

A discrete-domain approach to three-phase hysteresis in porous media

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November 22, 2022

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Key Points:

- Constrained energy minimization in a discrete-domain approach describes three-phase capillary pressure and hysteresis from pore to core scale
- Inclusion of saturation constraints leads to a variety of three-phase displacements with fluid redistribution, pressure- and saturation-jumps.
- A fast and flexible method to calculate three-phase capillary pressure for higher-order hysteresis loops.

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Abstract

We present a discrete-domain approach to three-phase displacements and hysteresis in porous media. Constrained energy minimization leads to evolution equations for local saturations that describe a wide range of three-phase displacements, including pressure- and saturation-controlled displacement with or without preservation of one of the defending phases. Under action of global saturation constraints, irreversible displacements lead to significant fluid redistribution, as well as abrupt fluctuations of both the three-phase saturation paths and the corresponding capillary pressures. These features are a consequence of Haines jumps with cooperative behavior that occur at pore scale in three-phase systems. The method is a fast and convenient way to investigate hysteresis behavior of three-phase displacement in porous media. As free energy is an extensive property, the framework links pore and core scales and provide a means to achieve upscaled three-phase displacements for higher-order hysteresis loops, which rarely is obtained in time-consuming three-phase measurements or pore-scale simulations.

Plain Language Summary

Knowledge of the way three fluids move through the pore space inside porous rocks is crucial to describe oil recovery and CO₂ storage processes in subsurface reservoirs. Because of the complex pore structure, interfaces between fluids do not generally recede (drainage) in the same way as they advance (imbibition), upon reversal of displacement direction. This means that the displacement is irreversible and depends on the history of fluid displacements. This is called hysteresis. At macroscopic scale, hysteresis is often quantified by the difference in capillary pressure-saturation curves between drainage and imbibition. The extent of hysteresis is a collective effect of many reversible and irreversible displacement events at pore scale. Hysteresis in two-phase fluid systems has been the subject of many previous studies. Here, we present a method to describe irreversible displacement and hysteresis in three-phase systems. Based on thermodynamics, we describe hysteresis as irreversible transitions across barriers in an energy landscape exhibiting metastability. Constrained minimization results in saturation evolution equations that collectively describe various irreversible three-phase displacements and corresponding capillary pressure-saturation curves. We envision that the approach is a suitable upscaling tool for relating three-phase hysteresis behavior from pore scale with macroscopic scale.

1 Introduction

An inherent challenge with multiphase flow processes in porous media, such as water-alternate-gas invasions for oil recovery or CO₂ injection for geologic storage, is that fluid displacements are irreversible, that is, they are history-dependent and exhibit hysteresis (Spiteri & Juanes, 2006). Hysteresis can be rate-dependent or rate-independent. Here, we examine rate-independent hysteresis in three-phase systems based on an energy landscape exhibiting metastability and barriers. Thus, we approach fluid displacements quasi-statically as a series of small changes of pressure or saturation. This is a reasonable approximation for slow displacement at pore scale where capillary forces typically dominate over viscous forces and gravity (Hilfer & Øren, 1996). At darcy (or, core) scale, hysteresis in two-phase systems emerges as the difference between drainage and imbibition capillary pressure curves ($P_{\alpha\beta}(S_\beta)$ -curves), where capillary pressure is the difference in phase pressures p between non-wetting (α) and wetting (β) phases (i.e., $P_{\alpha\beta} = p_\alpha - p_\beta$), and S_β is wetting-phase saturation. Collectively, the shape of $P_{\alpha\beta}(S_\beta)$ -curves depends on porous structure, pore-scale fluid displacements, saturation history and wetting state. Morrow (1970) interpreted $P_{\alpha\beta}(S_\beta)$ -curves thermodynamically as a sequence of reversible and irre-

versible pore-scale fluid displacements, termed “isons” and “rheons”, respectively, that describe transitions between capillary equilibrium states (i.e., local energy minima). Here, isons describe smooth changes of capillary pressure and saturation, while rheons, being responsible for energy dissipation and hysteresis (Morrow, 1970), describe instabilities that arise when a fluid invades a pore region accompanied by abrupt pressure jumps and spontaneous fluid redistributions in other parts of the pore space at almost constant saturation. This phenomenon, also called Haines jumps with cooperative behavior (Haines, 1930), has been investigated in two-phase flow in numerous experimental and numerical studies (e.g., Morrow, 1970; Måløy et al., 1992; Moebius & Or, 2012; Armstrong & Berg, 2013; Andrew et al., 2015; Berg et al., 2013; Zacharoudiou & Boek, 2016; Cueto-Felgueroso & Juanes, 2016; Helland et al., 2017; Holtzman et al., 2020, and others).

For three-phase flow, hysteresis and irreversible displacements are more complex and much less explored. This is due to several reasons. Displacement behavior vary significantly with immiscible and near-miscible fluid systems, spreading and non-spreading oils, and different wetting orders of the three phases (Keller et al., 1997; Hui & Blunt, 2000; van Dijke & Sorbie, 2002; Khishvand et al., 2016; Alhosani et al., 2019; Scanziani et al., 2020). At the pore scale, double displacements (Øren & Pinczewski, 1995; Keller et al., 1997; Khishvand et al., 2016; Helland & Jettestuen, 2016; Helland et al., 2019), where a continuous phase displaces a second isolated phase that displaces a third continuous phase, and multiple displacement chains (van Dijke & Sorbie, 2003; Scanziani et al., 2020; Jettestuen et al., 2020), where the continuous phases displace a chain of several isolated fluid ganglia, make three-phase flow different to two-phase flow. Further, three-phase experiments are time-consuming and challenging, while three-phase pore-scale simulations are computationally demanding (Helland et al., 2019; Jettestuen et al., 2020). They both rely on having established the relevant two-phase saturation history prior to the investigation. Finally, a two-phase displacement occurs with saturation change in one of two directions, while a three-phase saturation path can take infinitely many directions. Thus, measuring a sufficient amount of $P_{\alpha\beta}(S_\beta)$ -curves for main and nested hysteresis loops in three-phase systems at relevant conditions is hardly achievable.

