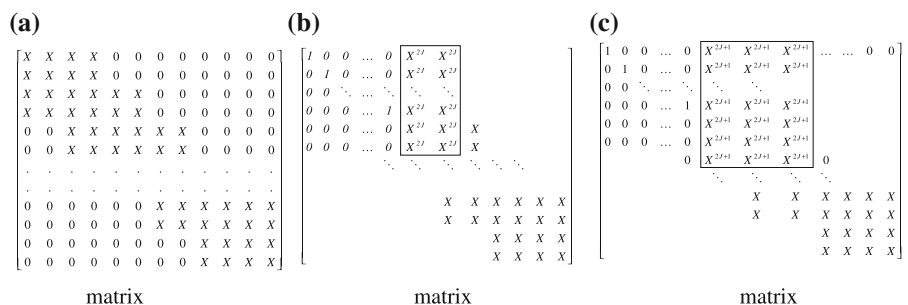


Fig. 2 Flow chart A

8 Model Verification

The algorithms presented above have been used to solve a variety of one-dimensional, two-phase flow

Fig. 3 Gauss elimination method for the matrix of coefficients



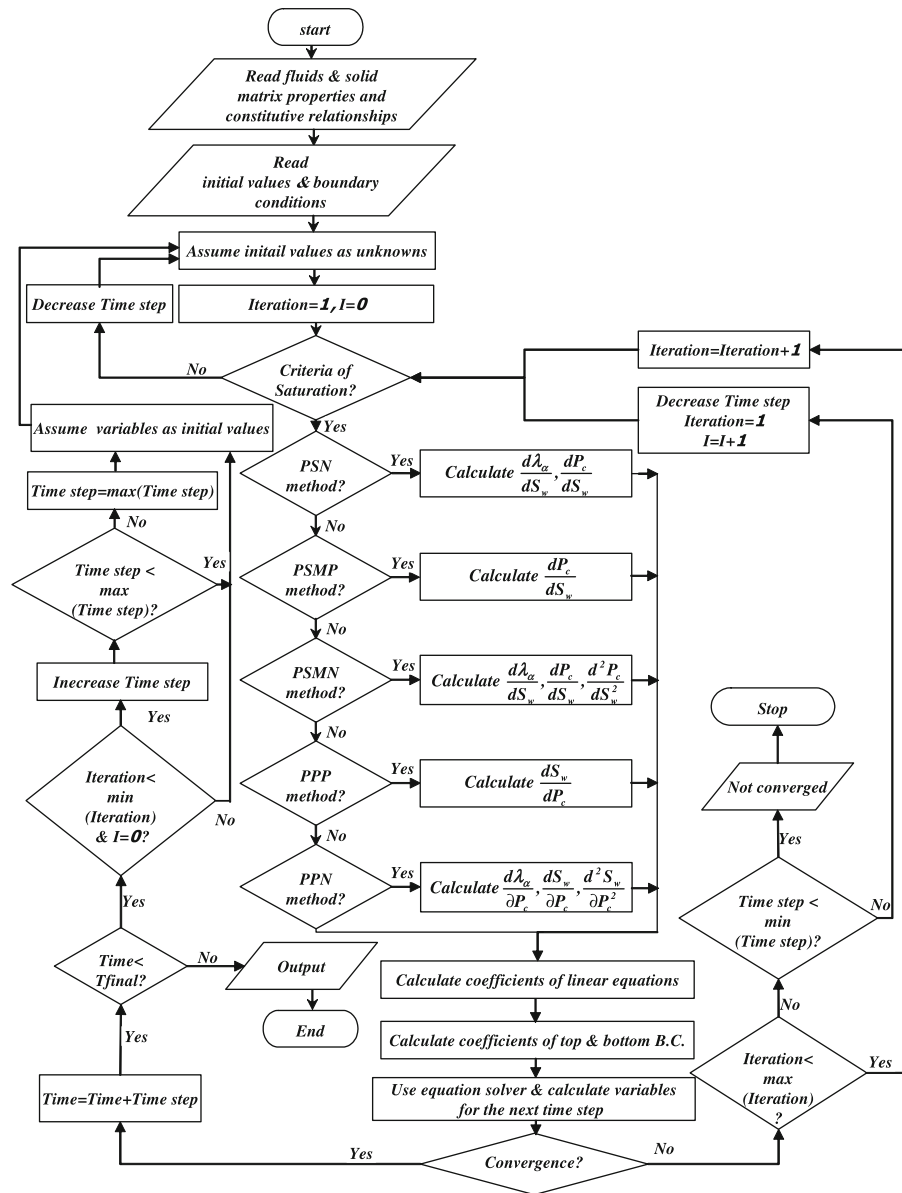
problems. Results are presented in this section to verify the developed model, to compare the numerical performance of algorithms to others reported in the literature, and to examine certain physical phenomena of interest. Two known solutions to the two-phase flow equations are available for this task, namely the Buckley and Leverett (1942) solution of the flow without capillary effects and the exact integral solution derived by McWhorter and Sunada (1990).

