

Article

Pore-Scale Dynamics of Water Imbibition and Residual-Gas Formation in Tight Gas Reservoir

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Abstract

Forced imbibition of a wetting liquid into a gas-filled tight rock is often expected to advance as a compact front because the liquid-to-gas viscosity ratio is favorable. This expectation can fail when narrow throats, pore-body/throat mismatch, capillary-valve pinning, and wall-associated wetting pathways reorganize the defending gas before it is displaced as a connected phase. We use a three-dimensional regularized color-gradient lattice Boltzmann model to examine these processes in a single, initially gas-saturated reconstructed tight-sandstone pore space. The simulations sample three capillary numbers, two or three Ohnesorge numbers depending on the capillary number, and two water-phase contact angles while keeping the water-to-gas viscosity ratio fixed at 26.11. The contact angle is measured through the aqueous phase, with $\theta = 20^\circ$ representing strongly water-wet conditions and $\theta = 60^\circ$ representing weakly water-wet conditions. For $\theta = 60^\circ$, terminal displacement efficiency changes little between the low and intermediate sampled capillary numbers and increases from approximately 0.660 to 0.736 at the highest sampled value. For $\theta = 20^\circ$, strong water-wetness is beneficial only after the bulk meniscus gains enough driving force to compete with precursor corner or wall flow; at a low capillary number, the same wetting affinity is associated with snap-off and premature gas isolation. The sampled Oh dependence is weaker than the Ca dependence and is consistent with conditional modulation of capillary-inertial damping and local interface relaxation; it is not interpreted as a new static entry criterion. Size-resolved and morphology-resolved statistics show contrasting terminal signatures: $\theta = 20^\circ$ is associated with more large-pore gas and snap-off-consistent fragmentation, whereas $\theta = 60^\circ$ is associated with more persistent small-pore gas and bypassing-consistent retention. Event-resolved phase-field sequences at one low- Ca condition directly show wall-first precursor advance, abrupt pore-body filling, gas-neck closure, persistent component splitting, and bypass-induced local entrapment. These events establish occurrence, not their frequency or dominance across parameter space. Because the study uses one pore-space realization and a sparse, non-factorial parameter matrix, the reported comparisons are restricted to the sampled conditions and do not define a continuous Ca – Oh – θ response surface or quantify structure-to-structure uncertainty.

Keywords: water-driven gas displacement; tight porous media; capillary-valve depinning; wettability; residual-gas topology; lattice Boltzmann method



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1. Introduction

A wetting liquid invading a connected gas phase is a canonical forced-imbibition problem in geometrically disordered porous media. It arises when water reaches gas-bearing tight formations and also in subsurface storage operations where aqueous phases contact gas-filled pore networks. The pore-scale issue is not limited to the final amount of gas left behind. The relevant state is whether the gas remains as a spanning backbone, as locally trapped ganglia in pore bodies, or as many small, disconnected remnants. Macroscopic quantities such as residual saturation and relative permeability therefore summarize the cumulative outcome of meniscus motion, connectivity loss, and trapping history [1,2]. At the reservoir scale, intelligent optimization has also been used to select fracturing parameters in unconventional formations [3].

Classical immiscible-displacement theory classifies invasion patterns as capillary fingering, viscous fingering, or stable displacement, mainly through capillary number and viscosity ratio [4,5]. Cieplak and Robbins [6,7] showed that quasistatic invasion changes through discrete bursts and cooperative filling events. They also showed that contact angle can reorganize the accessible invasion sequence. Primkulov et al. [8] subsequently extended the Lenormand framework by explicitly incorporating wettability. In patterned micromodels, Zhao et al. [9] demonstrated that wettability selects the pore-filling mode and displacement morphology. Holtzman and Segre [10] and Trojer et al. [11] showed that nonlocal cooperative filling and wettability alteration can stabilize invasion. Jung et al. [12] resolved local wetting-dependent interfacial instabilities, and Lei et al. [13] showed that depth variation can trigger instabilities during forced imbibition. Taken together, these studies show that a favorable water-to-gas mobility ratio suppresses classical viscous fingering but does not eliminate burst, touch, overlap, corner invasion, cooperative filling, or snap-off. Strong water-wetness may stabilize the bulk front while simultaneously promoting wall and corner flows that cut gas necks in narrow constrictions. At a different scale, evolutionary search combined with policy-gradient learning has been applied to hydraulic-fracturing optimization [14].

Tight porous media intensify this competition. Their pore systems contain small throats, large pore-body/throat contrasts, limited coordination, and strong capillary thresholds. When a water meniscus exits a small throat and enters a larger pore body, the interface curvature changes rapidly, and local capillary pressure can switch from a driving term to a resisting term. This capillary-valve effect can pin the meniscus at a pore-throat expansion and redirect water into wall-associated or corner-associated paths [15]. Dynamic capillary-pressure studies at geometric transitions further indicate that local acceleration and pore-junction shape can alter the apparent capillary barrier, although the reported configuration was drainage rather than imbibition [16]. The implication for water invasion is that a favorable viscosity ratio does not guarantee piston-like displacement; local pinning, depinning, snap-off, and bypassing can still produce residual gas.

The role of capillary-inertial damping during imbibition is also unresolved. Local inertia is often discussed in relation to Haines jumps during drainage, but wetting-phase invasion can also involve abrupt meniscus reconfiguration. In angular pores, irreversible reconfiguration may release surface energy into kinetic energy, generate local velocities far exceeding the sample-averaged Darcy velocity, and produce damped oscillations that influence the next pore-filling event [17]. Single-junction micromodel experiments and lattice Boltzmann simulations likewise show that spontaneous imbibition may depart from quasistatic Young–Laplace filling rules and that capillary number alone is insufficient; the Ohnesorge number is needed to quantify viscous damping of capillary-inertial interface motion [18].

Recent imbibition studies make this issue directly relevant to water-driven gas displacement. Dynamic capillary-barrier analyses show that pore-body filling during spontaneous imbibition depends on transition-zone shape, contact angle, and fluid inertia. Within a barrier-limited contact-angle window, inertia can help the wetting meniscus cross a resisting capillary zone [19]. Short-capillary and sharp-edge studies further show that free-surface oscillation, contact-line pinning, and depinning are governed by the conversion between surface energy and inertia [20,21]. Forced-imbibition simulations indicate that Oh can influence two-phase distribution, post-breakthrough contribution, the Euler characteristic, and energy dissipation when local inertial effects are amplified by viscosity ratio or pore geometry [22]. Three-dimensional pore-throat simulations show that snap-off during spontaneous imbibition depends on pore-to-throat size ratio, contact angle, and Oh , because Oh changes the speed difference between precursor corner flow and the bulk meniscus [23]. These results motivate a cautious interpretation. In water invasion of a tight rock, Oh is not expected to be the strongest control on terminal gas recovery. It can, however, regulate local depinning, meniscus relaxation, and snap-off when Ca and wettability bring the interface close to pore-scale capillary thresholds.

A further challenge is how to represent the trapped gas after water invasion. At the storage scale, Huppert and Neufeld [24] emphasized that trapping and migration must be interpreted together. At the pore scale, Wildenschild and Sheppard [25] established X-ray imaging workflows for quantifying phase configuration, while Raeini et al. [26] used direct simulations on micro-CT images to connect pore-scale forces with upscaled behavior. McClure et al. [27] demonstrated that phase connectivity changes the relationship among capillary pressure, saturation, and interfacial area, and Purswani et al. [28] showed why additional state information is needed for predictive relative permeability. These contributions imply that a single residual saturation can hide compact droplets, elongated throat-scale ganglia, several-pore bodies, and larger bypassed clusters with different interfacial areas and remobilization potentials. The unresolved link addressed here is therefore the connection among forced-imbibition dynamics, size-selective gas removal, and the morphology of the trapped nonwetting phase in an initially gas-saturated tight pore network. More broadly, theory-guided, data-driven strategies have been developed to connect physical understanding with fracturing-performance prediction [29].

Here, we use a three-dimensional regularized color-gradient lattice Boltzmann model to study the saturated end member of water–gas displacement in a reconstructed tight-sandstone digital rock. Water is the invading phase, gas is the defending phase, and the pore space contains no prescribed initial water saturation. This design isolates the sampled effects of Ca , Oh , and wettability from variations in the initial gas–water topology. We examine how changes among the simulated points are associated with (i) global displacement efficiency and front dynamics, (ii) size-selective gas depletion, and (iii) trapped-gas morphology. The working interpretation is that a favorable viscosity ratio suppresses classical viscous fingering but does not suppress local trapping; capillary-valve pinning/depinning, wall/corner water invasion, snap-off, and bypassing can contribute to the final gas configuration. The analysis is comparative: only one stochastic pore-space realization and a sparse, non-factorial Ca – Oh – θ matrix are considered, so no continuous response surface, formally separable interaction effect, or structure-independent law is inferred.

2. Numerical Methodology and Analysis Metrics

2.1. Digital Rock and Physical Problem

The computational domain is a three-dimensional reconstructed tight-sandstone pore space generated by a modified quadruple-parameter stochastic growth simulation strategy [30,31]. The model is a single stochastic reconstruction designed to represent

a low-porosity, low-permeability, throat-controlled tight-sandstone-like pore space. It is not a sample-specific micro-CT image and is not claimed to be statistically representative of all tight sandstones. The solid array contains $300 \times 300 \times 400$ lattice voxels and 4,875,144 connected pore voxels. It contains 768 pores and 1164 throats, with porosity 0.135421, permeability 0.201 mD, mean pore diameter $2.021 \mu\text{m}$, mean throat radius $0.381 \mu\text{m}$, and mean coordination number 3.031. These descriptors define a pore system with limited connectivity and a clear pore-body/throat mismatch. Pore-size-resolved analysis uses three equivalent pore-diameter classes: small pores, $1.30\text{--}6.96 \mu\text{m}$; medium pores, $6.96\text{--}12.64 \mu\text{m}$; and large pores, $12.64\text{--}18.29 \mu\text{m}$. Only this realization was simulated. The fixed geometry was used to isolate fluid-parameter effects without introducing simultaneous changes in network geometry. This design supports within-structure comparisons but does not provide an ensemble mean or variance. Quantitative values and rankings are therefore reported for this pore space only. Additional realizations may shift absolute thresholds and the strength of the observed rankings; structure-to-structure uncertainty remains unquantified.

The initial connected pore space is gas-saturated. Water is injected from the inlet and displaces the defending gas through the fixed solid skeleton. Gravity is omitted because the characteristic pore length is micrometric and the intended regime has a negligible Bond number compared with capillary and imposed viscous effects. The two fluids are density matched, $\rho_w = \rho_g = 1$ in lattice units, so the density ratio is $R_\rho = \rho_w / \rho_g = 1$. This numerical similarity assumption reduces stiffness and removes the phase-density contrast from the inertial response. Separately, the omission of gravity removes buoyancy-driven segregation, and the constant-density weakly compressible formulation does not represent real-gas compressibility. The model therefore isolates capillarity, viscous forcing, wettability, and local damping within these restrictions, which are discussed in Section 3.7.