The standard approach to deal with hysteresis of $P_{\alpha\beta}(S_\beta)$ -curves is to use correlations, equipped with a hysteresis loop logic model and a trapping model relating end-point saturations (e.g., Land, 1968; Lenhard, 1992; Skjæveland et al., 2000; Helland & Skjæveland, 2004; Spiteri et al., 2008; Lomeland & Ebeltoft, 2013, and others). While this is practical, it requires several fitting parameters that lacks a firm physical basis. Other approaches seek to eliminate hysteresis by adding new state variables based on Minkowski functionals (like interfacial area) in the incomplete $P_{\alpha\beta}(S_\beta)$ -function (Hassanizadeh & Gray, 1993; McClure et al., 2018), whereas emerging theories circumvent $P_{\alpha\beta}(S_\beta)$ -curves and hysteresis completely (Hansen et al., 2018). Cueto-Felgueroso and Juanes (2016) developed a two-phase discrete-domain model for hysteresis that describes Haines jumps as irreversible transitions among metastable states in a rugged energy landscape. The method envisions the porous medium as a discrete set of compartments, each with their own given energy function and local saturation. This facilitates simulations of pressure-controlled displacement, which calculates saturations for a prescribed series of capillary pressures, and saturation-controlled displacement, which mimics displacement at infinitesimally low rate and calculates capillary pressures for a prescribed series of global saturations. The latter displacement mode enforces a global saturation constraint that leads to fluid redistribution among compartments (cooperative behavior) and pressure fluctuations, consistent with saturation-controlled pore-scale simulations (Helland et al., 2017). Discrete-domain methods can be viewed as upscaling procedures from pore to core scales, as compartment energies are extensive properties (Cueto-Felgueroso & Juanes, 2016). These methods have also been used in other scientific fields (Puglisi & Truskinovsky, 2005; Dreyer et al., 2010, 2011;

Fraternali et al., 2011). In this work, we present a discrete-domain approach to characterize three-phase displacements with hysteresis. We show that metastability and the inclusion of various saturation constraints gives rise to irreversible three-phase displacements with cooperative behavior and fluid redistribution, accompanied by fluctuations of capillary pressures and saturation trajectories.

2 Method

We consider a porous medium saturated with three continuous fluids, gas (g), oil (o) and water (w), that are connected to their respective fluid reservoirs. Assuming the multiphase system is isothermal with incompressible fluids of constant composition, a thermodynamic potential for a Gibbs-like free energy is

$$G = \sum_{\alpha=g,o,w} (-p_{\alpha}V_{\alpha} + F_{\alpha}), \quad (1)$$

where p_{α} is pressure and V_{α} is volume of phase α . Here, we introduce the *phase-specific* Helmholtz free energy, F_{α} , which models the energy contribution from phase α to the fluid/fluid and fluid/solid interfacial free energies. This splitting strategy borrows ideas from pore-scale modelling of three-phase displacement where interfacial properties, like interfacial tension and contact angle, are formulated as the sum of individual phase contributions (Helland & Jetttestuen, 2016; Helland et al., 2019; Jetttestuen et al., 2020). We also assume this Helmholtz energy is a function of its own phase volume only, i.e., $F_{\alpha} = F_{\alpha}(V_{\alpha})$, in accordance with previous work (Cueto-Felgueroso & Juanes, 2016; Morrow, 1970).

Following Cueto-Felgueroso and Juanes (2016), let us now divide the porous medium into N compartments with equal pore volumes V_p . The global (or, average) phase saturation is $S_{\alpha} = \frac{1}{N} \sum_{i=1}^N s_{\alpha,i}$ where $s_{\alpha,i}$ is local saturation of phase α in compartment i . We introduce phase-specific compartment energy densities $f_{\alpha,i}$ as functions of their own saturations, $f_{\alpha,i} = f_{\alpha,i}(s_{\alpha,i})$, so that $F_{\alpha} = V_p \sum_{i=1}^N f_{\alpha,i}(s_{\alpha,i})$. Similarly, for Gibbs energy we obtain $G_{\alpha} = V_p \sum_{i=1}^N g_{\alpha,i}$. With this compartment description, equation (1) becomes

$$G = V_p \sum_{i=1}^N \left(\sum_{\alpha=g,o,w} g_{\alpha,i} \right) = V_p \sum_{i=1}^N \left(\sum_{\alpha=g,o,w} (-p_{\alpha}s_{\alpha,i} + f_{\alpha,i}(s_{\alpha,i})) \right). \quad (2)$$

Minimization of G with respect to $s_{\alpha,i}$ yields an equation per saturation per compartment. The resulting set of $3N$ equations is uncoupled and neglects that the sum of phase saturations must equal one in all compartments. To handle this problem, still by treating the compartment saturations $s_{\alpha,i}$ as independent variables, we introduce N constraints that couple the three saturations together in each compartment:

$$\frac{1}{2} \left(\sum_{\alpha=g,o,w} s_{\alpha,i} - 1 \right)^2 = 0, \quad i = 1, \dots, N. \quad (3)$$

In the numerical model, we set the left-hand side of equations (3) equal to a small positive number ϵ . The method of Lagrange multipliers is a suitable approach to solve such constrained minimization problems. Thus, we introduce the function

$$\mathcal{L}(\mathbf{s}, \boldsymbol{\lambda}) = V_p \sum_{i=1}^N \left(\sum_{\alpha=g,o,w} (-p_{\alpha}s_{\alpha,i} + f_{\alpha,i}(s_{\alpha,i})) - \frac{\lambda_i}{2} \left(\sum_{\beta=g,o,w} s_{\beta,i} - 1 \right)^2 \right), \quad (4)$$

where \mathbf{s} is a vector of the $3N$ compartment saturations and $\boldsymbol{\lambda} = [\lambda_1, \dots, \lambda_N]$ is a vector of Lagrange multipliers corresponding to the N constraints (3). Minimization of \mathcal{L}

with respect to each $s_{\alpha,i}$ amounts to solving $\frac{\partial \mathcal{L}}{\partial s_{\alpha,i}} = 0$. Parameterizing the solutions in iteration-time t yields $3N$ evolution equations for the compartment saturations:

$$\frac{\partial s_{\alpha,i}}{\partial t} = p_{\alpha} + \lambda_i \left(\sum_{\beta=g,o,w} s_{\beta,i} - 1 \right) - \frac{\partial f_{\alpha,i}}{\partial s_{\alpha,i}}, \quad (5)$$

where $\alpha = g, o, w$ and $i = 1, \dots, N$. We solve equations (5) for given pressures p_{α} and energies $f_{\alpha,i}$ to find equilibrium states of the compartment saturations, using the explicit Euler method for the iteration-time steps. We assume equations (5) have been made dimensionless by scaling with a characteristic pressure. As we calculate equilibrium states, this scaling will only impact the rate of convergence while the solutions remain the same.

