Nonlinearly preconditioned constraint-preserving algorithms for subsurface three-phase flow with capillarity

Haijian Yang\textsuperscript{a}, Yiteng Li\textsuperscript{b}, Shuyu Sun\textsuperscript{b,∗}

\textsuperscript{a}School of Mathematics, Hunan University, Changsha, Hunan 410082, PR China
\textsuperscript{b}Physical Science and Engineering Division, King Abdullah University of Science and Technology, Thuwal, 23955-6900, Saudi Arabia

Abstract

The multiphase flow model has been extensively used to describe complicated flow behaviors in subsurface formations, together with sophisticated reservoir models and well-defined fluid property. In this study, the fully implicit method, as one of most promising schemes for subsurface flow modeling, is employed to solve multiphase flow problems. In contrast to the conventional approach where mathematical models often include a pressure equation, the multiphase flow problems are modeled by up to three continuity equations so that mass conservation holds for all present phases. Another challenge that frequently shows up is the computed solution may sit outside its physically meaningful range, thereby leading to inaccurate predictions or even a failure of the simulation process. A simple remedy is to apply a cutting-off operation to the out-of-bound solution but such an action could ruin both local and global mass conservation. Instead, we replace the original model by a variational inequality formulation with box inequality constraints to protect the boundedness requirement on pressure and saturations from being violated. The variational inequality problem is then solved by a well-designed nonlinear solver consisting of the active-set reduced-space method and the nonlinear elimination preconditioning technique. A number of examples are presented to demonstrate that the proposed formulation is bound-preserving and mass-conservative for each of the present phases/components.

Keywords: Reservoir simulation, Fully implicit method, Bound-preserving, Mass conservation, Nonlinear preconditioning

1. Introduction

Modeling and simulation of subsurface flows in porous media have a variety of applications. In petroleum industry, it can be used to track flow patterns at various exploitation
stages of an oilfield, which could help optimization of the development plan for oil recovery enhancement. On the other hand, for those high-profile environmental issues, such as greenhouse gas emission and pollutant disposal, subsurface flow modeling sheds light on the migration behavior of carbon dioxide (CO$_2$), the main greenhouse gas, and underground pollutants (e.g. nuclear waste) in geological formations, and provides guidelines on how to effectively sequester CO$_2$ or controllably dispose the environmentally hazardous wastes. Clearly, all the aforementioned applications demand accurate simulation of subsurface flows, and also impose high requirement on efficient numerical algorithms due to increasingly complex flow and geological models.

Subsurface flow modeling consists of two components in an isothermal system, the mass conservation law that any physical process is supposed to satisfy and the Darcy’s law that describes fluid flow through a porous medium. When the fluid composition is fixed or slightly changes during simulation, the mass conservation equation is modeled based on phase; otherwise, the component-wise mass conservation equations are established since considerable mass transfer takes place between phases. Moreover, capillarity, gravity, heterogeneous rock property and complicated fluid property also play significant roles in the accurate description of flow behaviors [1]. For more realistic applications, some or all of them have to be taken into account. When numerically solving the partial differential equations (PDEs) of a subsurface flow problem, the local mass-conservation property is the key to selection of a spatial discretization scheme. Such discretization schemes include the mixed finite element method and cell-centered finite difference method.

There are three categories of time discretization methods to simulate the progress of fluid flow over time. Among them, the explicit scheme is easy to implement by treating all terms explicitly, thus making it much more straightforward than any other approaches. However, the Courant-Friedrichs-Lewy (CFL) condition imposes a strict restriction on the time step size. As a result, the explicit method is prohibitively expensive and impractical to simulate either long-term or large-scale problems with the tiny time steps. In comparison, the semi-implicit scheme relaxes the constraint on time stepping and meanwhile achieves enhanced stability, which makes it more extensively used than the fully explicit scheme in practice. Considering that the pressure information propagates more rapidly than the saturation information, the implicit pressure and explicit saturation (IMPES) scheme [2, 3, 4, 5, 6, 7, 8] was proposed by solving the linear pressure equation implicitly and nonlinear saturation equations explicitly. Analogous to the IMPES method, the implicit pressure and explicit concentration (IMPEC) scheme adopts a similar strategy to solve compositional flow problems [9]. In addition to porous media flow problems, similar semi-implicit methods are also applied to multiphase flow in a free space [10, 11, 12]. Unfortunately, these methodologies cannot completely get rid of the stability restriction caused by the CFL condition, which relates the time step size to the gridding size [4]. Moreover, a large splitting error might be introduced by decoupling the original flow problem with semi-implicit schemes [13, 14, 15, 16].

In spite of the popularity of semi-implicit methods, the fully implicit approach enables to solve all the coupled nonlinear equations simultaneously and implicitly with the relaxation of the stability requirement on the time step size, and has been successfully applied to several
classes of important applications [17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27]. Thanks to the simultaneous solution approach, it is allowed to account for more physical principles by readily introducing additional contributions to the existing mathematical model. Clearly, this shifts challenges from model itself to numerical solvers. In addition, theoretically it is possible to use very large time steps due to the unconditional stability of fully implicit methods. However, without a well-designed nonlinear solver, the simultaneous solution method might still yield enormous computation cost and memory consumption for those extreme-scale problems. In addition to the robust and efficient nonlinear solver, the adaptive time stepping strategy can effectively reduce the computational time and also extend the applicability of the fully implicit scheme.

When modeling subsurface flows in porous media, it is crucial to ensure that the predicted saturations/concentrations, as well as the pressure, stay inside their physically meaningful ranges. Generally, phase saturation, defined as the volume fraction of the pore space occupied by a certain fluid phase, ranges from 0 to 1, if not specified. Furthermore, the predicted pressure should sit between the bottomhole pressure of producer(s) and injector(s). If the phase saturation suffers nonphysical overshoot or undershoot during simulation, the relative permeability and capillary pressure, both of which are the nonlinear functions of saturation, become undefined and physically meaningless. This could result into incorrect predictions or even break down the whole simulation process. Despite of this, the commonly used algorithms still fail to guarantee the computed pressure, saturation or concentration within their ranges, due to strong nonlinearities that usually exhibit by pronounced permeability heterogeneity and highly spatially varying capillary pressure and relative permeability. To protect the boundedness requirement from violation, the commonly used fix is to apply a cut-off procedure by setting the value of the computed variable to its lower bound whenever it’s below the allowed minimum and setting it to the maximum if greater than the upper bound of the computed variable. Unfortunately, this treatment could ruin both local and global mass conservations, thus yielding unreliable simulation results. Therefore, it is of vital importance to make sure that the predicted saturation and pressure sit inside their physically meaningful range at each iteration.