2.2. Lattice Boltzmann Model

The numerical solver is a regularized color-gradient lattice Boltzmann scheme for immiscible two-phase flow. It uses a multiple-relaxation-time collision operator, a color-gradient perturbation and recoloring sequence to represent interfacial tension and maintain phase segregation, and a geometrically corrected interface normal to impose the prescribed contact angle at voxelized solid surfaces [32–37]. The regularization step filters nonhydrodynamic kinetic modes produced by curved interfaces, staircase walls, and strong local capillary forces while preserving the hydrodynamic moments [38]. Viscosity, interfacial tension, inlet velocity, and wettability are therefore varied independently within one fixed pore geometry.

The reconstructed rock is embedded in a $304 \times 304 \times 420$ computational lattice: two solid buffer nodes are placed on each transverse side, and 10-node fluid reservoirs are appended at the inlet and outlet. Flow is along the z direction. A uniform axial velocity, U_{in} , is prescribed at the z -min water inlet, and a fixed-reference-pressure open boundary is applied at z -max. The transverse exterior is impermeable. No slip at the voxelized mineral surface is imposed by halfway bounce-back, and the geometric wetting boundary sets θ measured through water. The governing lattice Boltzmann equations and the associated Laplace-pressure, wetting, imbibition, layered-flow, relative-permeability, corner-film, and micromodel benchmarks are documented in Refs. [39,40].

These calculations are transient, constant-flux simulations rather than steady-state solves; therefore, no steady-state residual-norm stopping criterion is imposed. All cases are advanced to the same injection horizon, and the terminal field used for pore-size and morphology statistics is the saved output nearest $PV = 1.2$. The 10-node inlet and outlet reservoirs are removed during post-processing. To avoid outlet-boundary contamination,

front, occupancy, and ganglion statistics are evaluated in the inlet-side 70% of the effective rock, containing 3,401,480 of the full 4,875,144 pore voxels; the *PV* coordinate is scaled consistently with the selected pore volume. Throughout this article, “residual gas” denotes this common operational terminal state and does not imply proof of an asymptotic equilibrium residual saturation.

2.3. Dimensionless Groups and Simulation Cases

Water is the invading phase, and gas is the defending phase. The capillary number, Reynolds number, and viscosity ratio follow conventional porous-media definitions [1,4,5], while the Ohnesorge number is used to quantify viscous damping of pore-scale capillary-inertial motion [18,22,23]:

$$Ca = \frac{\mu_w U_{in}}{\sigma} \quad (1)$$

$$Oh = \frac{\mu_w}{(\rho_w \sigma L_c)^{1/2}} \quad (2)$$

$$Re = \frac{\rho_w U_{in} L_c}{\mu_w} = \frac{Ca}{Oh^2} \quad (3)$$

$$M = \frac{\mu_w}{\mu_g} \quad (4)$$

Here, μ_w and μ_g are the dynamic viscosities of water and gas. U_{in} is the imposed inlet velocity, σ is the gas–water interfacial tension, ρ_w is the water density, and L_c is the reference pore length. All quantities in Table 1 are expressed in lattice units. We set $L_c = 10\Delta x = 10$ lu, corresponding to the nominal pore-body radius. This is one half of the 20-lu characteristic pore diameter used to construct the digital rock and approximately one half of the reported mean pore diameter, i.e., about 1.01 μm in the physical mapping. Substitution into $L_c = \mu_w^2 / (\rho_w \sigma Oh^2)$ reproduces $L_c = 10$ lu for every row of Table 1. At fixed fluid properties, $Oh \propto L_c^{-1/2}$ and $Re \propto L_c$, whereas Ca is independent of L_c . Choosing another common reference length would therefore rescale the reported Oh and Re values but would not change the simulated flow fields or the ordering of cases. The viscosity ratio is fixed at $M = 26.11$. The contact angle θ is measured through water; $\theta = 20^\circ$ denotes strongly water-wet conditions, and $\theta = 60^\circ$ denotes weakly water-wet conditions.

Table 1. Water-driven gas displacement simulation parameters in lattice units. Water is the invading phase, and gas is the defending phase. Re is a derived quantity defined by $Re = Ca/Oh^2$. The last-row value is reported as 4.90×10^{-3} after consistency checking with this definition.

Ca	Oh	Re	M	τ_{inj}	τ_{def}	σ
3.00×10^{-5}	8.00×10^{-2}	4.69×10^{-3}	26.11	0.692	0.507353	0.064
3.00×10^{-5}	1.26×10^{-1}	1.89×10^{-3}	26.11	0.81752	0.51216	0.07056
3.00×10^{-5}	2.00×10^{-1}	0.75×10^{-3}	26.11	1.100	0.522979	0.100
7.66×10^{-5}	1.26×10^{-1}	4.83×10^{-3}	26.11	0.810888	0.511906	0.067643
7.66×10^{-5}	2.00×10^{-1}	1.92×10^{-3}	26.11	1.001305	0.519199	0.069808
1.96×10^{-4}	1.26×10^{-1}	12.3×10^{-3}	26.11	0.7916	0.511168	0.05951
1.96×10^{-4}	2.00×10^{-1}	4.90×10^{-3}	26.11	0.928571	0.516413	0.05102

The three Ca values are approximately logarithmically spaced, with a successive ratio of about 2.55 and an overall range factor of 6.53. The Oh values 0.08, 0.126, and 0.20 are also approximately logarithmically spaced and span a factor of 2.5 in viscous damping. The lowest Ca cases emphasize capillary-threshold-controlled advance, the intermediate cases probe competition between capillary barriers and imposed viscous forcing, and the highest Ca cases provide stronger pore-body access. These points are intended to sample

a capillary-dominated forced-imbibition window rather than all possible tight-reservoir flow regimes.

Because the governing comparison is dimensionless, a dimensional mapping is not unique. For illustration, taking $L_c = 1.01 \text{ } \mu\text{m}$, $\rho_w = 1000 \text{ kg m}^{-3}$, and $\sigma = 0.03\text{--}0.07 \text{ N m}^{-1}$ maps $Oh = 0.08\text{--}0.20$ to $\mu_w \approx 0.44\text{--}1.68 \text{ mPa s}$. With $M = 26.11$, the corresponding gas viscosity is approximately $0.017\text{--}0.064 \text{ mPa s}$. For the actual $Ca\text{--}Oh$ combinations in Table 1, the imposed inlet velocity maps to approximately $0.82\text{--}12.95 \text{ mm s}^{-1}$. These values are best interpreted as local forced-invasion velocities near a fracture–matrix interface or near-well region, not as field-scale Darcy velocities throughout an undisturbed tight matrix. Because the numerical model is density matched, this mapping describes the viscous-capillary scales only and is not a complete thermodynamic reconstruction of reservoir gas.

A complementary classical measure of inertia relative to capillarity is $We = \rho_w U_{in}^2 L_c / \sigma = Re \cdot Ca = (Ca/Oh)^2$; equivalently, $Ca/Oh = \sqrt{We}$. Across the simulated cases, Ca/Oh ranges from 1.50×10^{-4} to 1.56×10^{-3} , and We ranges from 2.25×10^{-8} to 2.42×10^{-6} . Thus, all sampled points remain globally capillary-dominated. The observed Oh dependence is therefore interpreted as a change in the damping of local capillary-inertial reconfiguration, not as entry into a bulk inertia-dominated regime.

The parameter set is treated as a sparse, non-factorial sampling rather than a complete interaction design. Three Oh values are available only at $Ca = 3.00 \times 10^{-5}$, whereas the intermediate and high Ca levels contain two Oh values; wettability is represented by only $\theta = 20^\circ$ and 60° . Therefore, the analysis does not define a continuous $Ca\text{--}Oh\text{--}\theta$ response surface, identify a wettability transition angle, or statistically separate main and interaction effects. Statements about parameter coupling are restricted to direct comparisons among the sampled cases.

2.4. Metrics

We define injected pore volume, used here as the dimensionless time coordinate, as

$$PV = \frac{Q_{in} t}{V_p} \quad (5)$$

where Q_{in} is the imposed inlet volumetric flow rate, and V_p is the connected pore volume of the reported analysis region. Because the pore space is initially gas-saturated, we define displacement efficiency as the volume fraction of gas removed from that connected pore space:

$$E_d(t) = \frac{S_g(0) - S_g(t)}{S_g(0)} \quad (6)$$

where S_g is gas saturation. For the present initial condition, $S_g(0)$ is approximately unity, so E_d is also the invaded-water saturation in the connected pore volume. Equations (5) and (6) are operational definitions used in this study rather than constitutive laws adopted from another source.

Front roughness quantifies streamwise heterogeneity of the inlet-connected water front [41]:

$$W = \left\langle \left[x_f - \langle x_f \rangle \right]^2 \right\rangle^{1/2} \quad (7)$$

where x_f is the local streamwise front location, and angle brackets denote an average over the transverse section [41]. Connectivity changes are quantified using the Euler characteristic [2,27,28],

$$\chi = \beta_0 - \beta_1 + \beta_2 \quad (8)$$

Here, β_0 counts disconnected phase domains, β_1 counts independent loops, and β_2 counts enclosed cavities [27,28]. Negative shifts in χ reflect the development of looped connectivity, whereas positive shifts indicate breakup into more isolated components.

For each pore-size class k , we define gas occupancy as

$$O_{g,k}(t) = \frac{V_{g,k}(t)}{V_{p,k}} \quad (9)$$

where $V_{g,k}$ is the gas volume in pore-size class k , and $V_{p,k}$ is the total pore volume of that class. Equation (9) is an operational statistic defined for the present analysis.

After water injection, each residual-gas body is labeled using 26-neighbor, three-dimensional connected-component analysis. Its morphology is described by shape factor G , Euler characteristic χ , and occupied-pore count N_p , consistent with topology-based descriptions of disconnected phases [2,25–27]. Pore regions are segmented by the SNOW2 marker-based watershed procedure [42,43] using Gaussian smoothing $\sigma = 0.8$ lu and a maximum search radius of 6 lu, and N_p is the number of unique positive pore-region labels overlapped by a gas body. The dimensionless isoperimetric shape factor is computed as

$$G = \frac{A^3}{36\pi V^2} \quad (10)$$

where A is the gas-cluster surface area obtained from the 0.5 isosurface by marching cubes [44], and V is its voxel volume. The Euler characteristic is computed on the padded voxelized cluster using three-dimensional Minkowski functionals [45]. A compact sphere gives $G = 1$; a larger G denotes a more elongated or irregular body. The Table 2 cutoffs are operational rather than universal material constants. $G_c = 3$ separates compact from visibly noncompact bodies in the present descriptor distribution. $N_p \leq 2$ identifies local one- or two-pore bodies, $2 < N_p < 8$ denotes several-pore bodies, and $N_p \geq 8$ identifies spatially extended clusters. For a single connected body without enclosed cavities, $\chi = 1 - \beta_1$, so $\chi \leq -1$ corresponds to at least two independent loops. Enclosed cavities can also contribute to a general voxelized body. Therefore, $\chi \leq -1$ is used only as an operational marker of strongly looped topology, not as a universal loop criterion. Rules are evaluated hierarchically, and unmatched bodies are assigned to an unclassified fallback category. Because gas is the nonwetting phase in the water-wet pore space, a wall-film gas class is not used.