In order to evaluate the performances of the 6 different formulations available by the present code, five test cases are presented. In the first and third test cases, the infiltration results of water into an oil saturated soil, respectively, for both Buckley–Leverett and McWhorter problems, are presented. In the second and fourth test cases, the infiltration results of NAPL into a water saturated soil, respectively, with Brooks–Corey and van Genuchten models are presented. In the fifth test case, flow in the unsaturated subsurface region that is often modeled as a two-fluid-phase system, although usually with the simplified Richards’ equation model, are evaluated.

8.1 Test Case 1 (Two-phase Flow Without Capillary Pressure Effects—Buckley–Leverett Problem)

The analytical solution of Buckley and Leverett (1942), which describes the instationary displacement of oil by water, is a standard method for the verification of multiphase flow processes without capillary pressure effects. Figure 5 shows the numerical solutions in comparison to the analytical solution of saturation distribution S_w of the infiltrating water phase after a period of 1,500 days with the following parameters (Tables 6, 7):

Fig. 4 Flow chart of numerical algorithm of solving two phase fluid in porous media



8.2 Test Case 2 (Two-phase Flow with Capillary Pressure Effects—McWhorter Problem)

Model verification is carried out by comparison to an analytical solution, based on one by McWhorter and Sunada (1990), which differs from the Buckley–Leverett solution in that it fully incorporates the effect of capillarity. The physical Scenario used here for model verification involves a one dimensional, horizontal column of a non deforming porous medium initially completely saturated by an incompressible wetting fluid. Figure 6 illustrates the agreement

between the numerical model and analytical solution for the distribution of fluid saturations in the column at various times for all six methods. As is evident, the agreement is excellent at all times. Sand and fluid properties, and simulation parameters are shown in following tables (Tables 8, 9).

8.3 Test Case 3 (Initially NAPL Saturated—McWhorter Problem)

The physical Scenario used here for model verification involves a one dimensional, horizontal column of

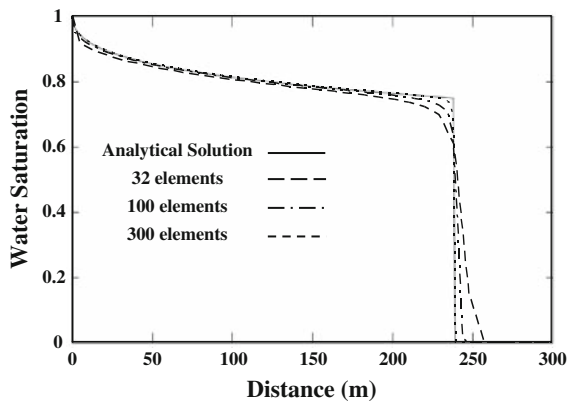


Fig. 5 Numerical solution of the Buckley-Leverett problem

Table 6 Sand and fluid properties of test case

Property	Units	Value
Permeability, k	$[m^2]$	10^{-7}
Porosity, ϕ	$[-]$	0.2
Capillary pressure, P_c	[Pa]	0.0
Pore size distribution, λ	$[-]$	2.0
Residual saturation, $S_{rz}, \alpha = w, nw$	$[-]$	0.0
Viscosity $\mu_{\alpha}, \alpha = w, nw$	[Pa.s]	0.001
Density $\rho_{\alpha}, \alpha = w, nw$	$[kg/m^3]$	1,000

Table 7 Boundary and initial condition of test case 1

Boundary condition	Units	Value
Boundary $x = 0$ m		
Water saturation S_w	$[-]$	1.0
Oil pressure P_{nw}	[Pa]	2×10^5
Boundary $x=300$ m		
Water saturation S_w	$[-]$	0.0
Flow rate of oil Q_{nw}	[m/s]	3×10^{-4}
Initial condition		
Water saturation S_w	$[-]$	0.0
Oil pressure P_{nw}	[Pa]	2×10^5

initially completely NAPL saturated by an incompressible non wetting fluid (Fig. 7; Tables 10, 11).

8.4 Test Case 4 (McWhorter Problem with van-Genuchten Fitting Parameters)

Comparisons were made for 1-D unidirectional displacement of water by trichloroethane in Borden Sand. The closed form solutions requires a decaying organic influx given by $q_{nw}(0, t) = A/\sqrt{t}$ where

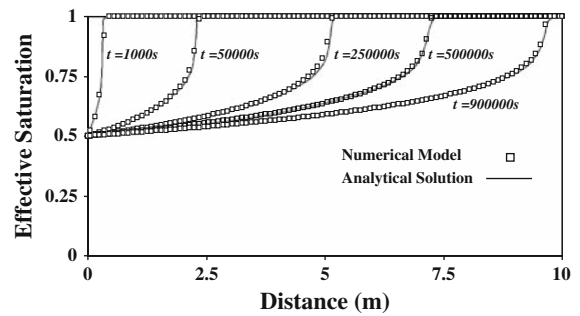


Fig. 6 Comparison between numerical and analytical results for fluid distribution within column

Table 8 Sand and fluid properties of test case 2

Property	Units	Sand
Permeability, k	$[m^2]$	5.0×10^{-11}
Porosity, ϕ	$[-]$	0.35
Entry pressure P_d	[Pa]	2,000.0
Pore size distribution, λ	$[-]$	2.0
Residual saturation, S_r	$[-]$	0.05
Nonwetting viscosity μ_{nw}	[Pa.s]	0.5×10^{-3}
Wetting viscosity μ_w	[Pa.s]	1×10^{-3}

Table 9 Boundary and initial condition of test case 2

Boundary condition		
Boundary $x = 0$ m		
Water saturation S_w	$[-]$	0.525
Flow rate of q_w	[m/s]	0.0
Boundary $x = 10$ m		
Water saturation S_w	$[-]$	1.0
Oil pressure P_{nw}	[Pa]	0.0
Initial condition		
Water saturation S_w	$[-]$	1.0
Oil pressure P_{nw}	[Pa]	0.0

q_{nw} is the organic injection rate, and A is a constant associated with the steady boundary saturation $S_o = S_w(0, t)$. For all numerical model comparisons S_o was prescribed as 0.5 and the associated value of A was 0.017187 (Fig. 8; Table 12).