In this study, to accurately simulate multiphase flow problems, the mathematical model is formulated by up to three continuity equations to replace the conventional formulation that often includes a pressure equation. All the continuity equations are discretized by the upwind scheme so that we can capture the information along flow direction for all present phases unbiasedly. As a result, the proposed multiphase flow model is mass-conservative, which is key to success of modeling subsurface flow in porous media. To protect the pressure and saturations from being violated, we reformulate the original problem using the variational inequality formulation [28, 29, 30, 31] with the box inequality constraints. Recent research has shown that the variational inequality method is of great potential to enhance the robustness and efficiency of reservoir simulation combining with well-designed nonlinear and linear solvers [32, 33, 34, 35]. Similar to our previous work, after reforming a nonlinear complementarity problem [36, 37], it is then solved by the active-set reduced space method [38, 35, 38, 39] with nonlinear elimination preconditioner [14, 21, 31, 33, 34, 40, 41], the latter of which eliminates the impact of imbalanced nonlinearities in a field-split approach to
accelerate the convergence of the active-set reduced-space method. However, a straightforward application of the nonlinear elimination method to the multiphase flow problems such as the black-oil model does not work well probably because it introduces much complicated dynamics of the subsurface flow in porous media. Hence, we propose an adaptive sophisticated elimination strategy and the region corresponds to the complexity of the fluid. The new method outperforms the classical method in terms of global nonlinear iterations. We also numerically show that our new method is more robust and efficient for both standard benchmarks as well as realistic problems in highly heterogeneous media.

The remainder of this paper is organized as follows. In Section 2 the original multiphase flow model is presented first and then transformed into the variation inequality formulation by introducing box inequality constraints. In Section 3 on the basis of inexact Newton methods, we build the nonlinear solver using the active-set reduced-space method with nonlinear elimination to efficiently solve the resultant nonlinear system. Numerical examples are presented in Section 4 to show the bound-preserving and mass-conservative properties of the proposed formulation and the robust performance of the well-designed nonlinear solver. At the end, we make concluding remarks in Section 5.

2. Mathematical model

2.1. Original multiphase flow formulation

The multiphase flow model [13, 42, 43], as a family of simplified compositional multiphase flow problems where the computational efficiency is heavily dominated by flash calculation [44], reduces to three phases and three components (oil, gas and water). Let the reservoir be isothermal, g be the gravitational acceleration constant and $z$ be the depth where the phase locates, then, by taking into account the mass transfer between phases, the generalized multiphase flow model includes the following continuity equation for each phase $\alpha$ with $\alpha = o, w, g$,

\[
\begin{align*}
\frac{\partial}{\partial t} (\phi \rho_o S_o + \phi \rho_o S_o) & - \nabla \cdot \left( \frac{\kappa_0 \rho_o}{\mu_o} \mathbf{K} \nabla \Theta_o \right) = q_o, \\
\frac{\partial}{\partial t} (\phi \rho_g S_o + \phi \rho_g S_g + \phi \rho_g S_w) & - \nabla \cdot \left( \frac{\kappa_0 \rho_g}{\mu_g} \mathbf{K} \nabla \Theta_o + \frac{\kappa_g \rho_o}{\mu_g} \mathbf{K} \nabla \Theta_g + \frac{\kappa_{rg} \rho_g}{\mu_w} \mathbf{K} \nabla \Theta_w \right) = q_g, \\
\frac{\partial}{\partial t} (\phi \rho_w S_w) & - \nabla \cdot \left( \frac{\kappa_{rw} \rho_w}{\mu_w} \mathbf{K} \nabla \Theta_w \right) = q_w,
\end{align*}
\]

(1)

where $\phi$ is the porosity of the porous medium, $S_\alpha$ and $q_\alpha$ are the saturation and external mass flow rate of phases. Moreover, $\kappa_{ra}, \mu_\alpha$ and $p_\alpha$ denote the relative permeability, viscosity and pressure of the phase $\alpha$, $\Theta_\alpha = p_\alpha + \rho_\alpha g z$ is the phase potential, and $\mathbf{K}$ is the absolute permeability tensor.

In the above formulation, $\rho_o^g$, $\rho_w^g$ and $\rho_g$ represent the density of solution gas in oil and water and the density of free gas, while $\rho_o^g$ and $\rho_o$ denote the density of vaporized oil and the density of fluid oil respectively. It can be seen gas is allowed to dissolve into water while hydrocarbons exhibit very low solubility in water. Meanwhile, the water component
is assumed in the water phase only. Since the pore space is fully saturated with fluids, the saturations of all three phases should sum up to one, i.e.,

\[ S_o + S_g + S_w = 1. \]  

(2)

The absolute permeability tensor is defined as \( K = K I \), where \( I \) is the identity matrix and \( K \) is a positive real number. The saturations are normalized as follows:

\[ S_{nw} = S_w - S_{rw}, \quad S_{no} = S_o - S_{ro}, \quad S_{ng} = \frac{S_g}{1 - S_{rw} - S_{ro}}, \]

with \( S_{rw} \) being the irreducible water saturation and \( S_{ro} \) being the residual oil saturation.

The relative permeability functions for the water and the gas phase are given by the following analytical expressions:

\[ \kappa_{rw} = S_{nw}^2, \quad \kappa_{rg} = S_{ng}^2, \]

and the relative permeability of oil \( \kappa_{ro} \) is defined by Stone’s model [13]. In addition, the pressures between any two phases are linked by capillary pressure relations shown below by regarding the gas phase as the nonwetting phase and the aqueous phase as the wetting phase,

\[
\begin{cases}
    p_{cow} = p_o - p_w = \frac{B_{cw}}{\sqrt{K}} \log(S_{nw}), \\
    p_{cgo} = p_g - p_o = \frac{B_{cg}}{\sqrt{K}} \log(S_{no}),
\end{cases}
\]

(3)

where \( B_{cw} \) and \( B_{cg} \) are positive parameters. The boundary conditions are assumed to be impervious, implying the phase velocity \( u_\alpha = 0 \) on boundary \( \partial \Omega \) with the computational domain denoted by \( \Omega \in \mathbb{R}^d, d = 1, 2, 3 \). Instead, the inflow and outflow boundaries are modeled as injectors and producers, respectively.