Table 2. Operational classification criteria for residual-gas occurrence types. When criteria overlap, the priority is clustered, multi-pore, columnar, and droplet; unmatched bodies are retained as unclassified.

Type	Criteria	Main Geometric/Topological Meaning
Droplet gas	$G \leq 3, \chi > 0$	Compact, isolated gas body with simple topology, commonly occupying one local pore region.
Columnar gas	$G > 3, \chi > 0, N_p \leq 2$	Elongated gas body spanning one or few pores or a throat-like connection.
Multi-pore gas	$G > 3, \chi > -1, 2 < N_p < 8$	Gas body spanning several neighboring pores without a strongly looped network.
Clustered gas	$(G > 3 \text{ and } \chi \leq -1) \text{ or } N_p \geq 8$	Large gas cluster with broad pore coverage and/or looped internal connectivity.

We assessed threshold sensitivity by reclassifying all 6335 gas bodies from the 14 terminal cases. We used $G_c = 2.5, 3.0$, and 3.5 and the extended-cluster pore-count

cutoff $N_c = 6, 8$, and 10 , while retaining the Euler cutoffs and the local-body cutoff $N_p \leq 2$. At the baseline $G_c = 3$ and $N_c = 8$, 29 of the 6335 bodies (0.46% by count) did not satisfy any of the four physical class rules and were retained as unclassified. Thus, 6306 bodies were included in the four-class count statistics reported later, and the corresponding four-class volume fractions were normalized by the total classified residual-gas volume. At the baseline thresholds, the pooled droplet-gas volume fractions are 36.78% for $\theta = 20^\circ$ and 15.92% for $\theta = 60^\circ$. The pooled multi-pore-plus-clustered fractions are 53.61% and 63.92%, respectively. Individual class fractions are threshold-dependent. The largest absolute changes are 14.13 percentage points for $\theta = 20^\circ$ and 7.52 percentage points for $\theta = 60^\circ$. Nevertheless, the higher droplet fraction at $\theta = 20^\circ$ and the higher combined multi-pore-plus-clustered fraction at $\theta = 60^\circ$ persist in all 9/9 tested G_c – N_c combinations. This analysis establishes robustness only over the tested G_c and N_c ranges; it does not establish invariance to every possible Euler or occupied-pore threshold. The class percentages and mechanistic labels should therefore be interpreted comparatively and conditionally.

2.5. Transient Pore-Scale Diagnostic Analysis

To obtain event-resolved pore-scale evidence without altering the original parameter matrix, two high-temporal-resolution diagnostic reruns were performed at the existing condition $Ca = 3.00 \times 10^{-5}$ and $Oh = 1.26 \times 10^{-1}$, for $\theta = 20^\circ$ and $\theta = 60^\circ$. The pore geometry, boundary conditions, fluid properties, and numerical parameters were unchanged. The diagnostic runs were terminated before breakthrough, and only the phase field φ was written every 13,000 lattice time steps. Solid nodes are represented by NaN values, whereas $\varphi < 0$ and $\varphi > 0$ denote the invading water and displaced gas, respectively; the $\varphi = 0$ contour defines the local fluid–fluid interface. Gas connectivity was evaluated primarily using 26-neighbor, three-dimensional connected-component analysis. Snap-off was recorded only when a gas neck closed and a gas region previously belonging to the outlet-connected parent gas became a persistent disconnected component. Sensitivity was evaluated by varying the phase threshold around zero (± 0.2 for the $\theta = 20^\circ$ snap-off event and ± 0.25 for the $\theta = 60^\circ$ bypass event) and by using 6-, 18-, and 26-neighbor connectivity. A pinned-to-burst event was operationally identified as an interface remaining within the same local throat region for multiple outputs, followed by abrupt pore-body filling. These pre-breakthrough diagnostics are used only as transient mechanism evidence and do not replace the terminal-state statistics reported at $PV = 1.2$.

2.6. Grid-Resolution Sensitivity Assessment

To assess resolution sensitivity under the present simulation conditions, the intermediate case $Ca = 7.66 \times 10^{-5}$, $Oh = 1.26 \times 10^{-1}$, $\theta = 20^\circ$, and $M = 26.11$ was selected. This point lies within the sampled parameter range and contains wetting-sensitive wall/corner advance, pore-throat expansion, and snap-off, making it a demanding test of pore-throat and diffuse-interface resolution.

The same physical digital-rock realization is consistently resampled, rather than regenerated, to $150 \times 150 \times 200$ ($0.5\times$), $300 \times 300 \times 400$ ($1.0\times$), and $450 \times 450 \times 600$ ($1.5\times$) rock arrays. The physical pore space, boundary conditions, M , Ca , Oh , and θ are kept fixed. With ρ and σ fixed in lattice units, the lattice-unit characteristic length scales with resolution; therefore, μ_w and U_{in} are scaled as $\mu_w \propto L_c^{1/2}$ and $U_{in} \propto L_c^{-1/2}$, preserving both Ca and Oh . For each grid, injected pore volume is normalized by the connected pore volume of the corresponding resampled geometry, and the displacement-efficiency curves are compared on a common $0 \leq PV \leq 1.2$ coordinate. Under the physical mapping used in this study, the mean throat diameter corresponds to approximately 3.77, 7.54, and 11.31 lattice nodes on the $0.5\times$, $1.0\times$, and $1.5\times$ grids, respectively.

Figure 1 compares the three computed displacement-efficiency curves. At $PV = 1.2$, the displacement efficiencies are 0.6865, 0.7098, and 0.7134 on the $0.5\times$, $1.0\times$, and $1.5\times$ grids, respectively. Taking the $1.0\times$ grid as the reference, the endpoint relative differences are 3.28% for $0.5\times$ and 0.50% for $1.5\times$. Over $0 \leq PV \leq 1.2$, the corresponding maximum absolute curve differences are 7.01 and 0.58 percentage points, and the curve-wise RMSE values evaluated on the common PV coordinates are 3.92 and 0.43 percentage points. Both maximum differences occur near $PV = 0.50$. The $1.0\times$ and $1.5\times$ curves remain close throughout injection, whereas the $0.5\times$ grid yields substantially lower displacement efficiency during the intermediate stage. This coarse-grid deviation is consistent with the mean throat diameter being represented by only about 3.77 lattice nodes on the $0.5\times$ grid, compared with 7.54 and 11.31 nodes on the $1.0\times$ and $1.5\times$ grids. The $300 \times 300 \times 400$ lattice was therefore retained as an accuracy-cost compromise for the global displacement-efficiency metric in this tested case. Because the refinement ratios are unequal, this assessment is reported as a direct resolution sensitivity comparison rather than a Richardson/GCI estimate, and it does not establish convergence of every local snap-off or depinning pathway or of all Ca – Oh – θ combinations.

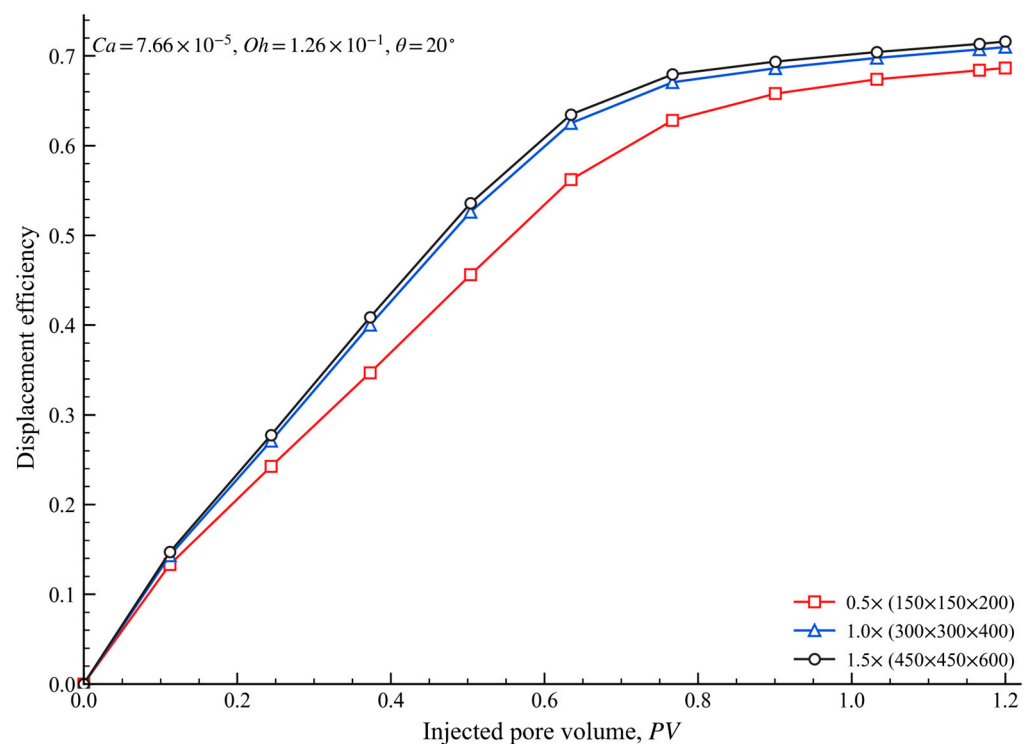


Figure 1. Grid-resolution sensitivity of displacement efficiency for $Ca = 7.66 \times 10^{-5}$, $Oh = 1.26 \times 10^{-1}$, $\theta = 20^\circ$, and $M = 26.11$. The curves correspond to $0.5\times$ ($150 \times 150 \times 200$), $1.0\times$ ($300 \times 300 \times 400$), and $1.5\times$ ($450 \times 450 \times 600$) consistently resampled representations of the same physical pore space. The $1.0\times$ and $1.5\times$ results remain close over $0 \leq PV \leq 1.2$, whereas the $0.5\times$ grid exhibits a larger intermediate- PV deviation.

3. Results and Discussion

3.1. Global Displacement Dynamics and Ca -Dependent Trends in the Sampled Cases

Figure 2 compares displacement efficiency, front roughness, terminal efficiency, and interface-curvature distributions for $\theta = 60^\circ$ and $\theta = 20^\circ$. The terminal quantities correspond to the saved field nearest $PV = 1.2$ in the inlet-side 70% analysis region defined in Section 2.2. The displacement is globally efficient because water is more viscous than gas, which suppresses classical viscous fingering. Nevertheless, the front is not piston-like. At low Ca ,

water first advances through small throats and wall-adjacent pathways before some larger pore bodies are fully swept. This early advance is a local capillary-access effect rather than a macroscopic viscous finger.