8.5 Test Case 5 (Two-phase Flow of Air–Water Problem of Touma and Vauclin (1986))

In hydrology, boundary conditions are frequently specified in each phase separately. A common

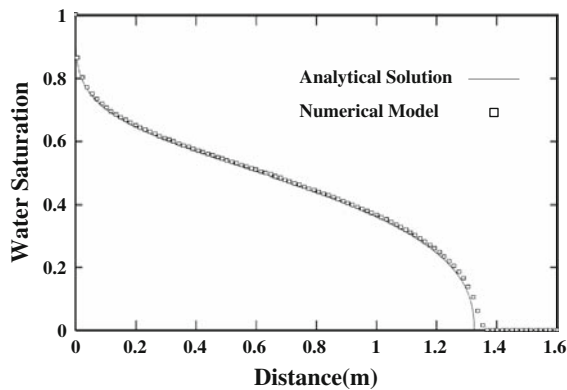


Fig. 7 Comparison between numerical and analytical results for Initially NAPL saturated problem

Table 10 Sand and fluid properties for test case 3

Property	Units	Value
Permeability, k	[m ²]	10 ⁻¹⁰
Porosity, ϕ	[-]	0.3
Entry pressure P_d	[Pa]	5,000.0
Pore size distribution, λ	[-]	2.0
Residual saturation, $S_{r2}, \alpha = w, nw$	[-]	0.0
Viscosity $\mu_{\alpha}, \alpha = w, nw$	[Pa.s]	0.001
Density $\rho_{\alpha}, \alpha = w, nw$	[kg/m ³]	1,000

Table 11 Boundary and initial condition for test case 3

Boundary condition	Unit	Value
Boundary $x = 0$ m		
Water saturation S_w	[-]	1.0
Oil pressure P_{nw}	[Pa]	2×10^5
Boundary $x = 1.6$ m		
Water saturation S_w	[-]	0.0
Flow rate of oil Q_{mw}	[m/s]	0.0
Initial condition		
Water saturation S_w	[-]	0.0
Oil pressure P_{nw}	[Pa]	2×10^5

problem specifies a flux in the water phase and a pressure in the air phase. For the present example, a column of soil is considered with a normalized initial saturation of 0.1655. The boundary conditions for the problem are that the water flux is fixed at 8.3 cm/h and the air pressure equal to 0 cm water at the soil surface. The air pressure is set to be 0.1204 cm and the water pressure -99.8796 cm at the bottom of the soil column. The air boundary conditions are chosen

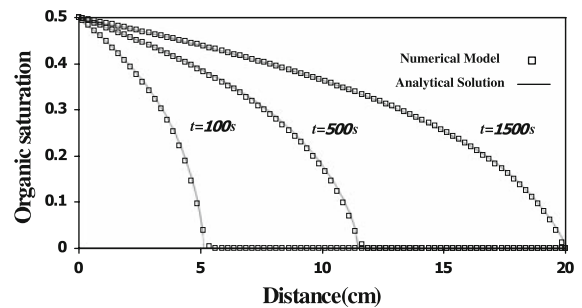


Fig. 8 Comparisons of analytical and numerical solutions for 1-D unidirectional water displacement problem at time 100, 500 and 1,500 s

Table 12 Soil and fluid parameters used in simulations for test case 4

Property	Units	Value
Permeability, k	[cm ²]	8.36×10^{-8}
Porosity, ϕ	[-]	0.33
van Genuchten α fitting parameters	[Pa ⁻¹]	5.2×10^{-4}
Pore size distribution, n	[-]	5.62
Residual saturation, S_r	[-]	0.204
Non wetting viscosity μ_{mw}	[Poise]	0.00119
Wetting viscosity μ_w	[Poise]	0.001

Table 13 Soil and fluid parameters used in simulations for test case 5

Property	Units	Value
Touma parameters A_w	[-]	18,130
Touma parameters B_w	[-]	6.07
Touma parameters A_a	[-]	3.86×10^{-5}
Touma parameters B_a	[-]	-2.4
Touma parameters K_{ws}	[cm/h]	18,130
Touma parameters K_{mws}	[cm/h]	2,800
Porosity, ϕ	[-]	0.37
van Genuchten α fitting parameters	[cm ⁻¹]	0.044
Pore size distribution, n	[-]	2.2
Residual saturation, S_{rw}	[-]	0.0176
Residual saturation, S_{rmw}	[-]	0.157
Nonwetting viscosity μ_{mw}	[Pa.s]	1.83×10^{-5}
Wetting viscosity μ_w	[Pa.s]	0.001

to be those for a static equilibrium in the air phase and the bottom boundary condition on the water phase is chosen to match the initial water content of the column. The Column is filled with a coarse sand, having the properties given in Table 13. The problem