Under an assumption that no mass transfer takes place between phases, the above multiphase flow problem can be further simplified as below

\[
\begin{cases}
    \frac{\partial}{\partial t} \left( \phi \rho_o S_o \right) - \nabla \cdot \left( \frac{\kappa_{ro}}{\mu_o} K \nabla \Theta_o \right) = q_o, \\
    \frac{\partial}{\partial t} \left( \phi \rho_g S_g \right) - \nabla \cdot \left( \frac{\kappa_{rg}}{\mu_g} K \nabla \Theta_g \right) = q_g, \\
    \frac{\partial}{\partial t} \left( \phi \rho_w S_w \right) - \nabla \cdot \left( \frac{\kappa_{rw}}{\mu_w} K \nabla \Theta_w \right) = q_w.
\end{cases}
\]

(4)

Let the primary variables for the numerical solution of the multiphase flow problems be \( X_c = (p_w, S_w, S_g, S_o)^T \), then the mass conservation of all phases yields the following multi-component system

\[
F_c(X_c) = \begin{bmatrix}
    F_{c}(p_w) (X_c) \\
    F_{c}(S_g) (X_c) \\
    F_{c}(S_w) (X_c) \\
    F_{c}(S_o) (X_c)
\end{bmatrix} = \begin{bmatrix}
    \frac{\partial}{\partial t} \left( \phi \rho_o S_o \right) - \nabla \cdot \left( \frac{\kappa_{ro}}{\mu_o} K \nabla \Theta_o \right) - q_o \\
    \frac{\partial}{\partial t} \left( \phi \rho_g S_g \right) - \nabla \cdot \left( \frac{\kappa_{rg}}{\mu_g} K \nabla \Theta_g \right) - q_g \\
    \frac{\partial}{\partial t} \left( \phi \rho_w S_w \right) - \nabla \cdot \left( \frac{\kappa_{rw}}{\mu_w} K \nabla \Theta_w \right) - q_w \\
    S_o + S_w + S_g - 1
\end{bmatrix} = 0.
\]

(5)
Here, the subscript \(c\) indicates that the system (3) is the continuous form of the equations. And in a similar way we can build the corresponding continuous multicomponent system for the generalized multiphase flow model (1).

### 2.2. Bounding-preserving formulation

It is required that the phase saturations during simulation should sit inside the interval \([0, 1]\), unless the lower bound of phase saturation, such as the residual oil/gas saturation or connate water saturation, and accordingly the upper-bound values are specified. Similarly, the pressure is supposed to range from the bottom hole pressure at the production well \(p^b\) to the bottom hole pressure at the injection well \(p^u\). In light of the pressure and saturation constraints, Lagrange multipliers are introduced to reformulate the constrained problem into an unconstrained one, see the references [28, 29, 30, 31] for more details. As a result, we obtain the box constrained variational inequality formulation for the multiphase flow model. Again, we use the model problem (4) to build its bounding-preserving formulation for the convenience of introduction. For example, the variational inequality formulation for the gas saturation \(S_g\) is expressed as

\[
\begin{cases}
S_g = S^b_g, & \text{and } F_c(S_g)(X_c) = \frac{\partial \left( \phi \rho_g S_g \right)}{\partial t} - \nabla \cdot u_g - q_g \geq 0, \\
S_g = S^a_g, & \text{and } F_c(S_g)(X_c) = \frac{\partial \left( \phi \rho_g S_g \right)}{\partial t} - \nabla \cdot u_g - q_g \leq 0, \\
S_g \in (S^b_g, S^a_g), & \text{and } F_c(S_g)(X_c) = \frac{\partial \left( \phi \rho_g S_g \right)}{\partial t} - \nabla \cdot u_g - q_g = 0,
\end{cases}
\]

under the gas volume constraint \(S^b_g \leq S_g \leq S^a_g\), which also applies to oil and water saturations. Similarly, the variational inequality formulation for the water pressure \(p_w\) is given as follows

\[
\begin{cases}
p_w = p^b_w, & \text{and } F_c(p_w)(X_c) \geq 0, \\
p_w = p^a_w, & \text{and } F_c(p_w)(X_c) \leq 0, \\
p_w \in (p^b_w, p^a_w), & \text{and } F_c(p_w)(X_c) = 0.
\end{cases}
\]

In this study, we employ a mixed finite element method (MFEM) for accurate characterization of pressure and saturation variations along the flow direction. Let \(\Omega\) be the domain that partitioned by a finite number of mesh cells. In the proposed spatial discretization scheme, the finite element space for the pressure unknown denotes \(Q_\kappa\), which is the space of piecewise tensor-product polynomials of order \(\kappa\). The Raviart-Thomas space \(RT_\kappa\) of order \(\kappa\) is the smallest polynomial space such that the divergence maps \(RT_\kappa\) onto \(Q_\kappa\). For the velocity unknown, we approximate \(\hat{u}_\alpha := u_\alpha / (k_\alpha \rho_\alpha)\) using the Raviart-Thomas space \(RT_\kappa\), which exhibits higher continuity than \(u_\alpha\) in the normal direction by excluding the effect of saturation discontinuity. This is the best solution to model fluid velocity for each phase in the conventional framework, while a new framework has been proposed recently to approximate the total velocity since it is more continuous in normal direction [45]. Here, we solve \(\hat{u}_\alpha\) as the direct unknown instead of the original mass flux rate \(u_\alpha = k_\alpha \rho_\alpha \hat{u}_\alpha\). Let the finite-dimensional velocity space (which vanishes on \(\Gamma_N\)) be \(V_h \subset RT_\kappa\), and the finite-dimensional
pressure space be denoted by $W_h = Q_\alpha$. Then we want to find $S_\alpha(\cdot, t) \in W_h$, $p_\alpha(\cdot, t) \in W_h$, and $\hat{u}_\alpha(\cdot, t) \in V_h$, such that

\[
\left( \frac{\partial}{\partial t} (\phi \rho \alpha S_\alpha), w \right) + \langle k^*_r \rho \alpha \hat{u}_\alpha \cdot n, w \rangle_{\Gamma_D} - \langle k_{ra} \rho \alpha \hat{u}_\alpha, \nabla w \rangle = (q_\alpha, w), \quad \forall w \in W_h,
\]

\[
\left( \mu \alpha K^{-1} \hat{u}_\alpha, v \right) - \langle p_\alpha, \nabla \cdot v \rangle + \langle p_\alpha, v \cdot n \rangle_{\Gamma_D} + \langle \rho \alpha g \nabla z, v \rangle = 0, \quad \forall v \in V_h,
\]

\[
(S_{\alpha} + S_w + S_\gamma - 1, w) = 0, \quad \forall w \in W_h,
\]

\[
(p_g - p_\alpha, w) = (p_{ego}, w), \quad \forall w \in W_h,
\]

\[
(p_\alpha - p_w, w) = (p_{cow}, w), \quad \forall w \in W_h,
\]

where $k^*_r$ and $\rho^*_\alpha$ represent the upwind values of $k_{ra}$ and $\rho_\alpha$ based on the direction of the velocity $\hat{u}_\alpha$. Note that we use the Raviart-Thomas space $RT_\kappa$ to approximate $\hat{u}_\alpha$ instead of $u$, because $\hat{u}_\alpha$ is a smooth function, while $u$ can be a function with discontinuities or sharp gradients. To get a fully discretized system, we adopt the implicit backward Euler scheme with adaptive time stepping for the temporal integration. And then the implicit first order scheme (Backward Euler) is used for the time differencing approximation, to relax the constraint on time step size imposed by the CFL condition that usually dominates the time step in the fully explicit or semi-implicit schemes, the detailed process of the discretization can be found \[35\].