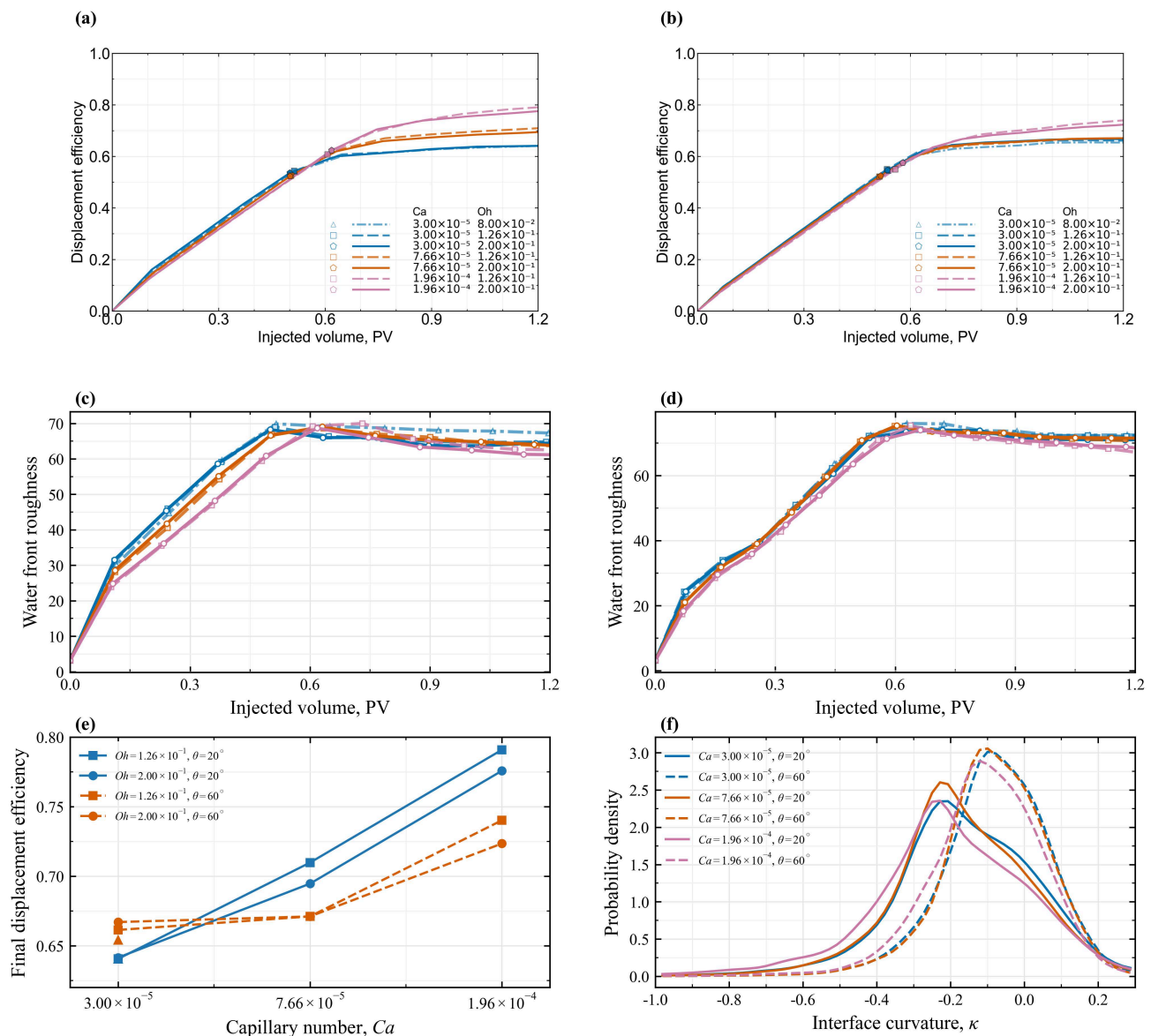


Figure 2. Global displacement dynamics during water invasion: (a) displacement efficiency for $\theta = 60^\circ$; (b) displacement efficiency for $\theta = 20^\circ$; (c) front roughness for $\theta = 60^\circ$; (d) front roughness for $\theta = 20^\circ$; (e) terminal displacement efficiency at $PV = 1.2$ as a function of Ca for the sampled Oh and θ values; (f) interface-curvature distributions at $Oh = 0.126$ for the sampled Ca and θ values.

At $\theta = 60^\circ$ and $Oh = 0.126$, the number of streamwise slices in which small-pore water arrival precedes large-pore arrival decreases from 44 to 32 and then to 21 as Ca increases. This trend indicates that low- Ca water invasion is biased toward small throats, while increasing Ca reduces the dominance of small-throat capillary access. The observed trend is consistent with the throat-to-pore-body transition being an important local constraint. As water exits a small throat, meniscus curvature decreases, and the local capillary pressure can become a resisting barrier; when the imposed viscous pressure drop is insufficient, the interface can remain pinned at the expansion. This interpretation is consistent with capillary-valve simulations [15], dynamic capillary-barrier models for imbibition [19], and dynamic capillary-pressure studies at geometric transitions [16].

Across the three sampled Ca values, increasing Ca is associated with a stronger imposed viscous pressure drop and with invasion of more pore-body regions separated by geometric capillary barriers. For $\theta = 60^\circ$, final displacement efficiency increases only weakly from approximately 0.660 to 0.674 between the low and intermediate Ca cases but increases to approximately 0.736 at the highest sampled value. The sampled response is therefore weak between the first two points and larger at the third. Because only three Ca values were simulated, this pattern may be described as threshold-like but does not establish a sharp or universal depinning threshold. The roughness curves and curvature distributions in Figure 2 are consistent with reduced front heterogeneity and a smaller contribution from strongly pinned configurations as Ca increases.

The $\theta = 20^\circ$ cases show a different terminal response. Strong water-wetness increases wall affinity and promotes water spreading along corners and narrow throats. At low Ca , this stronger capillary driving does not automatically improve displacement. Wall- and corner-associated water can advance ahead of the bulk meniscus, merge in constrictions, and close gas necks before adjacent pore bodies are fully swept. This class of precursor-bulk competition has been identified in three-dimensional spontaneous-imbibition snap-off simulations [23] and in prior work on corner-film-controlled transport [40]. The event-resolved sequences presented in Section 3.3 directly document wall-first precursor advance followed by abrupt pore-body filling and gas-neck closure followed by persistent gas-component separation in one selected $\theta = 20^\circ$ diagnostic event. These sequences establish that the processes occur under that condition but do not quantify their frequency across the sampled cases.

Across the sampled Ca values at $\theta = 20^\circ$, front roughness decreases from about 65.5 to 63.9 and then to 61.7, a stronger change than in the $\theta = 60^\circ$ cases. The terminal-state trends are consistent with the bulk meniscus becoming more competitive with wall-associated wetting pathways and with a reduced contribution from premature isolation at higher Ca . However, the event-resolved diagnostic sequences were obtained only at $Ca = 3.00 \times 10^{-5}$ and therefore do not directly demonstrate a cross- Ca suppression mechanism or a change in event frequency.

3.2. Sampled Ohnesorge-Number Dependence of Interface Relaxation

Figures 2 and 3 show that terminal displacement efficiency varies less with Oh than with Ca over the sampled points. This does not imply that capillary-inertial effects are absent. Rather, final gas volume appears to be constrained mainly by capillary thresholds, wetting-dependent access, and the connectivity of this pore space, while the observed Oh dependence is interpreted as a conditional response of interfaces close to local reconfiguration. It is not a direct measurement of depinning dynamics.

This interpretation follows the imbibition literature. In angular or sharp-edged pore spaces, meniscus reconfiguration releases surface energy, generates damped oscillations, and may alter the subsequent filling sequence [17,20,21]. Single-junction imbibition experiments and simulations show that Ca alone cannot describe spontaneous pore filling because Oh controls the damping of local capillary-inertial motion [18]. Dynamic capillary-barrier models further show that inertia can help the wetting phase pass through a resisting transition zone, but only when the contact angle and geometry place the system within a barrier-limited window [19]. Therefore, the present Oh trends should be interpreted as conditional interface-relaxation effects rather than changes in static capillary-entry pressure.

At low Ca , the water front advances slowly and is strongly constrained by capillary-valve pinning, wall/corner invasion, and local gas isolation. The nearly coincident terminal efficiencies of the lowest Ca , $\theta = 20^\circ$ cases indicate little detectable Oh sensitivity at the sampled points. This may reflect geometric accessibility dominating over changes in

interface damping, and it is consistent with forced-imbibition simulations in which inertial effects remain weak under relatively stable conditions but become more visible when local velocities or displacement heterogeneity are amplified [22].