The compartment saturations reach equilibrium states when $\frac{\partial s_{\alpha,i}}{\partial t} = 0$. Equations (5) imply that this occurs when the capillary pressures for all fluid pairs $\alpha\beta = go, ow, gw$ satisfy

$$P_{\alpha\beta} = p_{\alpha} - p_{\beta} = - \left(\frac{\partial f_{\beta,i}}{\partial s_{\beta,i}} - \frac{\partial f_{\alpha,i}}{\partial s_{\alpha,i}} \right), \quad i = 1, \dots, N. \quad (6)$$

When the third phase is absent or immobile, $ds_{\alpha,i} = -ds_{\beta,i}$, and we can write equations (6) as $P_{\alpha\beta} = - \frac{\partial(f_{\alpha,i} + f_{\beta,i})}{\partial s_{\beta,i}}$. This is the equilibrium states for a two-phase system, consistent with the single saturation approach of Cueto-Felgueroso and Juanes (2016).

The energy functions $f_{\alpha,i}(s_{\alpha,i})$ contain concave and convex segments (peaks and valleys) to describe metastability in a rugged energy landscape. Stable and metastable states satisfy equations (6). In addition, the free interfacial energy must belong to convex segments with local minima of Gibbs free energy. In the two-phase case these valleys satisfy $\frac{\partial^2 f_i}{\partial s_{\beta,i}^2} \geq 0$ where $f_i = f_{\alpha,i} + f_{\beta,i}$. A peak in f_i represents an energy barrier that must be overcome in a transition from the current to the next, adjacent, metastable state. In the three-phase system, where $f_i = f_{g,i} + f_{o,i} + f_{w,i}$, the metastable states satisfy equations (6) while the second derivative of the interfacial free energy with respect to the relevant compartment saturation is positive for all phase pairs go , ow , and gw , respectively:

$$\left(\frac{\partial^2 f_i}{\partial s_{o,i}^2} \right)_{s_{w,i}} \geq 0, \quad \left(\frac{\partial^2 f_i}{\partial s_{w,i}^2} \right)_{s_{g,i}} \geq 0, \quad \text{and} \quad \left(\frac{\partial^2 f_i}{\partial s_{w,i}^2} \right)_{s_{o,i}} \geq 0. \quad (7)$$

Here, the subscripted variable outside the parenthesis is held constant in the derivation. Equation (7) is the equilibrium locus, that is, the states that correspond to equilibrium compartment saturations for any phase pressure combination.

3 Three-phase displacement protocols

Equations (5) offer the opportunity to investigate various three-phase displacement modes, like invasion under preservation of a constant global saturation, or invasion controlled by prescribed global saturations. Introducing a global saturation constraint for one or more phases α ,

$$S_{\alpha} = \frac{1}{N} \sum_{i=1}^N s_{\alpha,i} = \text{const}, \quad (8)$$

will couple the saturation equations for the different compartments together. Despite global saturations are fixed under such constraints, significant redistribution of local saturations among compartments can occur, possibly accompanied by three-phase capillary pressure fluctuations. Here we apply equations (5) to a range of different three-phase displacement protocols.

3.1 Gas-pressure controlled displacement (PG)

This case prescribes all phase pressures p_g , p_o and p_w . Gas invasion (retraction) occurs by increasing (decreasing) p_g in small specified steps Δp after each converged state of equations (5). The N compartment constraints (3) must hold for all iteration times. Thus,

$$\frac{d}{dt} \left(\frac{1}{2} \left(\sum_{\alpha=g,o,w} s_{\alpha,i} - 1 \right)^2 \right) = \left(\sum_{\alpha=g,o,w} s_{\alpha,i} - 1 \right) \sum_{\alpha=g,o,w} \frac{\partial s_{\alpha,i}}{\partial t} = 0. \quad i = 1, \dots, N. \quad (9)$$

Combining equations (5) and (9) yields expressions for the Lagrange multipliers that we update in every iteration step:

$$\lambda_i = - \frac{\sum_{\alpha=g,o,w} \left(p_{\alpha} - \frac{\partial f_{\alpha,i}}{\partial s_{\alpha,i}} \right)}{3 \left(\sum_{\alpha=g,o,w} s_{\alpha,i} - 1 \right)}, \quad i = 1, \dots, N. \quad (10)$$

3.2 Gas-pressure controlled displacement with constant global oil saturation (PGSO)

This case prescribes phase pressures p_g and p_w . As for the previous case, gas invasion (retraction) occurs by increasing (decreasing) p_g stepwise after each equilibrium state. We preserve global oil saturation S_o by enforcing constraint (8) on the oil phase, while treating the oil pressure p_o as the associated Lagrange multiplier. Together with equations (3) we now have $N + 1$ constraints that must hold for all iteration times. Equation (8) implies that

$$\frac{\partial S_o}{\partial t} = \frac{\partial}{\partial t} \left(\frac{1}{N} \sum_{i=1}^N s_{o,i} \right) = \frac{1}{N} \sum_{i=1}^N \frac{\partial s_{o,i}}{\partial t} = 0. \quad (11)$$

By inserting the evolution equations (5) into equations (11) and (9), we obtain

$$p_o + \frac{1}{N} \sum_{i=1}^N \lambda_i \left(\sum_{\alpha=g,o,w} s_{\alpha,i} - 1 \right) = \frac{1}{N} \sum_{i=1}^N \frac{\partial f_{o,i}}{\partial s_{o,i}} \quad (12)$$

and

$$p_g + p_o + p_w + 3\lambda_i \left(\sum_{\alpha=g,o,w} s_{\alpha,i} - 1 \right) = \sum_{\alpha=g,o,w} \frac{\partial f_{\alpha,i}}{\partial s_{\alpha,i}}, \quad i = 1, \dots, N, \quad (13)$$

respectively. Equations (12) and (13) constitute $N + 1$ equations that we solve for the Lagrange multipliers p_o and $\lambda_1, \dots, \lambda_N$ in every iteration step.