Suppose that $\mathcal{S} = \{1, 2, 3, \ldots, N\}$ is an index set, and $X \in \mathbb{R}^N$ is the solution vector with respect to $\mathcal{S}$, which is defined by

\[
X = (p_w, S_w, S_g, S_o, \ldots, p_w, S_w, S_g, S_o) = (X_1, X_2, X_3, \ldots, X_N).
\]

After the spatial and temporal discretizations, the above fully implicit formulation results in a nonlinear algebraic system with the pointwise (field-coupling) order

\[
F(X) = (F_1(X), F_2(X), F_3(X), \ldots, F_N(X)) \in \mathbb{R}^N,
\]

(6)

Here, the system \[6\] denotes the discretized form of \[5\] by using the aforementioned fully implicit scheme. The lower- and upper-bound vectors for the solution $X$ have the following forms

\[
\begin{align*}
\varphi &= (p^b_w, S^b_w, S^b_g, S^b_o, \ldots, p^b_w, S^b_w, S^b_g, S^b_o) = (\varphi_1, \varphi_2, \varphi_3, \ldots, \varphi_N) \in \mathbb{R}^N, \\
\psi &= (p^a_w, S^a_w, S^a_g, S^a_o, \ldots, p^a_w, S^a_w, S^a_g, S^a_o) = (\psi_1, \psi_2, \psi_3, \ldots, \psi_N) \in \mathbb{R}^N,
\end{align*}
\]

(7)

Then the variational inequality formulation for \[5\] is defined to compute a vector $X \in \mathbb{R}^N$ such that

\[
\begin{align*}
X_i &= \varphi_i, & F_i(X) &\geq 0, \\
X_i &= \psi_i, & F_i(X) &\leq 0, \\
X_i &\in (\varphi_i, \psi_i), & F_i(X) &= 0,
\end{align*}
\]

(8)

holds for all $i$ belonging to the index set $\mathcal{S}$. 

7
It is worth mentioning that the variational inequality formulation is the key to success for the simulation of multiphase flow and enables all the pressures and saturations to stay inside their physically meaningful ranges. Otherwise, some rock/fluid properties, like capillary pressure and relative permeability, become undefined, leading to a failure of numerical simulation. On the other hand, in order to eliminate those unexpected overshoots or undershoots from the numerical solution, the conventional approach applies a cut-off operator by, for example, setting the saturation to zero when it is negative and to one whenever it is greater than one. Unfortunately, this not only destroys the local mass conservation but also damages the global mass conservation. In addition, the conventional numerical algorithm usually consists of one pressure equation and two continuity equations, but the pressure equation cannot capture the information along the flow direction because no upwind scheme is applied. Furthermore, two continuity equations have to be selected in a biased approach while the new formulation avoids this issue. We also want to mention that conventionally one phase pressure and two phase saturations are selected as the primary variables and the third saturation has to be computed based on [2]. However, the variational inequality approach cannot guarantee the third saturation sits within its lower- and upper-bound, which explains why the saturation constraint is introduced as an additional residual function. Moreover, the system [3] is a coupled elliptic-hyperbolic nonlinear system of equations that often appears in porous media simulations. The nature of this distinguishing feature, accompanied by the complicated model parameters such as nonlinear relative permeabilities and viscosity differences, instigates highly nonlinear structures in the solution, and these nonlinearities are shared with more complex problems. Hence, in this study, we present a well-designed nonlinear solver consisting of the active-set reduced-space method and the nonlinear elimination technique for the solution of the resultant nonlinear algebra system.

Remark 1 The focus of this study is on the model (1), and we can build the corresponding bounding-preserving model and obtain its fully implicit discretization scheme as mentioned above in a similar way. Here, we omit its introduction for the sake of simplicity and convenience.

3. Nonlinearly preconditioned constraint-preserving algorithms

To efficiently solve the proposed nonlinear system, a bound-preserving solver is employed in this study. On the basis of inexact Newton methods, the active-set reduced-space method plays a crucial role in the nonlinear solver, preconditioned by the nonlinear elimination if necessary. In addition, the Generalized Minimal RESidual (GMRES) method [46, 47, 48, 49], as one of commonly used Krylov iterative methods, is used to solve the linear system. However, such linear solvers may not have satisfactory convergence rate, especially when the Jacobian matrix has a large condition number. Therefore, a properly designed linear preconditioner is desired to improve the convergence of the Krylov methods. Recently, one of linear preconditioning techniques, the restricted additive Schwarz preconditioner, has been extensively used to accelerate the Krylov iterations and increase the scalability of the linear solver on parallel computing, see references [10, 50, 51, 52, 53, 54, 55] for more details.
In this section, we mainly focus on the nonlinear solver, which consists of the active-set reduced-space method and the nonlinear elimination preconditioner.

3.1. Active-set reduced-space method

Due to the advantages, such as easy implementation and fast convergence rate, the family of inexact Newton methods has been extensively used to solve nonlinear problems. Despite this, the inexact Newton method still cannot prohibit the computed solution from jumping outside the physically meaningful range. Thus, by taking advantages of inexact Newton methods, we introduce the active-set reduced-space method to deal with those out-of-bound solutions. Suppose $X^k$ is the current approximate solution, in order to update the new solution $X^{k+1}$, the index set $S = \{1, 2, 3, \ldots, N\}$ is first divided into the active and inactive sets, yielding

\[
\begin{align*}
A_\varphi(X) &= \{ i \in S \mid X_i = \varphi_i \& F_i(X) \geq 0 \}, \\
A_\psi(X) &= \{ i \in S \mid X_i = \psi_i \& F_i(X) \leq 0 \}, \\
I(X) &= S \setminus (A_\varphi(X) \cup A_\psi(X)).
\end{align*}
\]

(9)

where $A_\varphi(X)$ and $A_\psi(X)$ denote the active sets of the variable indexes that reach the lower- and upper-bound respectively, $X_i = \begin{cases} \varphi_i, & \text{if } i \in A_\varphi(X), \\ \psi_i, & \text{if } i \in A_\psi(X), \end{cases}$

(10)

and $I(X)$ is the inactive set that contains the remaining variables for a reduced linear system. Let $\pi$ be a projecting operator that pull the overshoot or undershoot back to the variable bound $[\varphi, \psi]$. The new approximate solution $X^{k+1}$ can be computed by

\[
X^{k+1} = \pi \left[ X^k + \lambda^k d^k \right],
\]