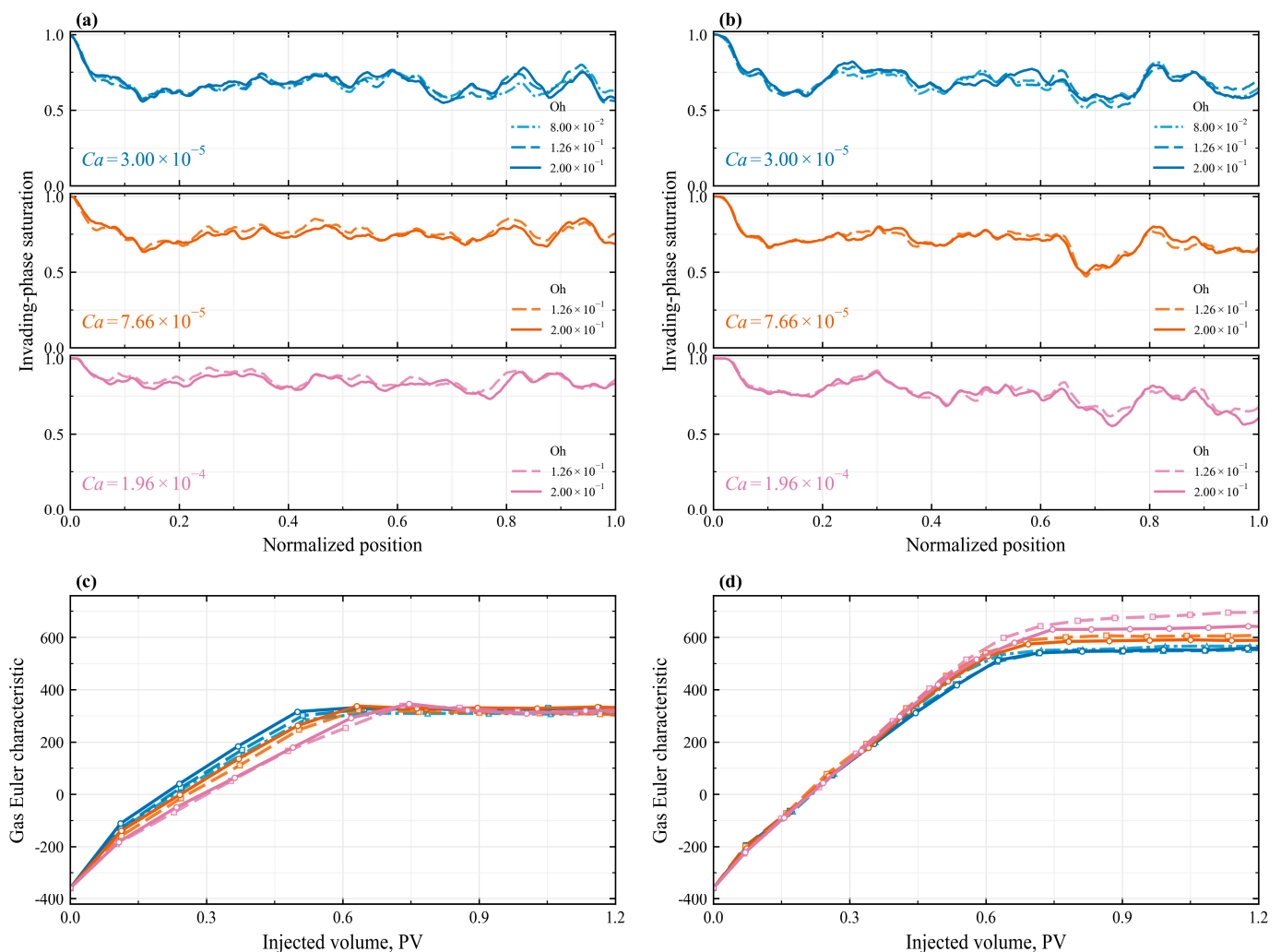


Figure 3. Saturation and topology evolution under different Ca – Oh combinations: (a) streamwise invading-phase saturation profiles for $\theta = 60^\circ$; (b) streamwise invading-phase saturation profiles for $\theta = 20^\circ$; (c) gas-phase Euler characteristic versus injected pore volume for $\theta = 60^\circ$; (d) gas-phase Euler characteristic versus injected pore volume for $\theta = 20^\circ$.

At the intermediate and high sampled Ca values, differences between the two available Oh values become more visible. Lower Oh corresponds to weaker viscous damping of capillary-inertial motion. At $\theta = 20^\circ$ and $Ca = 7.66 \times 10^{-5}$, lowering Oh from 0.200 to 0.126 increases large-pore water occupancy from approximately 0.632 to 0.664. At $Ca = 1.96 \times 10^{-4}$, it increases from approximately 0.794 to 0.819. These changes correspond to relative increases of about 5.1% and 3.1%, respectively. Over the same Oh change, Ca/Oh increases by 58.7%, and We increases by a factor of 2.52. The fixed- Ca trend is consistent with weaker damping and easier interface reconfiguration near pore-body expansions. It is a terminal-state proxy, not a direct measurement of meniscus relaxation time, oscillation frequency, local pressure threshold, or depinning probability. Without local pressure or velocity fields, and because the matrix is incomplete, capillary-valve depinning cannot be identified uniquely as the cause.

For $\theta = 60^\circ$, the observed Oh dependence is smaller. At low and intermediate Ca , final efficiency changes little between the sampled Oh values. Only at the highest Ca does lower

Oh slightly increase water occupancy in all pore-size classes. This weaker sensitivity may reflect the greater importance of geometric accessibility and sustained viscous forcing in these cases, but the present diagnostics do not establish a wettability-dependent difference in snap-off frequency or wall-associated acceleration.

The topological metrics in Figure 3 reinforce the conditional nature of this interpretation. Gas-phase Euler characteristic changes as water cuts the gas network, while the water-phase Euler characteristic reflects the formation of connected water paths and disconnected water pockets. Greater Oh sensitivity appears only in sampled cases where Ca and wettability also favor interface reconfiguration. This is a comparative pattern, not proof of a general activation criterion or a statistically separable Ca – Oh –wettability interaction. The caution is important because spontaneous-imbibition simulations found that increasing Oh can promote snap-off in some highly water-wet pore-throat geometries [23], whereas the present forced-invasion results are consistent with improved large-pore sweep at lower Oh for selected higher- Ca cases. The difference may reflect the balance among spontaneous precursor flow, forced bulk-front advance, and local capillary barriers.

The high-temporal-resolution diagnostic sequences were obtained only at $Oh = 1.26 \times 10^{-1}$ and contain no local pressure or velocity output. Consequently, the inferred roles of Oh in depinning, meniscus relaxation, and precursor–bulk competition are treated as physically consistent interpretations of the sampled global and terminal-state statistics. They are not direct local-field measurements or a general interaction law. A direct correlation between Oh and local depinning dynamics would require the same local throat to be sampled at multiple Oh values with higher-frequency interface, pressure, and velocity output. The present data do not support such a correlation analysis. We therefore report the fixed- Ca terminal proxies above and identify event-resolved multi- Oh diagnostics as future work.

3.3. Direct Pore-Scale Interface Evolution

Figure 4 presents event-resolved phase-field evidence from two diagnostic reruns at $Ca = 3.00 \times 10^{-5}$ and $Oh = 1.26 \times 10^{-1}$. The sequences were selected to determine whether precursor advance, abrupt pore filling, gas-neck closure, and bypassing occur in the simulated pore space; they were not designed to measure mechanism frequency across the parameter matrix.

Figure 4a shows a selected $\theta = 20^\circ$ local invasion event in $x = 208$ – 231 , $y = 112$ – 135 , and $z = 200$ – 223 . From steps 728,000 to 767,000, the water front on the $y = 124$ slice remained at $z = 203$ – 204 , and only 4–20 newly invaded water voxels appeared per output. At step 767,000, all 53 water voxels in the local region were within two lattice nodes of a solid surface; no water occupied the pore core defined by a wall distance greater than three lattice nodes. At step 780,000, 1721 newly invaded water voxels appeared within one output interval. The local water count increased from 53 to 1785, and the front advanced abruptly to $z = 219$; the pore body was nearly filled by step 793,000. Thus, the low-advance stage persisted for at least 39,000 lattice time steps, whereas the bulk-filling transition occurred within one 13,000-step output interval. The saved cadence therefore bounds the burst duration but does not resolve an oscillation period. The sequence documents wall-first advance followed by rapid bulk filling and provides a kinematic signature consistent with capillary-valve pinning/depinning or a local Haines-type jump. Because no local pressure field was written, it is not interpreted as a direct measurement of a capillary-pressure threshold.

Figure 4b shows direct snap-off evidence at $\theta = 20^\circ$. A gas neck centered near $(x, y, z) = (149, 77, 249)$ changed from gas at step 884,000 ($\varphi = 0.932$) to an interfacial state at step 897,000 ($\varphi = -0.0023$) and became water-filled at step 910,000 ($\varphi = -0.766$).

At step 897,000, a 34,629-voxel gas ganglion separated from the outlet-connected parent gas and remained disconnected with 33,821 gas voxels at step 923,000. The split was reproduced using 6-, 18-, and 26-neighbor connectivity, and changing the gas threshold from $\varphi > 0$ to $\varphi > -0.2$ or $\varphi > +0.2$ shifted the detected separation by no more than one output interval. The simultaneous gas-neck closure and persistent gas-component splitting therefore constitute direct topological evidence of snap-off.

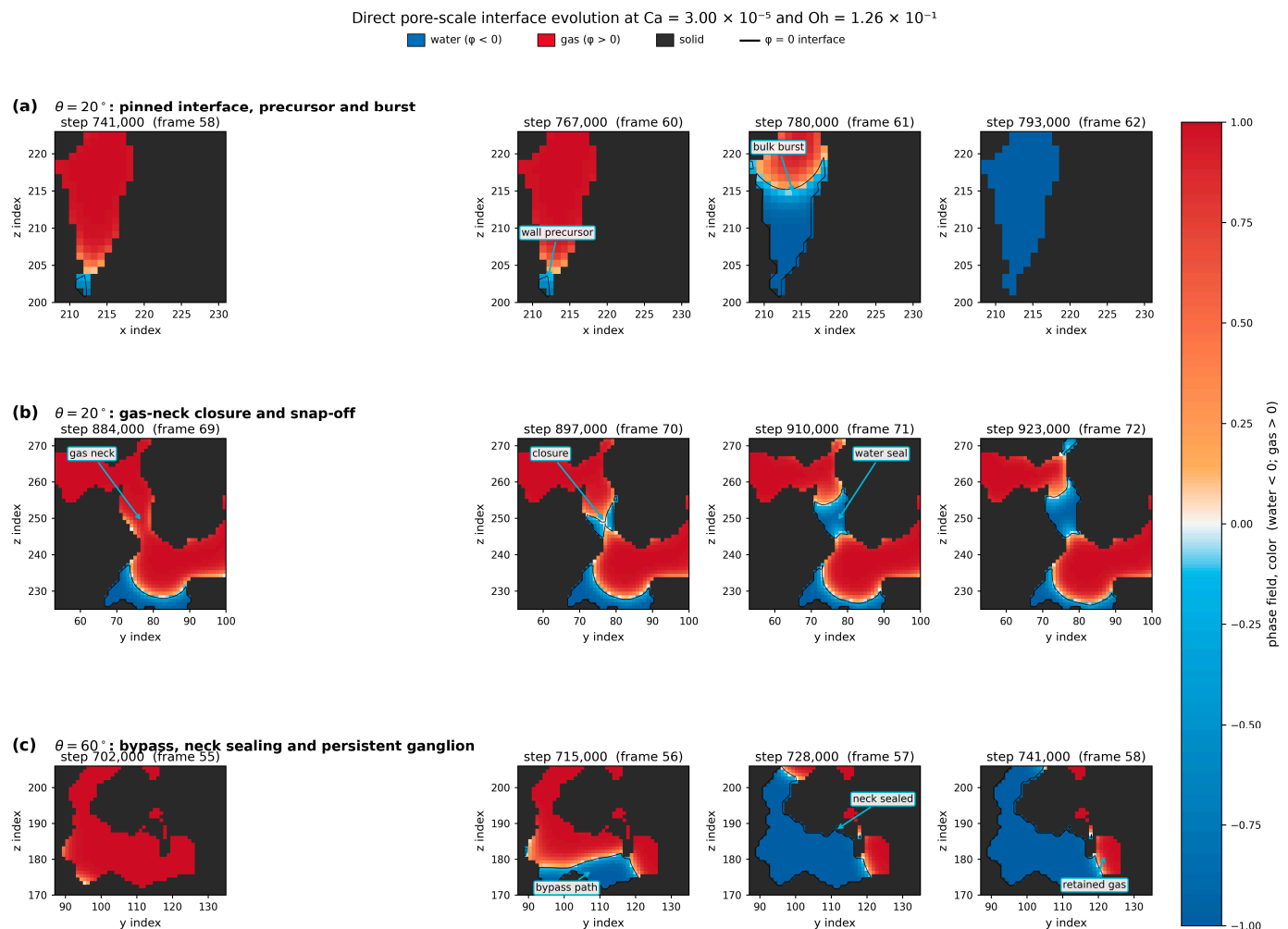


Figure 4. Direct pore-scale interface evolution at $Ca = 3.00 \times 10^{-5}$ and $Oh = 1.26 \times 10^{-1}$. The enlarged in-figure legend identifies water ($\varphi < 0$), gas ($\varphi > 0$), solid, and the $\varphi = 0$ interface: (a) at $\theta = 20^\circ$, a wall-adjacent precursor remains ahead of the bulk meniscus during steps 741,000–767,000, followed by abrupt pore-body filling at step 780,000, and near-complete filling at step 793,000. (b) at $\theta = 20^\circ$, a gas neck narrows at step 884,000, closes at step 897,000, and is fully water-sealed by step 910,000, leaving a persistent disconnected gas ganglion. (c) at $\theta = 60^\circ$, water bypasses a gas-filled branch, seals the connecting neck at step 728,000, and leaves a persistent ganglion. Coordinates are lattice indices.