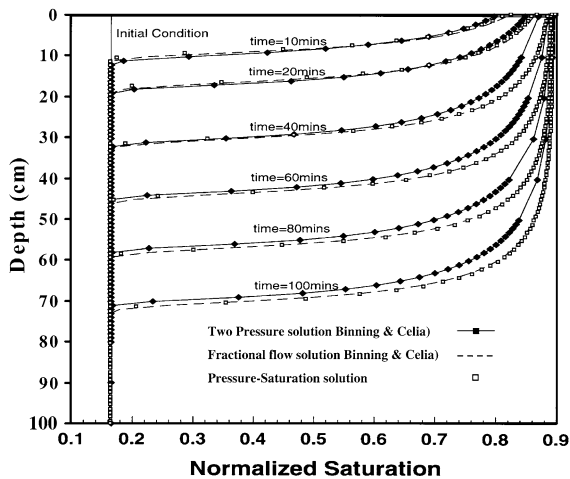


Fig. 9 Solution of a problem with constant saturation boundary conditions using three different numerical methods (Binning and Celia 1999)

is solved here using pressure–saturation approach and compared with both the fractional flow approach and the two-pressure solution (Fig. 9).

9 Validation

Tables 14, 15 and 16 lists the statistics for numerical performances of each formulation in solving the problem. In the present model the time steps increases if the iterations are less than a specific value, and decreases if the solution does not converge after a specific number of iterations. DT0 is the minimum time and DT is the maximum time step that is required for convergence. In these tables it can be observed that Newton–Raphson method is not a proper method of solution in terms of both the CPU_time and the number of iterations using pressure–saturation method. However this problem is obviated when modified pressure–saturation is used. Generally selecting pressures as

Table 14 Comparison of numerical results for test case 2

Method	CPU_times (s)	Iterations	Time steps	DT0–DT (s)
PSP	166.2031	14,677	7,342	17.8–127
PSN	2,043.219	207,471	34,634	4.22–26
PSMP	171.78	12,895	5,792	31.64–221
PSMN	15.15	1,760	566	42.19–6,495
PPP	33.28	4,156	663	75–5,199
PPN	32.81	3,962	630	75–6,344

Table 15 Comparison of numerical results for test case 3

Method	CPU_times (s)	Iterations	Time steps	DT0–DT (s)
PSP	183.6406	39,914	5,078	4.23E-03–2.28
PSN	2,714.25	621,450	103,579	1.79E-05–0.078
PSMP	23.71875	5,435	766	1.01E-05–26.8
PSMN	23.40625	6,469	953	1.97E-05–21.8
PPP	18.15625	3,642	555	5.66E-05–38.8
PPN	12.3125	2,142	305	5.63–58.6

Table 16 Comparison of numerical results for test case 4

Method	CPU_times (s)	Iterations	Time steps	DT0–DT (s)
PSP	61.84375	8,499	2,037	0.075–0.48
PSN	500.9688	82,996	7,806	0.017–0.19
PSMP	57.65625	5,393	1,128	0.075–2.18
PSMN	5.109375	779	189	0.17–10

primary variables yields better results in terms of both the CPU_time and the number of iterations and Newton–Raphson scheme is a better iterative method than picard.

The two pressure approach, in test case 2 and 4, in which the column is initially water saturated, does not converge and is not solvable. But in test case 2, with the assumption of $P_c = P_d$, the problem converges to an acceptable solution.

10 Conclusions

Six numerical methods have been tested for the evaluation of the three different forms of two-phase flow equations. The code presented allows the user to solve two-phase flow problems selecting different primary variables, iterative schemes (Newton–Raphson/Picard) and types of boundary conditions. The use of the six methods implemented in present code, resulted the following main points:

1. For the all test cases, the two-pressure approach shows better results compared to the pressure–saturation approach in terms of CPU_time and the number of iterations.
2. The modification of pressure–saturation approach improves the results.
3. The Newton–Raphson scheme shows better results compared to the Picard iteration scheme except for pressure–saturation method.

4. When the organic liquid is initially absent from a domain, the selection of the pressure-based formulation is not converged, but if the Brooks–Corey formula for capillary pressure is used, with the assumption of $P_c = P_d$, the problem will converge to an acceptable solution.