(11)

where $\lambda^k$ is the step length for line search, and $d^k$ is the direction vector consisting of three components: $d_{A_\varphi}, d_{A_\psi}$ and $d_I$. At each iteration of the active-set reduced-space method, the search directions with respect to the active sets $A_\varphi$ and $A_\psi$ are set to zero, i.e. $d_{A_\varphi} = d_{A_\psi} = 0$, while the search direction of the inactive set $d_I$ is the approximate solution of the following linear system

\[
(\nabla F(X^k))_{I^k} d_I^k = -F_I(X^k),
\]

(12)

where $(\nabla F(X^k))_{I^k} I^k$ is a submatrix of the Jacobian matrix $\nabla F(X^k)$ for the original multiphase flow problem, and $F_I(X^k)$ is a subvector of $F(X^k)$. In addition, the step length $\lambda^k$ is determined to achieve

\[
\|F_\Theta \left( \pi \left[ X^k + \lambda^k d^k \right] \right) \| \leq (1 - \omega \lambda^k) \|F_\Theta(X^k)\|,
\]

(13)

where $\omega$ is a constant to ensure a sufficient reduction for $\|F(X^k)\|$. The restriction operator $F_\Theta(X)$ is defined for each component individually

\[
[F_\Theta(X)]_i = \begin{cases} F_i(X), & \text{if } \varphi_i < X_i < \psi_i, \\ \min\{F_i(X), 0\}, & \text{others}. \end{cases}
\]

(14)
The nonlinear iterations are performed until it satisfies the following convergence criterion

\[ \|F_\Theta(X^{k+1})\| \leq \max\{\varepsilon_r\|F_\Theta(X^0)\|, \varepsilon_a\}, \]

where \(X^0\) is an initial approximation of the solution, \(\varepsilon_r\) is the relative tolerance and \(\varepsilon_a\) is the absolute tolerance. In summary, the framework of the active-set reduced-space method (ASRS) algorithm is described in Algorithm 1.

**Algorithm 1** Active-set reduced-space (ASRS) method

Choose an initial guess \(X^0 \in [\phi, \psi]\) and set \(k = 0\).

1: for \(k = 0, 1, 2, 3, \ldots\) until convergence do

2: Define the active and inactive sets

\[
\begin{align*}
A_\phi(X^k) &= \{i \in S \mid X_{i}^k = \phi_i \text{ and } F_i(X^k) > 0\}, \\
A_\psi(X^k) &= \{i \in S \mid X_{i}^k = \psi_i \text{ and } F_i(X^k) < 0\}, \\
I(X^k) &= S \setminus (A_\phi(X^k) \cup A_\psi(X^k)).
\end{align*}
\]

3: Set \(d_{A_\phi} = 0\) and \(d_{A_\psi} = 0\), and approximately solve the linear system

\[
(\nabla F(X^k))_{I^k, I^k} d_{I^k} = -F_{I^k}(X^k)
\]

to calculate a direction \(d_{I^k}\).

4: Set \(X^{k+1} = \pi [X^k + \lambda^k d^k]\), where \(\lambda^k \in (0, 1]\) is determined to satisfy

\[
\|F_\Theta(\pi [X^k + \lambda^k d^k])\| \leq (1 - \omega \lambda^k)\|F_\Theta(X^k)\|.
\]

5: end for

**Remark 2** In ASRS, we first solve the subspace linear system \((12)\) to obtain a search direction \(d^k\), and then update the approximate solution along this search direction. The step size \(\lambda_k\) is used to determine how far we should go from the current search direction, which is computed by the backtracking linesearch method \([61]\). And in practice the parameter \(\omega = 10^{-4}\) is employed to ensure that the reduction of \(\|F(X^k)\|\) is sufficient \([33]\). Moreover, if the active sets in \((9)\) are all through empty, i.e., \(A_\phi(X) = A_\psi(X) = \emptyset\) and \(I(X) = S\), then the active-set reduced-space method degrades into the classical inexact Newton with backtracking (INB) method \([40, 44, 56]\).

3.2 Nonlinear elimination preconditioner

The class of active-set reduced-space algorithms is a suitable generalized Newton-type method for the solution of the nonsmooth nonlinear system of equations. It is one of the standard methods for solving this kind of problems, since it appears to be quite reliable and efficient from the view of the numerical aspects. However, when it is used to solve the multiphase flow problems, the highly nonlinear relative permeability and capillary pressure
functions could result into heavily imbalanced nonlinearity of the system. As a consequence, very slow convergence or even divergence takes place in the aforementioned reduced-space method, which inexactly solves the reduced linear system. In order to improve the robustness and efficiency of the proposed bound-preserving solver, a class of adaptive nonlinear elimination preconditioner is employed, if necessary, to reduce the impact of local nonlinearity on the global system by implicitly removing those solution components that make troubles in Newton iterations.

In this study, the nonlinear elimination preconditioning is performed in a field-split approach, which decomposes the solution vector into two parts $X = (X_{S_b}, X_{S_g}) \in \mathbb{R}^N$. The subscripts $S_b$ and $S_g$ denote the index set for bad and good components respectively, with $S = S_b \cup S_g = \{1, 2, 3, \ldots, N\}$. Based on this partition strategy, the nonlinear system is reformulated as

$$F(X) = F(X_{S_b}, X_{S_g}) = \begin{bmatrix} F_{S_g}(X_{S_b}, X_{S_g}) \\ F_{S_b}(X_{S_b}, X_{S_g}) \end{bmatrix} = 0,$$

where $F_{S_b}(X_{S_b}, X_{S_g})$ and $F_{S_g}(X_{S_b}, X_{S_g})$ represent the nonlinear equations with imbalanced and well-balanced nonlinearities, respectively.

Let us define the subspaces $V_b$ and $V_g$ with respect to $S_b$ and $S_g$ as follows

$$\begin{align*}
V_b &= \{ v \mid v = (v_1, v_2, \ldots, v_n)^T \in \mathbb{R}^N, v_i = 0, \text{ if } i \not\in S_b \}, \\
V_g &= \{ v \mid v = (v_1, v_2, \ldots, v_n)^T \in \mathbb{R}^N, v_i = 0, \text{ if } i \not\in S_g \}.
\end{align*}$$

Moreover, two restriction operators $R_b$ and $R_g$ are designed to restrict the vector $v$ from $\mathbb{R}^N$ to $V_b$ and $V_g$, respectively. Consequently, we can define a sub-nonlinear function $F_{S_b} = R_b(F(X))$ for any given $X \in \mathbb{R}^N$, and define $T_b(X) : \mathbb{R}^N \to V_b$ as the solution of the following subspace nonlinear system

$$F_{S_b}(R_g(X) + T_b(X)) = 0. \tag{17}$$

Thus, by introducing a new global function $G(X) = R_g(X) + T_b(X)$, the good components of the solution vector are retained, while those bad ones are substituted by the solution of (17).