3.3 Gas-saturation controlled displacement (SG)

This case prescribes phase pressures p_o and p_w . Gas invasion (retraction) occurs by increasing (decreasing) global gas saturation S_g in small specified steps Δs after each converged state of equations (5), while we calculate p_g . For each target gas saturation, we initialize the compartment gas saturations as $s_{g,i} \pm \Delta s$ and adjust the compartment oil and water saturations correspondingly, $s_{o,i} \mp \Delta s/2$ and $s_{w,i} \mp \Delta s/2$. Obviously, the compartment saturations at equilibrium will differ from this initial configuration. Equation (8) enforces the target global gas saturation, so that p_g becomes the associated Lagrange multiplier. Thus,

$$p_g + \frac{1}{N} \sum_{i=1}^N \lambda_i \left(\sum_{\alpha=g,o,w} s_{\alpha,i} - 1 \right) = \frac{1}{N} \sum_{i=1}^N \frac{\partial f_{g,i}}{\partial s_{g,i}}. \quad (14)$$

Equations (13) and (14) constitute $N + 1$ equations that provide solutions for p_g and $\lambda_1, \dots, \lambda_N$ in every iteration step.

3.4 Gas-saturation controlled displacement with constant global oil saturation (SGSO)

This case prescribes water pressure p_w and calculates p_g and p_o . Gas invasion (retraction) occurs by increasing (decreasing) the global gas saturation S_g in small specified steps Δs after each equilibrium state, while global oil saturation S_o is fixed. For each target gas saturation, we initialize compartment saturations as $s_{g,i} \pm \Delta s$ and $s_{w,i} \mp \Delta s$. We enforce equation (8) on both the gas and oil phases, so that both p_g and p_o are Lagrange multipliers. Together with equations (3) we now have $N + 2$ constraints. Equations (12), (13) and (14) constitute the $N + 2$ equations from which we calculate the Lagrange multipliers $p_g, p_o, \lambda_1, \dots, \lambda_N$ in every iteration step.

4 Results

We apply the method to elucidate three-phase displacements and hysteresis behavior for the previously described displacement protocols, using oscillatory energy density functions to capture energy barriers and metastability. To this end, we make advantage of the energy functions employed in the single-saturation, two-phase approach (Cueto-Felgueroso & Juanes, 2016):

$$f_i(s_i) = s_i \log s_i + (1 - s_i) \log (1 - s_i) - \omega s_i - c_i \cos(K\pi s_i), \quad i = 1, \dots, N, \quad (15)$$

where s_i is the wetting-phase compartment saturation, ω represents the strength of the wetting state, K reflects the number of minima in each compartment, and $c_i, i = 1, \dots, N$, describe the barriers between energy minima that are responsible for the hysteresis. If ω varies among compartments, the system has a fractional wetting state, whereas a constant and uniform ω (as we use in this work) describes a uniform wetting state.

In the multiple saturation approach, we construct phase-specific energy contributions $f_{\alpha,i}(s_{\alpha,i})$ that ensure the equilibrium solutions (6) for fluid pair $\alpha\beta$ are consistent with the solutions from the single-saturation approach for two-phase systems using equation (15). We accomplish this with

$$f_{\alpha,i}(s_{\alpha,i}) = s_{\alpha,i} \log s_{\alpha,i} - \omega_{\alpha} s_{\alpha,i} - c_{\alpha,i} \cos(K_{\alpha} \pi s_{\alpha,i}), \quad \alpha = g, o, w, \quad i = 1, \dots, N, \quad (16)$$

where the parameters for each fluid pair $\alpha\beta$ satisfy $K = K_{\alpha} = K_{\beta}$, $\omega = \omega_{\beta} - \omega_{\alpha}$, and $c_i = c_{\alpha,i} + c_{\beta,i}$ (for even integers K). As we explore displacements constrained by stepwise saturation changes Δs , we specify a saturation interval $[s_{\min}, s_{\max}]$ that we require all compartment saturations to be located within. If a compartment saturation reaches one of these limits, that compartment is static and excluded from the further saturation evolution based on equations (5) and Lagrange multipliers. Thus, the number of possible metastable states decreases toward the end of the displacement process, possibly accompanied by more severe pressure fluctuations. Here, we use $s_{\min} = 0.001$ and $s_{\max} = 0.999$. This approach also offers a means to include residual saturations that may vary with compartment. The simulations presented here achieve equilibrium states when all compartment saturations change by less than 10^{-8} during an iteration step.

First, we demonstrate the discrete-domain method on a small number of compartments for a water-wet state where oil is intermediate-wet phase and gas is non-wetting phase (Hui & Blunt, 2000; van Dijke & Sorbie, 2002). This implies $\omega_w > \omega_o > \omega_g$ and $c_{w,i} > c_{g,i} > c_{o,i} > 0, i = 1, \dots, N$. We set $N = 3, K = 4, \omega_w = 11, \omega_o = 6, \omega_g = 1, c_w = [0.1, 0.2, 0.3], c_o = [0.001, 0.03, 0.05]$, and $c_g = (c_w + c_o)/2$. We simulate a two-phase oil/water hysteresis loop consisting of primary drainage and imbibition by applying evolution equations (5) on the two phases, using $\Delta p = 0.1$ for pressure-controlled displacement and $\Delta s = 0.005$ for saturation-controlled displacement. Figure 1(a)

shows that pressure-controlled Haines jumps create irreversible saturation jumps at constant pressure. Such an event is a jump in one of the compartment saturations across an energy barrier separating two metastable states of Gibbs free energy, while the other compartment saturations stay in their energy valleys. Overall, this generates a stepwise staircase shape on the $P_{ow}(S_w)$ -curves, where steep and smooth curve segments represent reversible displacements within the same energy valleys. Haines jumps in saturation-controlled mode occur as abrupt, irreversible pressure drops (drainage) or increases (imbibition) at constant global saturation. While these events also create a jump across an energy barrier in one compartment, the other compartment saturations move in the opposite direction to maintain the global target saturation. Hence, fluid redistribution among compartments occurs. Reversible displacements follow the same branches of the $P_{ow}(S_w)$ -curves as the pressure-controlled displacements. Overall, the $P_{ow}(S_w)$ -curves obtain nonmonotonic sawtooth shapes which we also observe in the evolution of compartment saturations.