Figure 4c shows bypassing and subsequent local isolation at $\theta = 60^\circ$ in $x = 124$ – 172 , $y = 87$ – 135 , and $z = 170$ – 206 . Water advanced along a lower alternative pathway during steps 702,000–715,000 and passed a gas-filled branch. At step 728,000, a 3623-voxel water-filled neck region separated a 14,731-voxel gas ganglion from its parent component. Of this ganglion, 14,702 voxels (99.80%) belonged to the same parent gas component in the preceding frame. The disconnected ganglion retained 14,625 voxels at step 780,000. The topology change was reproduced for gas thresholds of -0.25 , 0 , and $+0.25$ combined with 6-, 18-, and 26-neighbor connectivity. This sequence directly demonstrates bypassing, followed by neck sealing and persistent local gas entrapment.

These event-resolved observations demonstrate that the selected pore-scale processes occur at the low- Ca diagnostic condition. However, the two reruns have the same Ca and Oh and contain no local pressure or velocity output. They do not establish a Ca - or Oh -dependent suppression rate, the relative frequency of each mechanism, or their dominance across the sampled matrix. Broader parameter-dependent assignments are therefore treated as interpretations consistent with ensemble statistics rather than as direct local-field measurements.

3.4. Wettability-Dependent Contrast in Trapping Signatures

The central observed contrast between $\theta = 20^\circ$ and $\theta = 60^\circ$ concerns the pathway by which capillary driving is converted into pore occupancy. In the strongly water-wet case, the wetting phase can access corners and wall-adjacent regions more readily. This access is favorable when the bulk front remains coordinated with the wetting layers, but it can also promote gas-neck closure when wall-associated pathways advance ahead of the pore-core meniscus. Similar nonmonotonic wetting effects, in which stronger wetting shifts displacement toward corner-flow-related trapping, have been reported in microfluidic and pore-scale studies [9,12,13].

At $\theta = 20^\circ$ and low Ca , the selected event shows wall-associated advance and subsequent snap-off, while the ensemble terminal patterns are consistent with a larger contribution from snap-off-related isolation. Strong water-wetness therefore does not guarantee high efficiency: the same capillary affinity that improves access to small throats may also increase the likelihood of gas-neck closure when the imposed viscous pressure drop is weak. This interpretation is consistent with three-dimensional spontaneous-imbibition simulations in which pore-to-throat size ratio, contact angle, and Oh influence precursor–bulk competition [23]. The present data demonstrate occurrence but do not quantify a snap-off probability.

At $\theta = 60^\circ$, the selected diagnostic sequence shows water bypassing a gas-filled branch, sealing its connecting neck, and leaving a persistent ganglion. The terminal pore-size and morphology statistics are consistent with a greater contribution from incomplete access and bypassing-related retention than in the $\theta = 20^\circ$ cases. Small-pore gas can remain because local entry conditions are less favorable, throat connectivity is weak, or interfaces remain pinned at pore-throat expansions. The study does not measure snap-off frequency at $\theta = 60^\circ$ and therefore does not establish that snap-off is generally less frequent under this wettability.

Across the sampled Ca points, both wettability states show improved sweep, but their terminal changes have different signatures. For $\theta = 20^\circ$, the data are consistent with a reduced contribution from premature isolation as the bulk meniscus advances more effectively. For $\theta = 60^\circ$, higher Ca is associated with improved access to pore domains that remain poorly invaded at lower forcing. Because event-resolved diagnostics were performed at only one Ca , these cross- Ca mechanism assignments remain interpretations rather than direct measurements of mechanism frequency.

This wettability-dependent contrast indicates why terminal efficiency, pore-size occupancy, and ganglion morphology should be analyzed together. A lower terminal gas saturation does not imply uniform sweeping of all pore classes, and strong water-wetness can simultaneously improve small-throat access and increase gas fragmentation. The data support different trapping signatures at the two sampled wettability states; they do not identify a continuous wettability transition angle or uniquely partition every residual-gas body by formation mechanism.

3.5. Size-Selective Residual-Gas Retention

Figures 5–7 identify where the remaining gas is stored during water invasion and at the operational terminal state nearest $PV = 1.2$. In both wetting states, gas occupancy decreases with injected PV in all pore-size classes, but the decline sequence and terminal distribution are different.

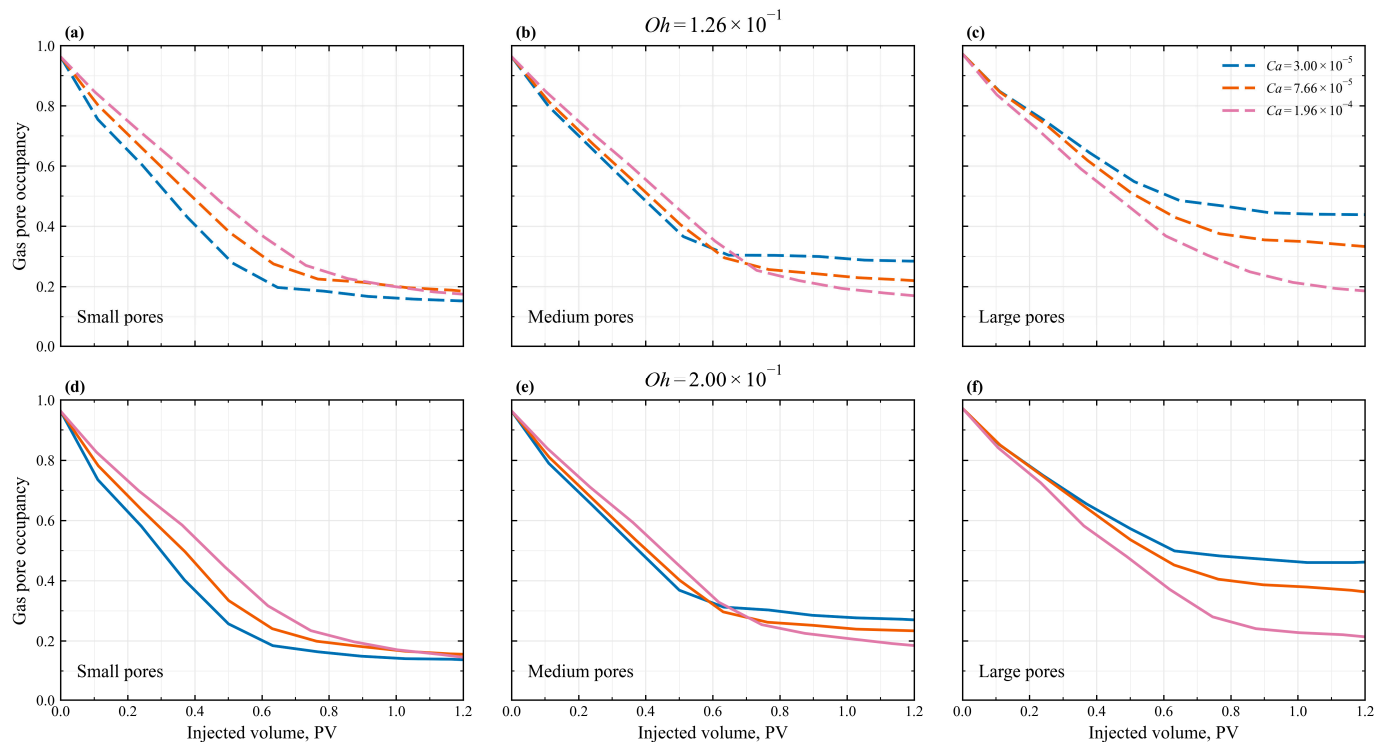


Figure 5. Temporal depletion of gas in the strongly water-wet case ($\theta = 20^\circ$): (a) small-pore gas occupancy at $Oh = 1.26 \times 10^{-1}$; (b) medium-pore gas occupancy at $Oh = 1.26 \times 10^{-1}$; (c) large-pore gas occupancy at $Oh = 1.26 \times 10^{-1}$; (d) small-pore gas occupancy at $Oh = 2.00 \times 10^{-1}$; (e) medium-pore gas occupancy at $Oh = 2.00 \times 10^{-1}$; (f) large-pore gas occupancy at $Oh = 2.00 \times 10^{-1}$. Dashed curves in panels (a–c) denote $Oh = 1.26 \times 10^{-1}$, solid curves in panels (d–f) denote $Oh = 2.00 \times 10^{-1}$, and colors distinguish the sampled Ca values. The pore-size intervals are 1.30–6.96 μm , 6.96–12.64 μm , and 12.64–18.29 μm .

For $\theta = 20^\circ$, small-pore gas declines most rapidly, medium-pore gas declines at an intermediate rate, and large-pore gas declines slowest. At the operational terminal state, gas occupancy follows the order large pores > medium pores > small pores. Strong water-wetness therefore enables early water entry into fine pore elements, but it does not ensure complete removal of gas from larger pore bodies. These observations are consistent with local isolation in pore bodies, including snap-off-related events, but terminal occupancy alone cannot uniquely identify formation history. The late-stage gas in the strongly water-wet cases is predominantly located in large pores; attributing it specifically to snap-off remains a mechanism-based interpretation supported by the selected event.

For $\theta = 60^\circ$, the terminal distribution reverses: small pores retain more gas than medium and large pores. The weakly water-wet system has less capillary affinity for entering fine throats, so that small-pore gas can be protected by local entry conditions, capillary-valve pinning, and limited connectivity. The contrast with $\theta = 20^\circ$ is consistent with a larger contribution from incomplete access and bypassing-related retention, but the terminal distribution does not exclude other trapping histories.