**Remark 3** For multi-component systems, there is no available theoretical guidelines of determining the bad components, and designing a good strategy is often problem-dependent. Hence, different strategies have been proposed to choose the bad components that slow down the convergence of the Newton method. A popular approach, presented in [31, 40], is to predetermine the to-be-eliminated based on the priori knowledge and initiate the nonlinear elimination from the very beginning. In comparison, the proposed nonlinear elimination method is implemented either when the line search fails, or when the parameter $\epsilon_{\text{switch}}$, used to control the activation of subspace correction, is invoked due to the slow convergence of the global iteration. If the subspace correction is ignored, it degenerates to the classical active-set reduced-space method.
3.3. Nonlinearity checking and subproblem construction for multiphase flow

It is noted that the nonlinear elimination method serves as a subproblem solver within the framework of the reduced-space method by eliminating locally large nonlinearities prior to the new global Newton iteration. The key to success in the nonlinear elimination preconditioning depends on the partition of $S_b$ and $S_g$, which further affects the construction of the subspaces $V_b$ and $V_g$.

In this study, we implicitly remove those high-nonlinearity components if they are present during the global nonlinear iterations. In the following, we construct the subproblem in an algebraic way. Now the nonlinear algebraic system (6) is re-organized by the componentwise (field-splitting) order

$$F(X) = (F^{(p_w)}(X), F^{(S_w)}(X), F^{(S_g)}(X), F^{(S_o)}(X)) \in \mathbb{R}^N,$$

where each field subvector $F^{(\beta)}(X), \beta = p_w, S_w, S_g, S_o$, is defined by

$$F^{(\beta)}(X) = (F_1^{(\beta)}(X), F_2^{(\beta)}(X), F_3^{(\beta)}(X), \ldots, F_M^{(\beta)}(X)) \in \mathbb{R}^M$$

with $M = N/4$ being the number of unknowns. Let $\|F^{(\beta)}(X)\|_{\text{max}}$ be the maximum norm of the residual function $F^{(\beta)}(X)$ and the component-wise residuals $\left|F_i^{(\beta)}(X)\right|$ with $i \in \{1, 2, 3, \ldots, M\}$, we use an algebraic-based approach to define the bad region of the component, which is determined by

$$\left|F_i^{(\beta)}(X)\right| > \frac{\rho^{(\beta)}}{M} \|F^{(\beta)}(X)\|_{\text{max}}, \beta = p_w, S_w, S_g, S_o,$$

where $\rho^{(\beta)} > 0$ is a pre-chosen tolerance for the field $\beta$. And then the following index set collects the degrees of freedom with large residual components, which is the so-called bad components:

$$S_b^{\beta} = \left\{ i \in S \mid \left|F_i^{(\beta)}(X)\right| > \frac{\rho^{(\beta)}}{M} \|F^{(\beta)}(X)\|_{\text{max}} \right\}, \beta = p_w, S_w, S_g, S_o.$$

Let $S_b = \cup S_b^{\beta}, \beta = p_w, S_w, S_g, S_o$, and $S_g = S \setminus S_b$, then based on the strategy (19), we build the following subspace nonlinear system for each $i \in S_b$:

$$\begin{cases} X_i = \varphi_i, & F_i(X_{S_b}, X_{S_b}) \geq 0, \\ X_i = \psi_i, & F_i(X_{S_b}, X_{S_b}) \leq 0, \\ X_i \in (\varphi_i, \psi_i), & F_i(X_{S_b}, X_{S_b}) = 0. \end{cases}$$

Note that the above system is solved by the active-set reduced-space method to update the bad components of the solution vector, while the good components of the solution vector are retained.
4. Numerical Experiments

In this section, we report a series of numerical experiments for understanding the performance of the proposed algorithms. The first one is the countercurrent imbibition, by which the proposed formulation exhibits advantages over the conventional pressure-equation-based formulation. In the other examples, the variational inequality formulation solved by the constraint-preserving algorithm is demonstrated to enable the computed solution to sit within the physically meaningful range.

4.1. Countercurrent imbibition

As one of the important oil recovery mechanism in fractured reservoirs, countercurrent imbibition, in which oil and water pass through the same side of the matrix but in opposite directions, is investigated in this example. Due to this particular flow behavior, the multiphase flow model is required to capture the accurate saturation propagation between the opposite flow directions and meanwhile hold mass conservation. Consider the countercurrent imbibition process takes place in a 1D water-wet matrix block where the left end is open to flow and the right end is closed. Both oil and water are assumed to be incompressible. Initially, the domain is saturated with oil and the initial normalized water saturation is 0.01. The oil pressure is assumed to be zero. Because of capillary pressure, the water pressure in the matrix can be computed by $p_w = p_o - p_c = -p_c$. With negligible viscous effect, the capillary force dominates the countercurrent imbibition process and imbibes water, with pressure of 14.7 psia (1 atm), into the matrix to displace oil. Considering the continuity of capillary pressure at the imbibition face, the capillary force is supposed null, meaning that oil and water pressures become equal at the water-contact surface. All the related parameters and functions (e.g. relative permeability and capillary pressure) can be found in [57].

Figure 1 shows the normalized water-saturation profiles after a 5-days countercurrent imbibition process with the time step $\Delta t = 0.1$ day. The black dots represent the numerical result of Pooladi and Firoozabadi at $\Delta t = 5$ days as well, which is highly consistent with the analytical solution as shown in Figure 2 of [57]. We perform the grid-size sensitivity analysis of the countercurrent imbibition at three different grid numbers: $m = 100$, $m = 200$ and $m = 300$. It can be seen the solution of the finer mesh approaches to the analytical solution.

It should be noted that, before the injected water flows out from the production end, the amount of injected water should be exactly same as the computed water saturation over
the entire domain. Therefore, at each time step, we check if the overall water saturation is equal to the amount of injected water. Figure 2 shows the injected water saturation (blue circles) agrees with the water saturation computed through the numerical simulation (solid line) very well. Moreover, the overall oil saturations in the computation domain (dash line) coincide with the initial oil saturation minus the produced oil saturation (red diamonds). It is verified that the proposed formulation holds the mass-conservative property not only for the water phase but also for the oil phase as well.

Figure 1: The normalized water-saturation profiles at $t = 5$ days. Three mesh sizes (100, 200 and 300) are tested for the mesh-size sensitivity analysis. The black dots represent the numerical result of Pooladi and Firoozabadi [57] with 300 gridblocks for the same problem.