Appendix A: Derivation of Coefficients of Two-fluid-phase Equations for Pressure–Saturation Formulations

PSP Elemental Matrices

Using iterative increment equations it is possible to put Eq. 15 in the form of Eq. 10 where:

$$B_{w_j}^{n+1,m} = -\frac{\lambda_{w_{j+\frac{1}{2}}}^{n+1,m}}{\Delta z^2}; \quad C_{w_j}^{n+1,m} = \frac{\varphi}{\Delta t} \tag{A1, 2}$$

$$D_{w_j}^{n+1,m} = \frac{\lambda_{w_{j+\frac{1}{2}}}^{n+1,m} + \lambda_{w_{j-\frac{1}{2}}}^{n+1,m}}{\Delta z^2}; \quad F_{w_j}^{n+1,m} = -\frac{\lambda_{w_{j-\frac{1}{2}}}^{n+1,m}}{\Delta z^2} \tag{A3, 4}$$

$$R_{w_j}^{n+1,m} = -f_w(S_w^{n+1}, P_w^{n+1})^m \tag{A5}$$

$$B_{nw_j}^{n+1,m} = -\frac{\lambda_{nw_{j+\frac{1}{2}}}^{n+1,m}}{\Delta z^2}; \quad C_{nw_j}^{n+1,m} = -\frac{\varphi}{\Delta t} \tag{A6, 7}$$

$$D_{nw_j}^{n+1,m} = \frac{\lambda_{nw_{j+\frac{1}{2}}}^{n+1,m} + \lambda_{nw_{j-\frac{1}{2}}}^{n+1,m}}{\Delta z^2}; \quad F_{nw_j}^{n+1,m} = -\frac{\lambda_{nw_{j-\frac{1}{2}}}^{n+1,m}}{\Delta z^2}; \tag{A8, 9}$$

$$R_{nw_j}^{n+1,m} = -f_{nw}(S_w^{n+1}, P_w^{n+1})^m \tag{A10}$$

The other coefficients of Eq. 10 are zero.

PSN Elemental Matrices

Applying the Newton–Raphson method to Eq. 15 yields

$$A_{w_j}^{n+1,m} = \frac{\partial R_{w_j}^{n+1,m}}{\partial S_{w_{j-1}}} = \frac{\partial R_{w_j}^{n+1,m} d\lambda_{w_{j-\frac{1}{2}}}^{n+1,m}}{\partial \lambda_{w_{j-\frac{1}{2}}}^{n+1,m} dS_{w_{j-1}}^{n+1,m}} = \frac{1 P_{w_j}^{n+1,m+1} - P_{w_{j-1}}^{n+1,m+1} - \rho_w g \Delta z d\lambda_{w_{j-1}}^{n+1,m}}{2 \Delta z^2 dS_{w_{j-1}}^{n+1,m}} \tag{A11}$$

$$C_{w_j}^{n+1,m} = \frac{\partial R_{w_j}^{n+1,m}}{\partial S_{w_j}} = \frac{dR_{w_j}^{n+1,m}}{dS_{w_j}^{n+1,m}} + \frac{\partial R_{w_j}^{n+1,m} d\lambda_{w_{j-\frac{1}{2}}}^{n+1,m}}{\partial \lambda_{w_{j-\frac{1}{2}}}^{n+1,m} dS_{w_j}^{n+1,m}} + \frac{\partial R_{w_j}^{n+1,m} d\lambda_{w_{j+\frac{1}{2}}}^{n+1,m}}{\partial \lambda_{w_{j+\frac{1}{2}}}^{n+1,m} dS_{w_j}^{n+1,m}} = \frac{\varphi}{\Delta t} + \frac{1}{2} \frac{\partial \lambda_{w_j}^{n+1,m}}{\partial S_{w_j}^{n+1,m}} \frac{-P_{w_{j+1}}^{n+1,m+1} + 2P_{w_j}^{n+1,m+1} - P_{w_{j-1}}^{n+1,m+1}}{\Delta z^2} - \frac{\rho_w g}{\Delta z} \tag{A12}$$

$$E_{w_j}^{n+1,m} = \frac{\partial R_{w_j}^{n+1,m}}{\partial S_{w_{j+1}}} = \frac{\partial R_{w_j}^{n+1,m} d\lambda_{w_{j+\frac{1}{2}}}^{n+1,m}}{\partial \lambda_{w_{j+\frac{1}{2}}}^{n+1,m} dS_{w_{j+1}}^{n+1,m}} = \frac{1}{2} \frac{P_{w_j}^{n+1,m+1} - P_{w_{j+1}}^{n+1,m+1} - \rho_w g \Delta z d\lambda_{w_{j+1}}^{n+1,m}}{\Delta z^2 dS_{w_{j+1}}^{n+1,m}} \tag{A13}$$

$$A_{nw_j}^{n+1,m} = \frac{\partial R_{nw_j}^{n+1,m}}{\partial S_{w_{j-1}}} = \frac{\partial R_{nw_j}^{n+1,m} d\lambda_{nw_{j-\frac{1}{2}}}^{n+1,m}}{\partial \lambda_{nw_{j-\frac{1}{2}}}^{n+1,m} dS_{w_{j-1}}^{n+1,m}} + \frac{\partial R_{nw_j}^{n+1,m} dP_{c_{j-1}}^{n+1,m}}{\partial P_{c_{j-1}}^{n+1,m} dS_{w_{j-1}}^{n+1,m}} \tag{A14}$$

$$C_{nw_j}^{n+1,m} = \frac{\partial R_{nw_j}^{n+1,m}}{\partial S_{w_j}} = -\frac{\varphi}{\Delta t} + \frac{\partial R_{nw_j}^{n+1,m} d\lambda_{nw_{j-\frac{1}{2}}}^{n+1,m}}{\partial \lambda_{nw_{j-\frac{1}{2}}}^{n+1,m} dS_{w_j}^{n+1,m}} + \frac{\partial R_{nw_j}^{n+1,m} d\lambda_{nw_{j+\frac{1}{2}}}^{n+1,m}}{\partial \lambda_{nw_{j+\frac{1}{2}}}^{n+1,m} dS_{w_j}^{n+1,m}} + \frac{\partial R_{nw_j}^{n+1,m} dP_{c_j}^{n+1,m}}{\partial P_{c_j}^{n+1,m} dS_{w_j}^{n+1,m}} \tag{A15}$$