We proceed with corresponding three-phase displacements by introducing gas at $S_w = 0.4$ after the pressure-controlled imbibition. Figure 1(b) presents results for a gas invasion-retraction hysteresis loop using both PG and SG displacement protocols. The $P_{go}(1 - S_g)$ - and $P_{gw}(1 - S_g)$ -curves have identical shapes and differ only by the constant P_{ow} . They display similar behavior as the two-phase case. Energy barriers connecting the equilibrium locus of Gibbs free energy represent instabilities. In three-phase systems we cannot construct these barriers because compartment-saturation paths are not known *a priori*. This differs from two-phase systems where saturation changes in one of two directions. A Haines jump in SG mode occurs when the saturation state in one compartment jumps across a barrier to another state in the neighbor energy valley, while compensating saturation changes occur in the other compartments to maintain the global, target gas saturation. For the transition of states during gas invasion marked by magenta and cyan circles in Figure 1(b), $s_{g,1}$ increases at the expense of lower $s_{o,1}$ and $s_{w,1}$ in compartment 1, while in the other compartments $s_{g,2}$ and $s_{g,3}$ decrease at the expense of higher $s_{o,2}$, $s_{w,2}$, $s_{o,3}$ and $s_{w,3}$. The global saturation paths show that the overall result for this change of states is slightly higher S_g and S_w and lower S_o . This emerges as a characteristic feature for Haines jumps in SG mode: Gas invasion (retraction) occurs with accompanying water invasions displacing oil, or oil invasions displacing water, leading to abrupt directional changes of the saturation path (that is, oil and water saturation jumps). Reversible displacements within the same energy valleys aim at driving the saturation path back on track so that equilibrium states in PG and SG modes coincide between Haines jumps. The main observation is that saturation paths in SG mode display a characteristic stepwise staircase shape, while in PG mode they consist of gas-saturation jumps intertwined with more steady saturation changes. Differences in compartment-saturation evolution confirm the behavior: SG mode shows significant fluid redistribution among compartments and saturation fluctuations, while PG mode shows stepwise, monotonically increasing or decreasing compartment saturations.

The parameters ω_α and $c_{\alpha,i}$ in equation (16) make it possible to explore hysteretic three-phase displacements at other realistic wetting states. A weakly oil-wet system (Hui & Blunt, 2000; van Dijke & Sorbie, 2002), where water is intermediate-wetting phase and gas non-wetting phase, requires $\omega_o > \omega_w > \omega_g$, $c_{g,i} > 0 > c_{o,i} > c_{w,i}$, and $c_{g,i} > |c_{w,i}|$, i, \dots, N . In a strongly oil-wet system (Hui & Blunt, 2000; van Dijke & Sorbie, 2002), where gas is intermediate-wetting phase and water non-wetting phase, we must have $\omega_o > \omega_g > \omega_w$, $c_{g,i} > 0 > c_{o,i} > c_{w,i}$, and $|c_{o,i}| < c_{g,i} < |c_{w,i}|$, i, \dots, N . To explore three-phase hysteresis for these oil-wet states, we use a slightly larger system with $N = 6$ and $K = 8$. Further, $\omega_o = 11$, $c_{w,i}$ is evenly spaced between $c_{w,1} = -0.15$ and $c_{w,6} = -0.01$, and $c_{o,i} = -0.001$, $i = 1, \dots, 6$. Then, for the weakly oil-wet state, $\omega_w = 6$, $\omega_g = 1$, and $c_{g,i} = -1.2c_{w,i}$, and for the strongly oil-wet state, $\omega_w = 1$, $\omega_g = 6$, and $c_{g,i} = -0.5c_{w,i}$, $i = 1, \dots, 6$. We add a water-wet case for comparison,

with parameters $\omega_w = 11$, $\omega_o = 6$, $\omega_g = 1$, $c_{w,i}$ evenly spaced between $c_{w,1} = 0.01$ and $c_{w,6} = 0.15$, $c_{o,i} = 0.001$, and $c_{g,i} = (c_{w,i} + c_{o,i})/2$, $i = 1, \dots, 6$. Figure 2 presents two- and three-phase results from simulations of these wetting states, using $\Delta p = 0.05$ in PG mode and $\Delta s = 0.0025$ in SG mode. These steps are sufficiently small to capture all metastable states. The three-phase hysteresis loops begin at $S_w = 0.5$ on the pressure-controlled two-phase imbibition curve. The capillary pressure curves capture the expected differences in pressure levels for the different wetting states, and they all show the same characteristic Haines jump behavior. In SG mode, the three-phase capillary pressure curves and saturation paths fluctuate due to Haines jumps. For intervals with reversible displacements both the capillary pressure curves and saturation paths coincide in PG and SG mode. The compartment-saturation profiles show fluctuations in SG mode, particularly for the water-wet state, which indicates fluid redistribution among compartments, while for PG mode, these curves are stepwise and monotonic curves. Further, the compartment-saturation profiles exhibit hysteresis and show that fluid distributions vary with wetting state.

Along with the hysteresis loops, we also simulate gas invasion in PG mode from $S_w = 0.3$ and $S_w = 0.7$ to investigate saturation-dependencies of the three-phase capillary pressures in the presence of hysteresis. Simple capillary-tube bundle models, where hysteresis is absent, predict that two of the capillary pressures are functions of one saturation, as follows (Hui & Blunt, 2000; van Dijke & Sorbie, 2002): $P_{go}(S_g)$ and $P_{ow}(S_w)$ (water-wet state), $P_{ow}(S_o)$ and $P_{gw}(S_g)$ (weakly oil-wet state), and $P_{go}(S_o)$ and $P_{gw}(S_w)$ (strongly oil-wet state). In each case, the remaining capillary pressure is a function of two saturations. However, our simulated results deviate from this idealized description, which we attribute to the inherent hysteresis of the method and chosen energy functions. Instead we find that all three capillary pressures depend on two saturations. For example, the simulated saturation paths at constant P_{ow} in Figure 2 shows that P_{ow} depends on two saturations although significant oil displacement (especially in the water-wet system) indicates strong S_w -dependency. Further, the $P_{go}(1 - S_g)$ -curves (water-wet state) and $P_{gw}(S_w)$ -curves (strongly oil-wet state) for the three PG-based gas invasions do not coincide, implying that also these capillary pressures are functions of two saturations.