4.2. Saturated three-phase flow

Secondly, we use a saturated flow example in [58] to validate our model embraces the bound-preserving property. Consider a 1D reservoir model of 300 m. The initial pressure is 1800 psi ($\approx 124$ bar) and absolute permeability is 100 md everywhere. At the very beginning, the domain is fully saturated with oil, gas and water with phase saturation of 0.8922, 0.0579 and 0.0499. The injected fluid, consisting of 5.13\% oil, 45.48\% gas and 49.39\% water in volume fraction, flows into the left end of the computational domain, and the reservoir fluid is produced from the right end. The injection and production pressure is 2000 psi ($\approx 138$ bar) and 1600 psi ($\approx 110$ bar), respectively. We discretize the computational domain into 500 uniform grid blocks and simulate the saturated three-phase flow for 150 days with the time step $\Delta t = 0.5$ day. In this example, the gas component can dissolve in both oil and
water phases, and the oil component is allowed to vaporize into the gas phase. We ignore the capillary effect and gravitational effect for comparison with the published result. The fluid properties, such as density and viscosity, and rock/fluid property (e.g. relative permeability and capillary pressure), can be computed using the functions presented in [58].

Figure 3 displays the distribution of oil, gas and water saturations. As can be seen, the computed gas and water saturations are consistent with the published results, which are easily obtained from Figure 1 in [58]. Accordingly, the computed oil saturation match up with Trangenstein and Bell’s result as well. Table 1 shows the oil pressure and all three phase saturations in the first six grids at the third iteration. As can be seen, with the help of the ASRS method, the proposed formulation makes the computed solution sit inside the physically meaningful range. In contrast, the INB method fails to protect the boundedness requirement from being violated, thus yielding the irrational pressure and saturation predictions. This could destroy the accuracy and reliability of the simulation results.

4.3. Black oil model

In this subsection, we focus on the black oil model, and suppose that the oil component only exists in the oil phase, i.e., $\rho^o_g = 0$ and $\rho^g_w = 0$ in (1). Fluid properties are adopted from the Ninth Society of Petroleum Engineers (SPE) Comparative Solution Project [51, 59]. In the tests, the porosity of the medium $\phi = 0.2$, the viscosities $\mu_w = 0.3$ cP, $\mu_o = 3.0$ cP and $\mu_g = 0.1$ cP. The void space of medium is initially fully saturated with oil and gas, i.e., the initial conditions are $S^o_w = 10^{-4}$, $S^g_g = 0.1$, and $S^o_o = 1 - S^o_w - S^g_g$. In the computation, the lower-bound in (7) for the saturations is $S^b_\alpha = 10^{-4}$, $\alpha = o, w, g$, which is the minimal value of saturations, while the upper bound is restricted to $S^u_\alpha = 1$; the lower-bound for the pressure is $p^b_w = 1.0135$ bar that denotes the bottomhole pressure at the production well, and there is no restriction to the upper bound, i.e., $p^u_w = +\infty$.  

![Figure 2: Comparison of the injected water saturation and computed water saturation using the mass-conservative bound-preserving formulation (left); the absolute error of the saturation constraint (right).](image-url)
4.3.1. Identical permeability test case

In the first test of this subsection (denoted by Model-1), we consider a black oil problem with the computational domain 300 m × 150 m. The permeability is fixed to the identical value $K = 100$ md. The parameters in the capillary pressure (3) are fixed to $B_{cw} = 10$ and $B_{cg} = 10 \text{ bar} \cdot \text{md}^{1/2}$. The flow is injected from the right side of the domain with the injection rate is 0.1 PV/year, and the production is generated from the left side, respectively. For the simulation of the black oil model, it is hard to construct an analytic solution for the nonlinear problems. One way to validate the result is to observe the mesh convergence of the numerical solutions. We generate three meshes for the correction test, denoting by Mesh#1, Mesh#2 and Mesh#3. The number of degrees of freedom defined on these meshes are $50 \times 25 \times 4$, $100 \times 50 \times 4$ and $200 \times 100 \times 4$, respectively. We plot the numerical solutions of displacement in Figure 4 for the gas-phase saturation along the vertical section $y = 50$. The problem is solved on a $200 \times 100$ mesh, and the time step size is fixed to $\Delta t = 10^{-3}$ year after 1000 time steps. It is clear that the computed solutions converge as the mesh is refined. We remark that, since the profiles for other saturations are the similar, for brevity we simply show the gas-phase saturation.

4.3.2. Layered permeability test case

In the following tests, we focus on the test cases in a horizontal layer with the permeability tensor $\mathbf{K}$ in (1) changing with the computational domain. In the second configuration of
Table 1: The values of the pressure and saturations in the first six mesh cells computed by either the ASRS or INB method at the third iteration.

<table>
<thead>
<tr>
<th>Method</th>
<th>Variable</th>
<th>(1, 1)</th>
<th>(1, 2)</th>
<th>(1, 3)</th>
<th>(1, 4)</th>
<th>(1, 5)</th>
<th>(1, 6)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ASRS</td>
<td>$p_o$</td>
<td>135.2471</td>
<td>135.0851</td>
<td>134.8157</td>
<td>134.6250</td>
<td>134.4075</td>
<td>134.1421</td>
</tr>
<tr>
<td></td>
<td>$S_o$</td>
<td>0.4603</td>
<td>0.4615</td>
<td>0.6664</td>
<td>0.7414</td>
<td>0.7133</td>
<td>0.8204</td>
</tr>
<tr>
<td></td>
<td>$S_g$</td>
<td>0.3245</td>
<td>0.4349</td>
<td>0.2609</td>
<td>0.2072</td>
<td>0.2398</td>
<td>0.1297</td>
</tr>
<tr>
<td></td>
<td>$S_w$</td>
<td>0.2152</td>
<td>0.1036</td>
<td>0.0726</td>
<td>0.0513</td>
<td>0.0469</td>
<td>0.0500</td>
</tr>
<tr>
<td>INB</td>
<td>$p_o$</td>
<td>137.8653</td>
<td>137.7930</td>
<td>138.0550</td>
<td>136.7461</td>
<td>137.1828</td>
<td>136.2728</td>
</tr>
<tr>
<td></td>
<td>$S_o$</td>
<td>-2.0981</td>
<td>1.8737</td>
<td>0.3697</td>
<td>1.6586</td>
<td>0.5348</td>
<td>1.8460</td>
</tr>
<tr>
<td></td>
<td>$S_g$</td>
<td>2.9496</td>
<td>-0.9443</td>
<td>0.5957</td>
<td>-0.7290</td>
<td>0.4298</td>
<td>-0.9122</td>
</tr>
<tr>
<td></td>
<td>$S_w$</td>
<td>0.1485</td>
<td>0.0706</td>
<td>0.0346</td>
<td>0.0704</td>
<td>0.0353</td>
<td>0.0622</td>
</tr>
</tbody>
</table>

Figure 4: The profile curves of the gas-phase saturation with different mesh sizes for Model-1.