$$E_{nw_j}^{n+1,m} = \frac{\partial R_{nw_j}^{n+1,m}}{\partial S_{w_{j+1}}} = \frac{\partial R_{nw_j}^{n+1,m} d\lambda_{nw_{j+\frac{1}{2}}}^{n+1,m}}{\partial \lambda_{nw_{j+\frac{1}{2}}}^{n+1,m} dS_{w_{j+1}}^{n+1,m}} + \frac{\partial R_{nw_j}^{n+1,m} dP_{c_{j+1}}^{n+1,m}}{\partial P_{c_{j+1}}^{n+1,m} dS_{w_{j+1}}^{n+1,m}} \tag{A16}$$

where the capillary capacity $c_w = \frac{dP_c}{dS_w}$ (Touma and Vauclin 1986) and $\frac{d\lambda_{nw}}{dS_w}$ is negative, and $\frac{d\lambda_w}{dS_w}$ is positive. The other coefficients of Eq. 10 are the same as those of equation PSP elemental matrix.

Appendix B: Derivation of Coefficients of Two-fluid-phase Equations for Pressure–Saturation-modified Formulations

PSMP Elemental Matrices

Using finite difference solution of the modified pressure–saturation equation with a Picard iteration

scheme for the nonlinear coefficients for Eq. 20 yields

$$\begin{aligned}
 & -\varphi \frac{S_w^{n+1} - S_w^n}{\Delta t} - \frac{(\lambda_{nw} \cdot \frac{\partial P_w}{\partial z})_{j+\frac{1}{2}}^{n+1} - (\lambda_{nw} \cdot \frac{\partial P_w}{\partial z})_{j-\frac{1}{2}}^{n+1} + (\lambda_{nw} c c_w \frac{\partial S_w}{\partial z})_{j+\frac{1}{2}}^{n+1} - (\lambda_{nw} c c_w \cdot \frac{\partial S_w}{\partial z})_{j-\frac{1}{2}}^{n+1}}{\Delta z} \\
 & + \rho_{nw} g \frac{\lambda_{nw}^{n+1} - \lambda_{nw}^n}{\Delta z} = 0
 \end{aligned} \tag{B1}$$

$$\begin{aligned}
 A_{nw_j}^{n+1,m} &= (\lambda_{nw} c c_w)_{j-\frac{1}{2}}^{n+1,m}; \\
 C_{nw_j}^{n+1,m} &= -\frac{\varphi}{\Delta t} - (\lambda_{nw} c c_w)_{j-\frac{1}{2}}^{n+1,m} - (\lambda_{nw} c c_w)_{j+\frac{1}{2}}^{n+1,m}; \\
 & \tag{B2, 3}
 \end{aligned}$$

$$E_{nw_j}^{n+1,m} = (\lambda_{nw} c c_w)_{j+\frac{1}{2}}^{n+1,m} \tag{B4}$$

Where the $c c_w = \frac{dS_w}{dP_c}$ is the inverse of capillary capacity c_w . The other coefficients of Eq. 10 are the same as those of equation PSP elemental matrix.

PSMN Elemental Matrices

Applying the Newton–Raphson method to Eq. 20 yields

$$\begin{aligned}
 A_{nw_j}^{n+1,m} &= \frac{\partial R_{nw_j}^{n+1,m}}{\partial S_{w_{j-1}}} \\
 &= \frac{\partial R_{wn_j}^{n+1,m} d\lambda_{nw_j}^{n+1,m}}{\partial \lambda_{nw_j}^{n+1,m} dS_{w_{j-1}}} + \frac{\partial R_{wn_j}^{n+1,m} d c c_w^{n+1,m}}{\partial c c_w^{n+1,m} dS_{w_{j-1}}} \tag{B5}
 \end{aligned}$$

$$\begin{aligned}
 C_{nw_j}^{n+1,m} &= \frac{\partial R_{nw_j}^{n+1,m}}{\partial S_{w_j}} \\
 &= \frac{\partial R_{wn_j}^{n+1,m} d\lambda_{nw_j}^{n+1,m}}{\partial \lambda_{nw_j}^{n+1,m} dS_{w_{j-1}}} + \frac{\partial R_{wn_j}^{n+1,m} d c c_w^{n+1,m}}{\partial c c_w^{n+1,m} dS_{w_{j-1}}} \tag{B6}
 \end{aligned}$$

$$\begin{aligned}
 E_{nw_j}^{n+1,m} &= \frac{\partial R_{nw_j}^{n+1,m}}{\partial S_{w_{j+1}}} \\
 &= \frac{\partial R_{wn_j}^{n+1,m} d\lambda_{nw_j}^{n+1,m}}{\partial \lambda_{nw_j}^{n+1,m} dS_{w_{j+1}}} + \frac{\partial R_{wn_j}^{n+1,m} d c c_w^{n+1,m}}{\partial c c_w^{n+1,m} dS_{w_{j+1}}} \tag{B7}
 \end{aligned}$$

where $\frac{d c c_w}{d S_w} = \frac{d^2 P_c}{d S_w^2}$ (Eq. 24a,b). The other coefficients of Eq. 10 are the same as those of equation PSP elemental matrix.