Finally, we explore three-phase PGSO and SGSO displacements in a large water-wet system with constant global oil saturation $S_o = 0.3$, established after a two-phase pressure-controlled imbibition. We use $N = 24$, $K = 14$, $\omega_w = 26$, $\omega_o = 14$, $\omega_g = 2$, $c_{w,i}$ evenly spaced between $c_{w,1} = 0.05$ and $c_{w,24} = 0.15$, $c_{o,i}$ evenly spaced between $c_{o,1} = 0.001$ and $c_{o,24} = 0.05$, and $c_{g,i} = (c_{o,i} + c_{w,i})/2$, $i = 1, \dots, 24$. To capture all metastable states of this large system, we use $\Delta s = 0.001$ (SGSO) and $\Delta p = 0.05$ (PGSO). Figure 3(a) shows $P_{ow}(S_w)$ -curves for two-phase hysteresis loops, as well as results from the subsequent PGSO- and SGSO-simulations of main and nested three-phase hysteresis loops for gas invasions and gas retractions. For these displacement protocols all three capillary pressures vary during the displacement. Even in PGSO mode, P_{go} and P_{ow} display nonmonotonic variations, implying significant redistribution of the globally preserved oil phase. A sharp increase (or, drop) of P_{go} leads to a corresponding drop (or, increase) of P_{ow} for prescribed P_{gw} . For gas invasion in PGSO mode P_{ow} increases almost monotonically, while P_{go} vary nonmonotonically around the same pressure level. Three-phase pore-scale simulations of the same process explain this observation (Helland et al., 2019): A double displacement in which gas displaces a disconnected oil phase through wide and narrow pore channels, that in turn pushes oil/water interfaces further into narrower pore spaces, leads to nonmonotonic P_{go} and increasing P_{ow} . The three-phase capillary pressure curves from SGSO simulations display a more irregular sawtooth structure than the two-phase curves due to significant oil redistribution among compartments. The $s_{o,i}(1 - S_g)$ -curves show that this redistribution generally is different in PGSO and SGSO simulations so that the corresponding three-phase capillary pressure curves also deviate from each other.

For this system we also simulate main and nested hysteresis loops with PG and SG mode, starting at $S_o = 0.7$ from the two-phase pressure-controlled imbibition. In this case, the capillary pressure curves for PG and SG modes are more aligned with each other and they also display a more regular sawtooth structure, see Figure 3(b). Because the saturation paths for gas invasion and gas retraction vary, nested hysteresis loops are not fully contained within the main hysteresis loop. This is in contrast to the PGSO and SGSO cases where the saturation path is enforced. The SG and SGSO simulations in Figure 3 display severe pressure fluctuations near the end of the displacement processes. This is an effect of excluding compartments where saturations have reached their limits s_{\min} or s_{\max} , which significantly reduces the number of possible metastable states in subsequent calculations. Still, SG simulations of this large system exhibit less significant capillary pressure fluctuations in most of the saturation interval, while the stepwise, staircase features of the saturation paths in SG mode are less prominent, compared with smaller systems (Figures 1 and 2). Thus, increasing the system size (that is, N and K) yields smaller fluctuations because the density and number of metastable states increases, while hysteresis persists. This shows the potential of the discrete-domain approach as a method for upscaling three-phase capillary pressure curves with hysteresis from pore to larger scales where such fluctuations vanish.

5 Conclusions

This work presents a discrete-domain approach to three-phase displacements with rate-independent hysteresis in porous media. Constrained energy minimization leads to evolution equations for compartment saturations that collectively describe a wide range of three-phase displacements, including reversible and irreversible pressure- and saturation-controlled displacements with or without preservation of one of the defending phases. Saturation-controlled invasion, which mimics flow controlled by low rate, shows that three-phase irreversible displacements occur with significant fluid redistribution among compartments. This leads to abrupt capillary pressure jumps as previously seen in two-phase systems, and in addition, abrupt saturation changes and fluctuating saturation paths, which we find is a new characteristic feature for three-phase displacements. Both pressure and saturation jumps decrease with increasing system size. Three-phase displacements with a preserved saturation exhibit the most substantial fluid redistributions, and in these cases both pressure- and saturation-controlled displacement generate nonmonotonic capillary pressure curves, consistent with quasi-static pore-scale simulations (Helland et al., 2019). The presented discrete-domain approach is a fast and tractable method to investigate three-phase hysteresis in porous media. A current drawback is that the compartments are not spatially correlated and hence they are all accessible for invasion. In future work we will use spatially dependent energy functions from pore-scale experiments and simulations to evaluate effects of wetting state on three-phase irreversible displacement. As compartment energies are extensive quantities, establishing a direct link between pore scale and the compartmental description will provide a reliable upscaling method. Finally, compartment energies tailored to match pore-scale data will reveal whether the energy functions themselves exhibit hysteresis and if they require other state variables (like interfacial area) to describe uniquely drainage and imbibition.

Acknowledgments

We would like to thank our colleague Olav Aursjø for intriguing discussions and helpful suggestions to the paper. Financial support was provided by the Research Council of Norway through Petromaks2 project “Foam dynamics in the presence of oil during multiphase flow in porous rock (grant no. 294886)”, and The National IOR Centre of Norway (grant no. 230303) with industry partners, ConocoPhillips Skandinavia AS,

Aker BP ASA, Vår Energi AS, Equinor ASA, Neptune Energy Norge AS, Lundin Norway AS, Halliburton AS, Schlumberger Norge AS, and Wintershall DEA. All numerical information is provided in the figures produced by solving the equations described in the paper. Data were not used, nor created for this research.

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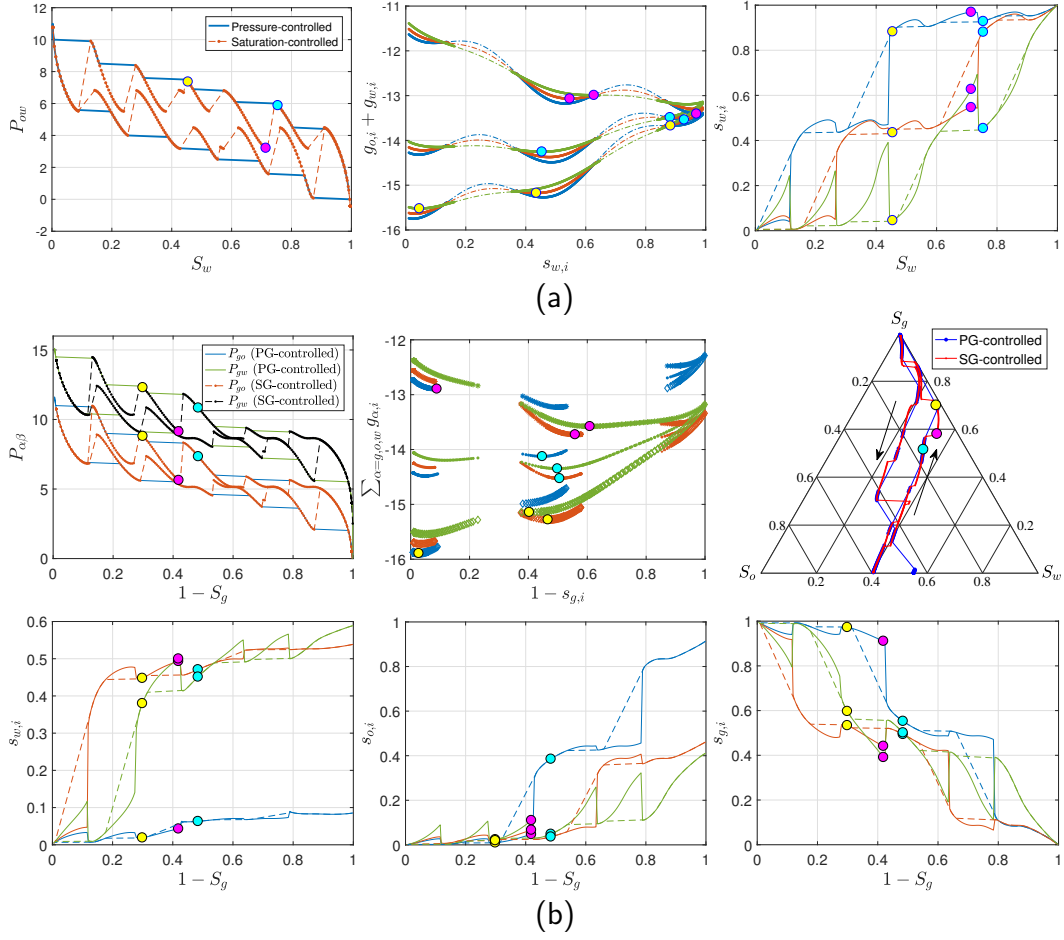