In this subsection, we use a more difficult test case (denoted by Model-2), in which its the domain with dimension (500 m × 270 m) is composed of layers of alternate permeabilities (1 md and 100 md), i.e.,

$$k = \begin{cases} 
1 \text{ md} & 30 + 60i \leq y \leq 60 + 60i, \ i = 0, 1, 2, 3, \\
100 \text{ md} & \text{otherwise.}
\end{cases}$$

In the simulation, we assume that the top and bottom boundaries of the domain are impermeable, and the flow system is is uniformly injected across the left-hand side of the layered domain with the production being across the opposite right-hand side. The injection rate is 0.1 PV/year. The parameters in the capillary pressure are fixed to $B_{cw} = 50$ and $B_{cg} = 100$. In Figure 5, we show the plots of the solution profiles that includes the pressure and the water, gas and oil saturations when the constraint-preserving black oil model is used.
The problem is solved on a 200 × 100 mesh, and the time step size is fixed to \( \Delta t = 10^{-3} \) year after 1000 time steps. We observe that the new model can successfully resolve the evolution of the black oil simulation, and meanwhile keep the boundedness requirement of the solution.

\[
\text{(a) } p_w \geq 1.0135 \text{ bar}
\]

\[
\text{(b) } 10^{-4} \leq S_w \leq 1
\]

\[
\text{(c) } 10^{-4} \leq S_g \leq 1
\]

\[
\text{(d) } 10^{-4} \leq S_o \leq 1
\]

Figure 5: Pressure and the saturation profiles by using the ASRS-NE method for Model-2.

Compared with the previous example, in this test case there are some layers and the value of permeabilities has a huge jump inside and outside the zone, which will trigger the nonlinear elimination preconditioning step. It is worthwhile to compare the performance of the classical ASRS method and its nonlinear elimination version (i.e, ASRS-NE) for this problem. In the ASRS-NE method, the role of the parameters \( \rho(\beta) \) in (19) is used to control the efficiency and robustness of the nonlinear elimination preconditioner by determining the subset indices of good and bad components. In our test cases through this section, the parameters in (19) are fixed to \( \rho(P_w) = \rho(S_w) = 10^{-1}, \rho(S_g) = +\infty \) and \( \rho(S_o) = +\infty \); and threshold \( \epsilon_{\text{switch}} = 3 \) is employed as a switch to determine the timing of turning on or off the subspace correction phase. In Figure 6, we show the histories of the nonlinear residuals by
using ASRS and ASRS-NE for Model-2. Results clearly show that the ASRS-NE method can reach the convergence after 15 global nonlinear iterations, while the nonlinear residual norm of the classical ASRS method stagnates around 10 without any progress after many nonlinear iterations and finally it fails to converge.

Figure 6: Nonlinear residual histories at the first time step for Model-2.

4.3.3. Quarter five-spot test case

In the third configuration of this subsection, denoted by Model-3, we use a random distribution of permeabilities in the domain as shown in Figure 7. In this flow model, the medium is highly heterogeneous, which significantly increases the nonlinearity of the system and imposes even greater challenges to the fully implicit solver. In this test case, the computational domain is $300 \text{ m} \times 300 \text{ m}$, the injection and production wells are located at the coordinates $(0, 0)$ and $(300 \text{ m}, 300 \text{ m})$, respectively. The injection rate is $0.01 \text{ PV/year}$. The parameters in the capillary pressure (3) are fixed to $B_{cw} = 50$ and $B_{cg} = 100$. In Figure 7, we display the distributions for the pressure and the saturations by using the variational inequality approach. Results clearly show the successful removal of overshoots and undershoots from the numerical solution when the constraint-preserving black oil model is used. The problem is solved on a $100 \times 100$ mesh, and the time step size is fixed to $\Delta t = 10^{-3} \text{ year}$. Moreover, Figure 8 shows the convergence history plots of the nonlinear residual norms at the first time step for Model-3. Again, the performance of the ASRS-NE method is better than its traditional approach in terms of the robustness and the efficiency.

4.3.4. SPE10 test case

In all of the above test cases, the porosity in the black-oil model (1) is assumed to a constant. In the final test case of this subsection, we import the porosity and the permeability from the Tenth SPE Comparative Project (SPE10) [60], which is a realistic realization
Figure 7: The permeability field, the pressure, and the saturation profiles for Model-3. We use the logarithmic scale for the permeability, i.e., log($K$) where $K$ has a unit of md.
with highly heterogeneous permeabilities and porosities. In the configuration, we import porosity and permeability data from the 20th layer of the model. As shown in Figure 9, the permeability ranges from $6.65 \times 10^{-4}$ md to $2 \times 10^4$ md and the porosity is varied in the interval $[0, 0.5]$. The reservoir domain is 2200 ft $\times$ 1200 ft. The injection well is located at the left hand side of the domain and the oil and gas are across the production well in the opposite right hand side. The injection rate is 0.01 PV/year. The capillary pressure parameters are fixed to $B_{cw} = 10$ and $B_{cg} = 20$. Figure [10] shows the convergence history plots of the nonlinear residual norms at the first time step for the SPE10 benchmark. With the help of the nonlinear elimination method, it is clear that the proposed approach can reach convergence much easier for this test case.

5. Conclusions

In this study, we present a bound-preserving mass-conservative formulation for the multiphase flow problem, which is solved by a well-designed nonlinear solver. The original model is transformed as a variational inequality formulation with the box inequality constraints to ensure the computed pressure and saturations sit within their physically meaningful ranges. In addition, the proposed formulation satisfies the local and global mass conservation. On the basis of inexact Newton methods, the active-set reduced-space method, preconditioned by the nonlinear elimination that eliminates the imbalanced nonlinearity, is employed to efficiently solve the nonlinear complementarity system at each implicit time step. The numerical results show that the proposed formulation preserves both the bound-preserving and mass-conservative properties. With properly introducing complexities, e.g. the mass transfer between hydrocarbon phases, the bound-preserving formulation for the multiphase flow model can be extended to the black oil model, which enables the more accurate char-
Figure 9: Permeability field for the 20th layer of the SPE10 model in the simulation.

Figure 10: Nonlinear residual histories at the first time step for the 20th layer of the SPE10 model.
acterization of the flow behavior in subsurface formations.

Acknowledgment

The authors would like to express their appreciations to the anonymous reviewer for the invaluable comments that have greatly improved the quality of the manuscript. This work is partially supported by the National Natural Science Foundation of China (No. 11971006, 11871069 and 51874262). The authors also greatly thank for the support from King Abdullah University of Science and Technology (KAUST) through the grants BAS/1/1351-01, REP/1/2879-01, and URF/1/3769-01. The first author was also supported in part by the PetroChina Innovation Foundation (2019D-5007-0213).

References


[27] Y. Liu, H. Yang, Z. Xie, P. Qin, R. Li, Parallel simulation of variably saturated soil water flows by fully implicit domain decomposition methods, J. Hydrol. 582 (2020) 124481.