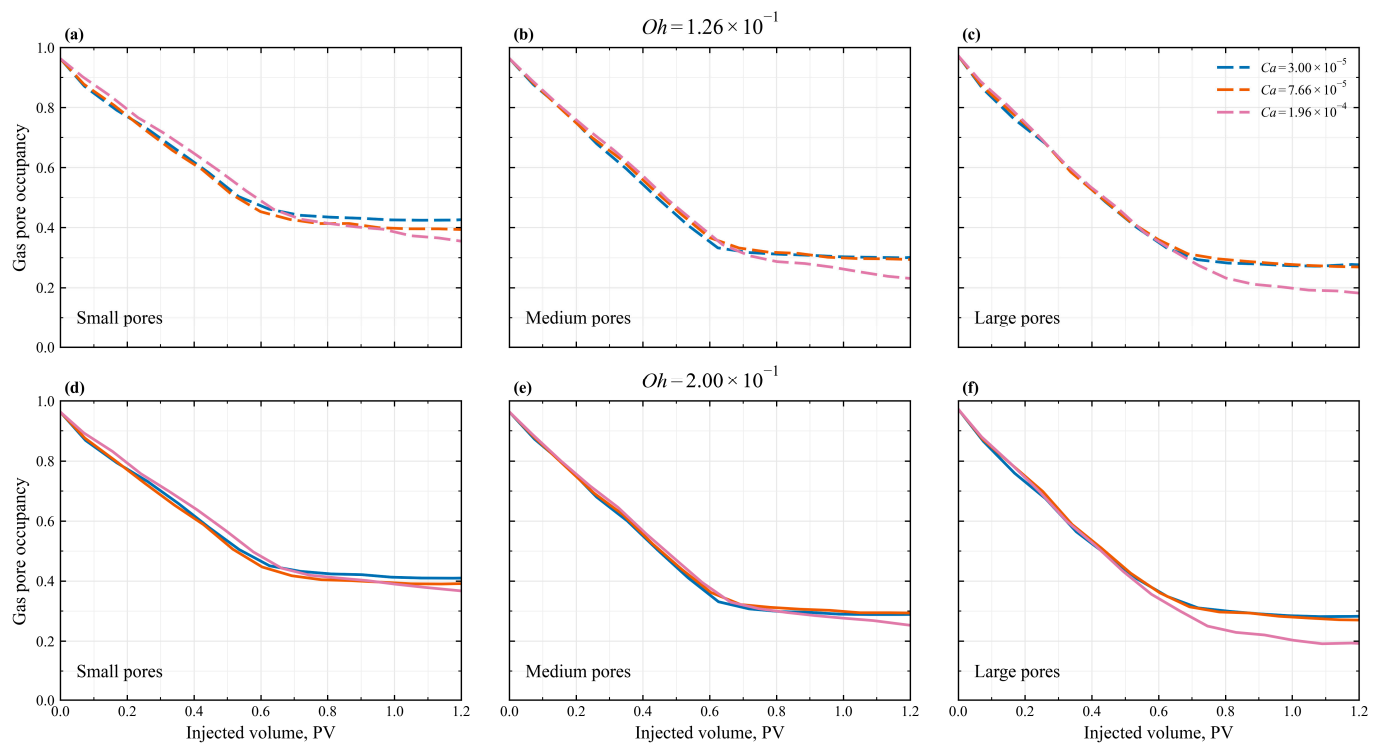


Figure 6. Temporal depletion of gas in the weakly water-wet case ($\theta = 60^\circ$): (a) small-pore gas occupancy at $Oh = 1.26 \times 10^{-1}$; (b) medium-pore gas occupancy at $Oh = 1.26 \times 10^{-1}$; (c) large-pore gas occupancy at $Oh = 1.26 \times 10^{-1}$; (d) small-pore gas occupancy at $Oh = 2.00 \times 10^{-1}$; (e) medium-pore gas occupancy at $Oh = 2.00 \times 10^{-1}$; (f) large-pore gas occupancy at $Oh = 2.00 \times 10^{-1}$. Dashed curves in panels (a–c) denote $Oh = 1.26 \times 10^{-1}$, solid curves in panels (d–f) denote $Oh = 2.00 \times 10^{-1}$, and colors distinguish the sampled Ca values. Compared with Figure 5, the weakly water-wet case retains a larger fraction of gas in the small-pore class.

Increasing Ca lowers terminal gas occupancy in all pore classes, but the largest change depends on wettability. Under $\theta = 20^\circ$, the most visible improvement occurs in large pores, consistent with enhanced invasion of regions that were poorly swept or locally isolated at lower forcing. This does not directly demonstrate remobilization of previously formed snap-off ganglia. Under $\theta = 60^\circ$, increasing Ca reduces large- and medium-pore gas occupancy, while small-pore gas remains comparatively persistent. Higher viscous forcing improves global sweep but does not eliminate local access limitations.

Within the sampled cases, changes in Oh are associated mainly with the redistribution of terminal gas among pore-size classes. Under $\theta = 20^\circ$, larger Oh tends to reduce gas in small and medium pores while slightly increasing gas in large pores. One physically consistent explanation is that stronger damping smooths local advance in fine elements while reducing interface reconfiguration near larger pore-body barriers. Under $\theta = 60^\circ$, the observed Oh dependence is weaker. These statements describe sampled associations and should not be read as a uniquely identified causal mechanism or a complete Ca – Oh interaction.

These results show why a volume-only residual-gas measure can be ambiguous. Large-pore ganglia and small-pore remnants may have different responses to subsequent forcing, but remobilization was not simulated here. Any statement about recoverability or relative-permeability impact is therefore an upscaling hypothesis rather than a directly tested outcome.

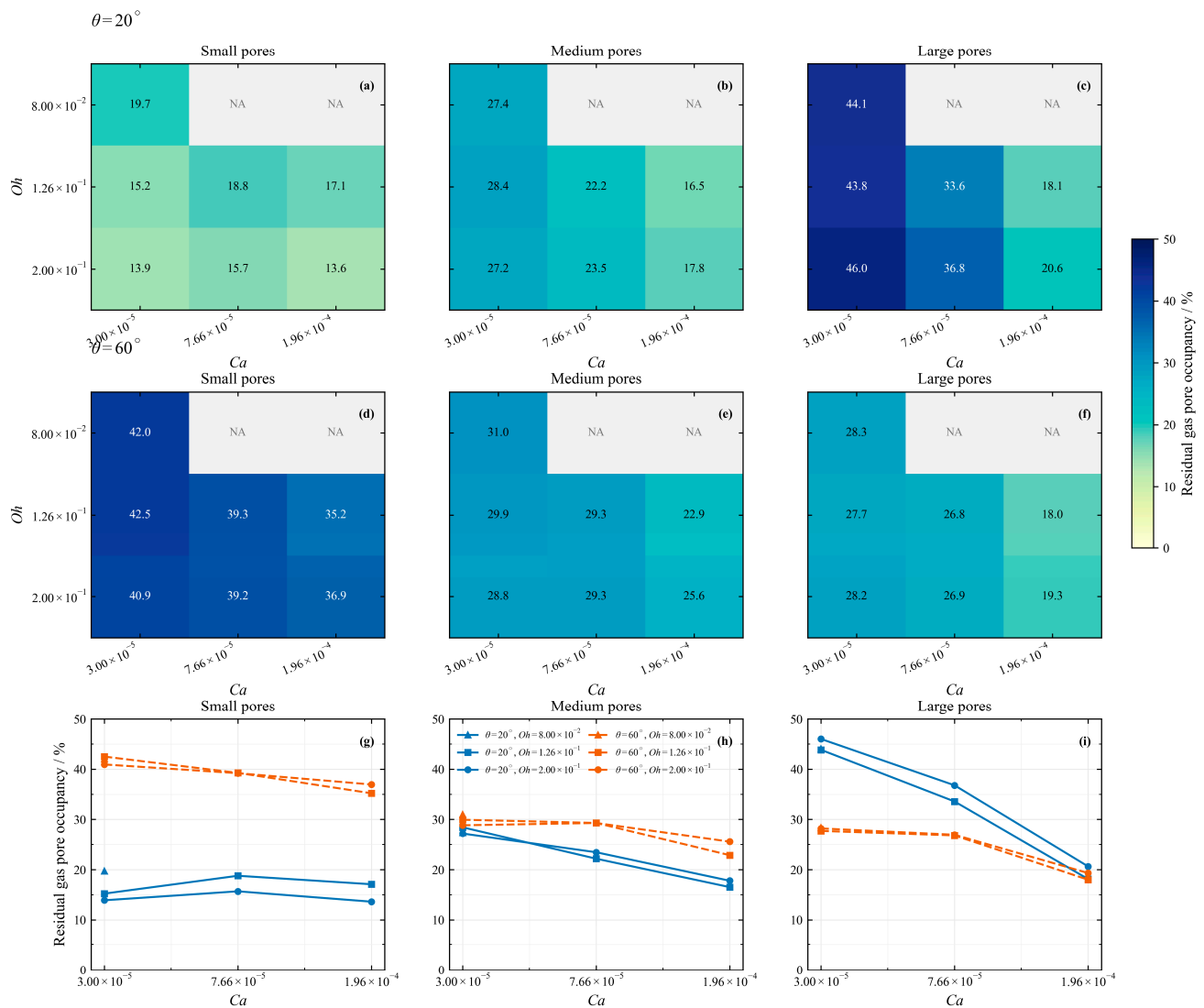


Figure 7. Residual-gas pore occupancy at the operational terminal state nearest $PV = 1.2$: (a) small-pore occupancy map for $\theta = 20^\circ$; (b) medium-pore occupancy map for $\theta = 20^\circ$; (c) large-pore occupancy map for $\theta = 20^\circ$; (d) small-pore occupancy map for $\theta = 60^\circ$; (e) medium-pore occupancy map for $\theta = 60^\circ$; (f) large-pore occupancy map for $\theta = 60^\circ$; (g) small-pore occupancy as a function of Ca ; (h) medium-pore occupancy as a function of Ca ; (i) large-pore occupancy as a function of Ca . The terminal distributions show that $\theta = 20^\circ$ leaves more large-pore gas, whereas $\theta = 60^\circ$ leaves more small-pore gas.

3.6. Trapped-Ganglion Morphology and Comparative Trapping Signatures

We separate trapped gas into four nonwetting-gas ganglion classes: droplet, columnar, multi-pore, and clustered gas. Film-type gas is not used because gas is nonwetting in the water-wet pore space and does not persist as a wall-adsorbed film. Figure 8 shows the three-dimensional spatial distribution of the four classes under the minimum Ca – Oh condition, and Figure 9 reports the morphology metrics used for classification.

Droplet gas has a low shape factor and simple topology and usually occupies one local pore region. Columnar gas is elongated but spans only one or a few pores, often reflecting gas retained in throats or narrow pore-body connections. Multi-pore gas spans several neighboring pores without developing a broad looped network. Clustered gas has the largest occupied-pore count or a more complex Euler characteristic, indicating a larger connected body with loops or a broad spatial extent. This classification follows

the topology-based view that connected components, loops, and cluster geometry carry information that saturation alone cannot provide [2,27,28].