Figure 1. Demonstration of the discrete-domain approach with $N = 3$ and $K = 4$. (a) *Left:* Capillary pressure curves for primary drainage and imbibition in a two-phase oil-water system. *Middle:* Gibbs free energy for compartment 1 (blue), 2 (red) and 3 (green), as functions of compartment water saturations for the three P_{ow} shown by large circles on the $P_{ow}(S_w)$ -curves. The convex segments are the equilibrium locus (bold curves), the concave segments are energy barriers (dash-dotted curves), and the circles show the three metastable compartment states for the corresponding three P_{ow} shown on the $P_{ow}(S_w)$ -curves. *Right:* Evolution of local saturations for compartment 1 (blue), 2 (red) and 3 (green). (b) *Top, left:* Three-phase capillary pressure curves for a gas invasion-retraction hysteresis loop, using PG and SG displacement modes. Gas invasion occurs at $S_w = 0.4$ after oil/water imbibition. *Top, middle:* Equilibrium locus of Gibbs free energy, obtained from equation (7), for compartment 1 (blue), 2 (red) and 3 (green), as functions of compartment liquid saturations for the three capillary pressures shown by large circles on the $P_{\alpha\beta}(1 - S_g)$ -curves. *Top, right:* Three-phase saturation paths. *Bottom row:* Evolution of local saturations for compartment 1 (blue), 2 (red) and 3 (green) for the gas invasions with displacement modes SG (solid curves) and PG (dashed curves).