Appendix C: Derivation of Coefficients of Two-fluid-phase Equations for Pressure–Pressure Formulations

PPP Elemental Matrices

Applying the Picard method to Eq. 25a,b yields

$$\left\{ \begin{aligned}
 & \varphi c_w^{n+1} \frac{P_{nw_j}^{n+1} - P_{nw_j}^n - P_{w_j}^{n+1} - P_{w_j}^n}{\Delta t} \\
 & - \frac{(\lambda_w \cdot \frac{\partial P_w}{\partial z})_{j+\frac{1}{2}}^{n+1} - (\lambda_w \cdot \frac{\partial P_w}{\partial z})_{j-\frac{1}{2}}^{n+1} + \rho_w g \frac{\lambda_w^{n+1} - \lambda_w^n}{\Delta z}}{\Delta z} = 0 \\
 & - \varphi c_w^{n+1} \frac{P_{nw_j}^{n+1} - P_{nw_j}^n - P_{w_j}^{n+1} - P_{w_j}^n}{\Delta t} \\
 & - \frac{(\lambda_{nw} \cdot \frac{\partial P_{nw}}{\partial z})_{j+\frac{1}{2}}^{n+1} - (\lambda_{nw} \cdot \frac{\partial P_{nw}}{\partial z})_{j-\frac{1}{2}}^{n+1}}{\Delta z} \\
 & + \rho_{nw} g \frac{\lambda_{nw}^{n+1} - \lambda_{nw}^n}{\Delta z} = 0
 \end{aligned} \right. \tag{C1}$$

$$\left\{ \begin{aligned}
 & y_w (P_{nw}^{n+1}, P_w^{n+1})^{m+1} \\
 & = \varphi c_w^{n+1,m} \frac{P_{nw_j}^{n+1,m+1} - P_{nw_j}^n - P_{w_j}^{n+1,m+1} - P_{w_j}^n}{\Delta t} \\
 & - \frac{\lambda_w^{n+1,m} \frac{P_{w_{j+1}}^{n+1,m+1} - P_{w_j}^{n+1,m+1}}{\Delta z} - \lambda_w^{n+1,m} \frac{P_{w_j}^{n+1,m+1} - P_{w_{j-1}}^{n+1,m+1}}{\Delta z}}{\Delta z} \\
 & + \rho_w g \frac{\lambda_w^{n+1,m} - \lambda_w^{n+1,m}}{\Delta z} = 0 \\
 & y_{nw} (P_{nw}^{n+1}, P_w^{n+1})^{m+1} \\
 & = -\varphi c_w^{n+1,m} \frac{P_{nw_j}^{n+1,m+1} - P_{nw_j}^n - P_{w_j}^{n+1,m+1} - P_{w_j}^n}{\Delta t} \\
 & - \frac{\lambda_{nw}^{n+1,m} \frac{P_{nw_{j+1}}^{n+1,m+1} - P_{nw_j}^{n+1,m+1}}{\Delta z} - \lambda_{nw}^{n+1,m} \frac{P_{nw_j}^{n+1,m+1} - P_{nw_{j-1}}^{n+1,m+1}}{\Delta z}}{\Delta z} \\
 & + \rho_{nw} g \frac{\lambda_{nw}^{n+1,m} - \lambda_{nw}^{n+1,m}}{\Delta z} = 0
 \end{aligned} \right. \tag{C2}$$

$$C_{w_j}^{n+1,m} = \frac{\varphi c_{w_j}^{n+1,m}}{\Delta t}; \tag{C3, 4}$$

$$D_{w_j}^{n+1,m} = -\frac{\varphi c_{w_j}^{n+1,m}}{\Delta t} + \frac{\lambda_{w_{j+\frac{1}{2}}}^{n+1,m} + \lambda_{w_{j-\frac{1}{2}}}^{n+1,m}}{\Delta z^2};$$

$$R_{w_j}^{n+1,m} = -\gamma_w (S_w^{n+1}, P_w^{n+1})^m \tag{C5}$$

$$C_{nw_j}^{n+1,m} = -\frac{\varphi c_{nw_j}^{n+1,m}}{\Delta t} + \frac{\lambda_{nw_{j+\frac{1}{2}}}^{n+1,m} + \lambda_{nw_{j-\frac{1}{2}}}^{n+1,m}}{\Delta z^2}; \tag{C6, 7}$$

$$D_{nw_j}^{n+1,m} = \frac{\varphi c_{nw_j}^{n+1,m}}{\Delta t};$$

$$R_{nw_j}^{n+1,m} = -f_{nw} (S_w^{n+1}, P_w^{n+1})^m \tag{C8}$$

PPN Element Matrices

Applying the Newton–Raphson method to Eq. 25a,b yields

$$A_{\alpha_j}^{n+1,m} = \frac{\partial R_{\alpha_j}^{n+1,m}}{\partial P_{nw_{j-1}}} = \frac{\partial R_{\alpha_j}^{n+1,m}}{\partial \lambda_{\alpha_{j-\frac{1}{2}}}^{n+1,m}} \frac{\partial \lambda_{\alpha_{j-\frac{1}{2}}}^{n+1,m}}{\partial P_{nw_{j-1}}} \frac{dP_{c_{j-1}}^{n+1,m}}{dP_{nw_{j-1}}} \tag{C9}$$