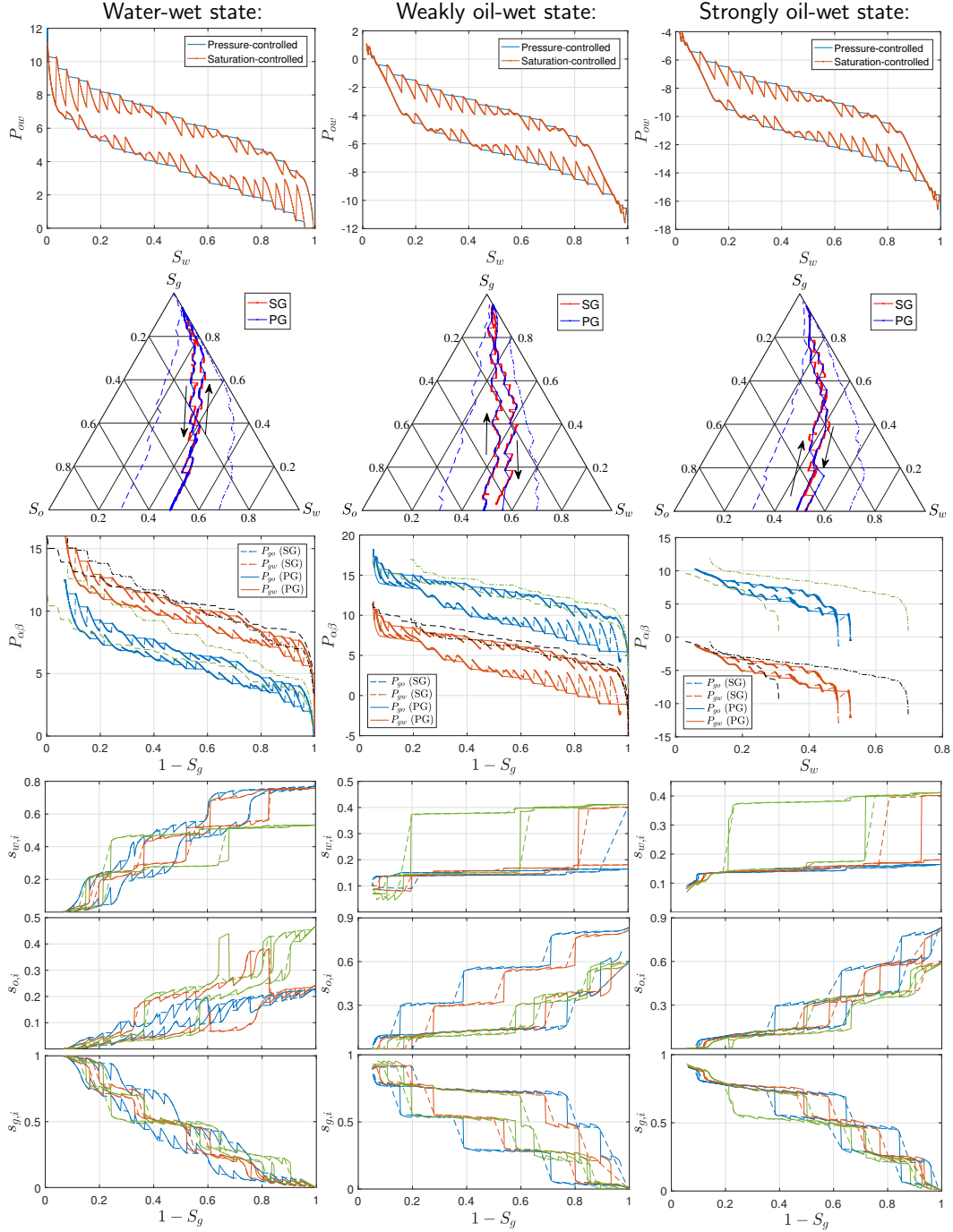


Figure 2. Application of the discrete-domain approach to water-wet (*left column*), weakly oil-wet (*middle column*), and strongly oil-wet (*right column*) states, using $N = 6$ and $K = 8$. *First row:* Two-phase oil/water capillary pressure curves for primary drainage and imbibition from pressure- and saturation-controlled simulations, representing the displacement history before gas invasion. *Second row:* Saturation paths for hysteresis loops of gas invasion (from $S_w = 0.5$) and gas retraction from PG- and SG-simulations, as well as saturation paths from PG-simulations of gas invasions at $S_w = 0.3$ (dashed curves) and $S_w = 0.7$ (dash-dotted curves). *Third row:* Capillary pressure curves for the hysteresis loops and the gas invasions from $S_w = 0.3$ (dashed curves, P_{go} in green and P_{gw} in black) and $S_w = 0.7$ (dash-dotted curves, P_{go} in green and P_{gw} in black). *Fourth, fifth and sixth row:* Evolution of local saturations in a compartment subset $\{1, 2, 3\}$ during the hysteresis loops with SG (solid curves) and PG (dashed curves) displacement protocols.

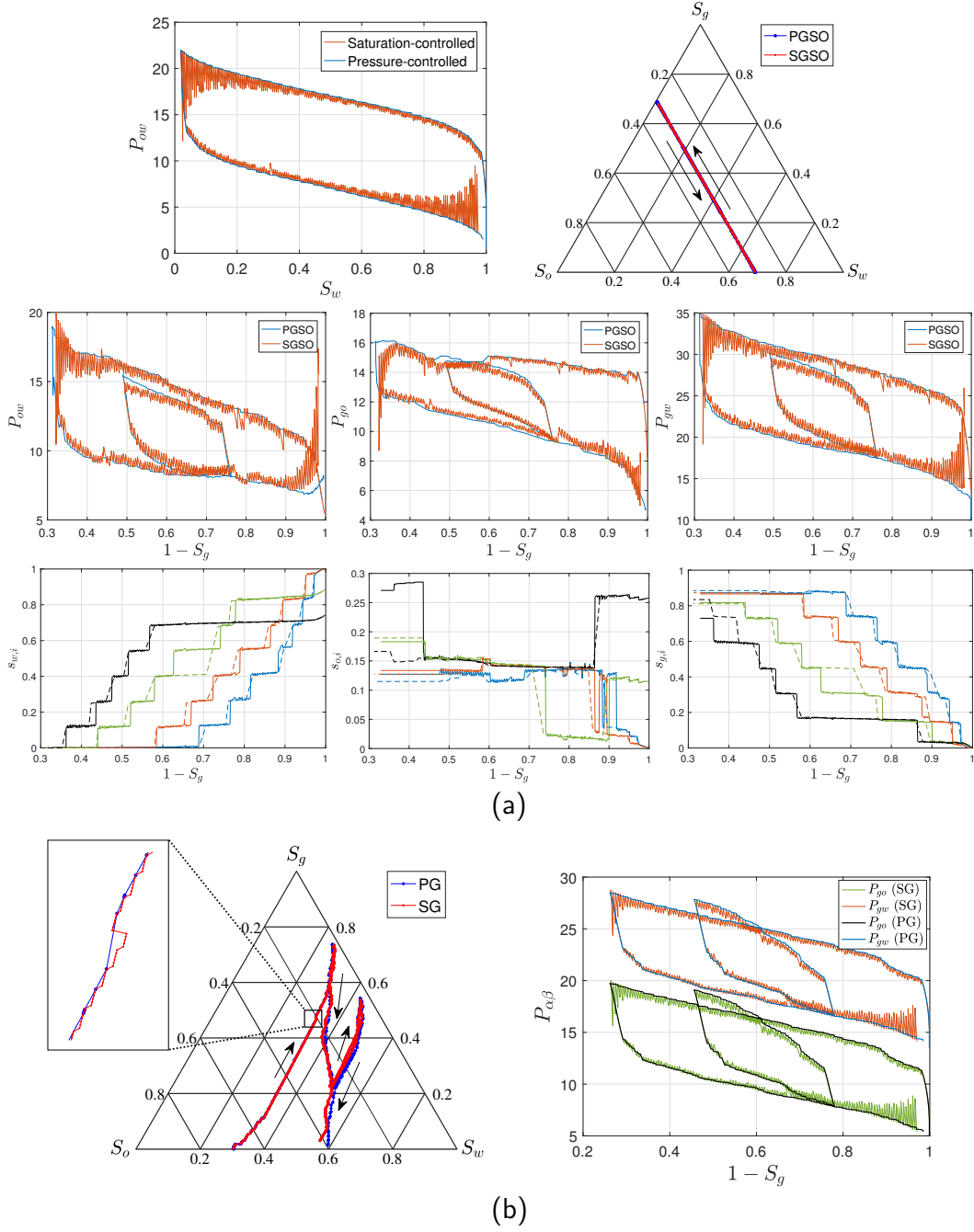


Figure 3. Three-phase hysteresis behavior during alternate gas invasions and gas withdrawals for the case with $N = 24$ and $K = 14$. (a) *Top, left:* Two-phase oil/water capillary pressure curves for primary drainage and imbibition representing the displacement history before gas invasion. *Top, right:* Three-phase saturation paths from simulations with constant global oil saturation (PGSO and SGSO). *Second row:* Three-phase capillary pressure curves for the main hysteresis loop and a nested hysteresis loop from PGSO and SGSO simulations. *Third row:* Evolution of local saturations in a subset of compartments $\{1, 4, 10, 14\}$ during the first gas invasion for displacement protocols SGSO (solid curves) and PGSO (dashed curves). (b) Saturation paths (*left*) and capillary pressure curves (*right*) from PG- and SG-simulations of two gas invasion/withdrawal cycles, demonstrating nested hysteresis-loop behavior for three-phase displacements. Initial global water saturations for the first gas invasions are $S_w = 0.7$ (PGSO and SGSO) and $S_w = 0.3$ (PG and SG).