$$B_{\alpha_j}^{n+1,m} = \frac{\partial R_{\alpha_j}^{n+1,m}}{\partial P_{w_{j-1}}} = \frac{\partial R_{\alpha_j}^{n+1,m}}{\partial \lambda_{\alpha_{j-\frac{1}{2}}}^{n+1,m}} \frac{\partial \lambda_{\alpha_{j-\frac{1}{2}}}^{n+1,m}}{\partial P_{w_{j-1}}} \frac{dP_{c_{j-1}}^{n+1,m}}{dP_{w_{j-1}}} \tag{C10}$$

$$C_{\alpha_j}^{n+1,m} = \frac{\partial R_{\alpha_j}^{n+1,m}}{\partial P_{nw_j}} = \frac{dR_{\alpha_j}^{n+1,m}}{dP_{nw_j}^{n+1,m}} + \frac{\partial R_{\alpha_j}^{n+1,m}}{\partial \lambda_{\alpha_{j-\frac{1}{2}}}^{n+1,m}} \frac{\partial \lambda_{\alpha_{j-\frac{1}{2}}}^{n+1,m}}{\partial P_{nw_j}^{n+1,m}} \frac{dP_{c_j}^{n+1,m}}{dP_{nw_j}^{n+1,m}}$$

$$+ \frac{\partial R_{\alpha_j}^{n+1,m}}{\partial \lambda_{\alpha_{j+\frac{1}{2}}}^{n+1,m}} \frac{\partial \lambda_{\alpha_{j+\frac{1}{2}}}^{n+1,m}}{\partial P_{nw_j}^{n+1,m}} \frac{dP_{c_j}^{n+1,m}}{dP_{nw_j}^{n+1,m}} + \frac{\partial R_{\alpha_j}^{n+1,m}}{\partial c_{\alpha_j}^{n+1,m}} \frac{\partial c_{\alpha_j}^{n+1,m}}{\partial P_{nw_j}^{n+1,m}} \frac{dP_{c_j}^{n+1,m}}{dP_{nw_j}^{n+1,m}} \tag{C11}$$

$$D_{\alpha_j}^{n+1,m} = \frac{\partial R_{\alpha_j}^{n+1,m}}{\partial P_{w_j}} = \frac{dR_{\alpha_j}^{n+1,m}}{dP_{w_j}^{n+1,m}} + \frac{\partial R_{\alpha_j}^{n+1,m}}{\partial \lambda_{\alpha_{j-\frac{1}{2}}}^{n+1,m}} \frac{\partial \lambda_{\alpha_{j-\frac{1}{2}}}^{n+1,m}}{\partial P_{w_j}^{n+1,m}} \frac{dP_{c_j}^{n+1,m}}{dP_{w_j}^{n+1,m}}$$

$$+ \frac{\partial R_{\alpha_j}^{n+1,m}}{\partial \lambda_{\alpha_{j+\frac{1}{2}}}^{n+1,m}} \frac{\partial \lambda_{\alpha_{j+\frac{1}{2}}}^{n+1,m}}{\partial P_{w_j}^{n+1,m}} \frac{dP_{c_j}^{n+1,m}}{dP_{w_j}^{n+1,m}} + \frac{\partial R_{\alpha_j}^{n+1,m}}{\partial c_{\alpha_j}^{n+1,m}} \frac{\partial c_{\alpha_j}^{n+1,m}}{\partial P_{w_j}^{n+1,m}} \frac{dP_{c_j}^{n+1,m}}{dP_{w_j}^{n+1,m}} \tag{C12}$$

$$E_{\alpha_j}^{n+1,m} = \frac{\partial R_{\alpha_j}^{n+1,m}}{\partial P_{nw_{j+1}}} = \frac{\partial R_{\alpha_j}^{n+1,m}}{\partial \lambda_{\alpha_{j+\frac{1}{2}}}^{n+1,m}} \frac{\partial \lambda_{\alpha_{j+\frac{1}{2}}}^{n+1,m}}{\partial P_{nw_{j+1}}} \frac{dP_{c_{j+1}}^{n+1,m}}{dP_{nw_{j+1}}} \tag{C13}$$

$$F_{\alpha_j}^{n+1,m} = \frac{\partial R_{\alpha_j}^{n+1,m}}{\partial P_{w_{j+1}}} = \frac{\partial R_{\alpha_j}^{n+1,m}}{\partial \lambda_{\alpha_{j+\frac{1}{2}}}^{n+1,m}} \frac{\partial \lambda_{\alpha_{j+\frac{1}{2}}}^{n+1,m}}{\partial P_{w_{j+1}}} \frac{dP_{c_{j+1}}^{n+1,m}}{dP_{w_{j+1}}} \tag{C14}$$

These coefficients above are applied for wetting and nonwetting phase ($\alpha = w, nw$).

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