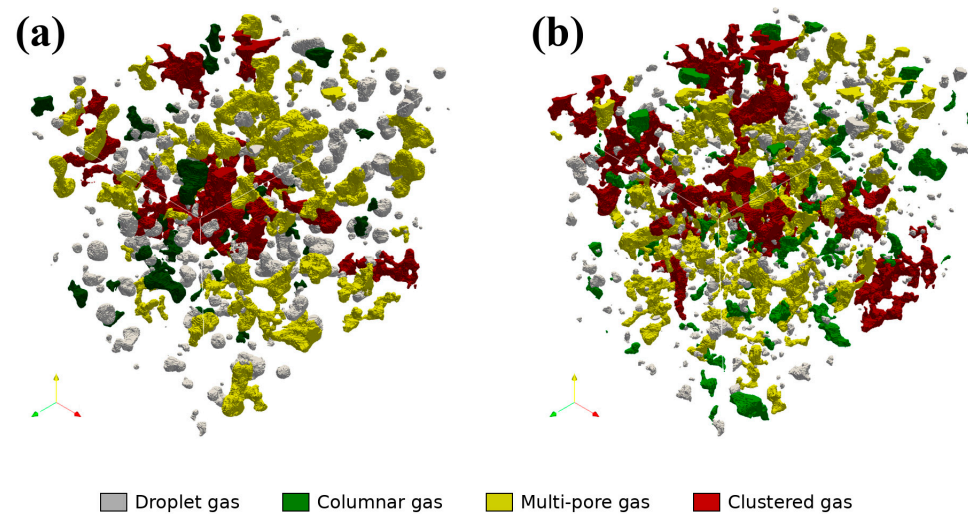


Figure 8. Three-dimensional residual-gas occurrence maps at the lowest $Ca-Oh$ condition and $PV = 1.2$: (a) $\theta = 20^\circ$; (b) $\theta = 60^\circ$. Gray, green, yellow, and red denote droplet, columnar, multi-pore, and clustered gas, respectively.

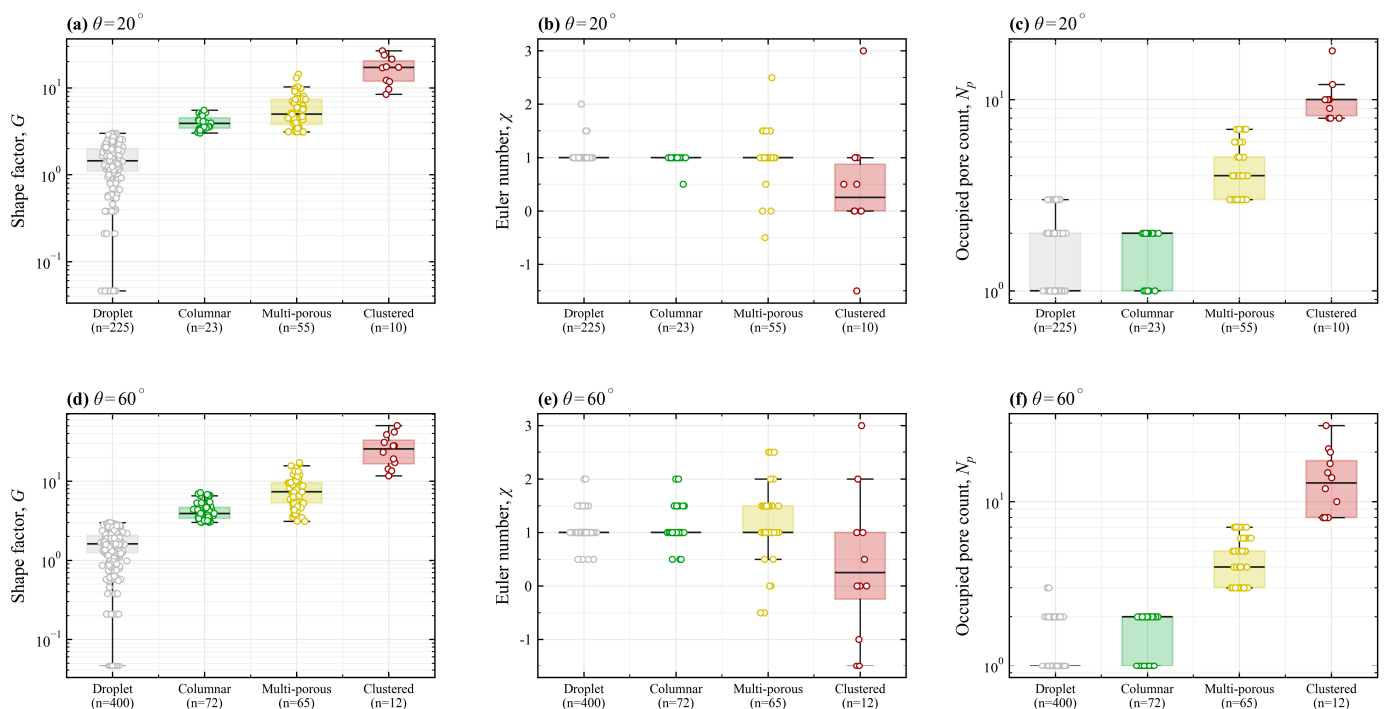


Figure 9. Statistical separation of residual-gas occurrence types at the lowest $Ca-Oh$ condition: (a) shape factor G for $\theta = 20^\circ$; (b) Euler characteristic χ for $\theta = 20^\circ$; (c) occupied-pore count N_p for $\theta = 20^\circ$; (d) shape factor G for $\theta = 60^\circ$; (e) Euler characteristic χ for $\theta = 60^\circ$; (f) occupied-pore count N_p for $\theta = 60^\circ$. Box limits enclose the interquartile range, center bars are medians, whiskers span the extrema, and points denote individual clusters.

Under $\theta = 20^\circ$, residual gas volume is dominated by droplet and multi-pore forms. Droplet gas contributes 31.03–40.73% of classified residual-gas volume, and multi-pore gas contributes 30.88–44.92%. Columnar gas is lower, about 7.47–14.75%, while clustered gas varies from about 11.55% to 22.48%. This distribution is consistent with a larger contribution from snap-off-related fragmentation. Strong water-wetness promotes water invasion

through corners and small throats, and the selected event shows that these pathways can close a gas neck. However, morphology alone does not uniquely identify formation history, so individual droplet or multi-pore bodies are not treated as proven snap-off products.

Under $\theta = 60^\circ$, multi-pore gas contributes about 33.71–36.53% of classified residual-gas volume, while clustered gas is high at low Ca , reaching about 31.66–33.20%, and decreases across the sampled Ca values. Droplet and columnar fractions increase. This pattern is consistent with bypassing-related retention of larger gas domains followed by partial invasion or fragmentation at higher forcing. Because event frequency was not measured across Ca , the shift is interpreted from terminal morphology rather than as direct evidence of a universal breakup pathway.

The residual-gas volume partitions in Figure 10 and the corresponding body counts in Figure 11 reveal a number–volume asymmetry. Droplet gas is numerous but typically small in individual volume. Clustered gas is less numerous but can contribute a large fraction of the residual volume. A displacement process that produces many droplets may have a high cluster count but limited recoverable volume, whereas a process that leaves a few clustered gas bodies may have fewer clusters but a larger remobilization target.

Across the sampled cases, the most evident Ca -associated morphology change is a reduction in the volume fraction of larger clustered bodies and an increase in smaller classified forms, especially for $\theta = 60^\circ$. This is consistent with additional throat invasion disturbing the connectivity of larger gas bodies, but it may represent partial removal, fragmentation, or both. The terminal statistics cannot uniquely distinguish these histories.

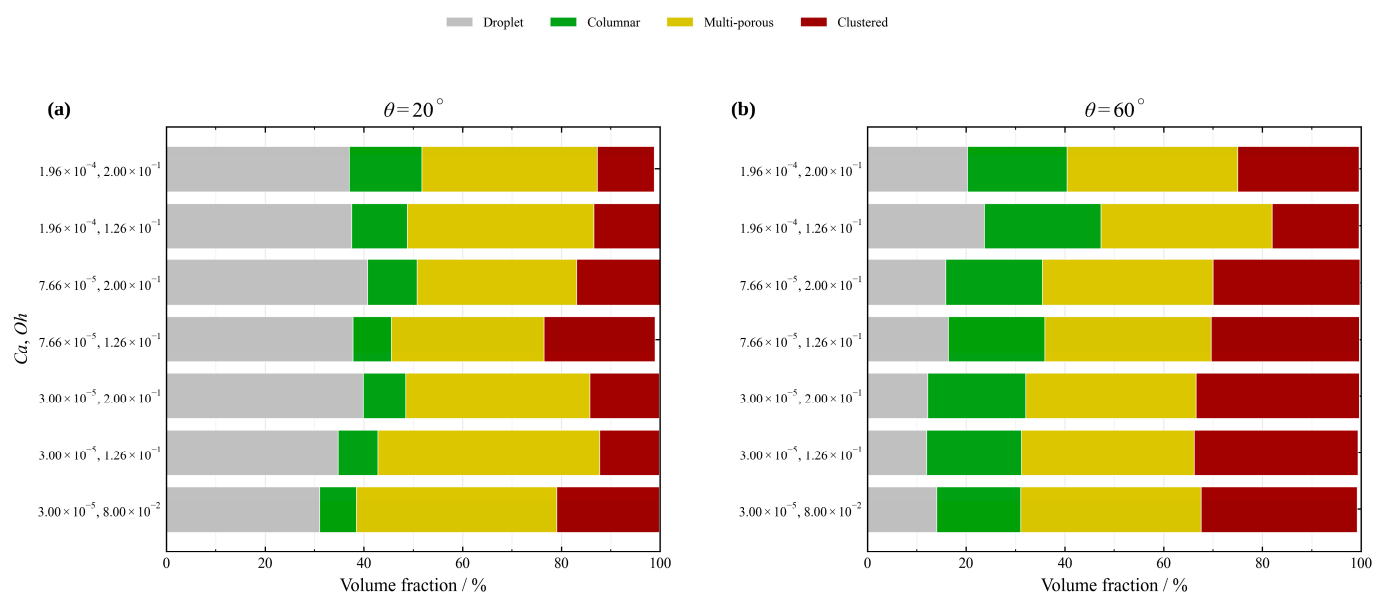


Figure 10. Residual-gas volume partition among the four classified forms for all sampled Ca – Oh – θ cases: (a) classified volume fractions for $\theta = 20^\circ$; (b) classified volume fractions for $\theta = 60^\circ$. Fractions are normalized by the total classified residual-gas volume; 29 baseline bodies assigned to the unclassified fallback are not included in the four-class partition and are not assigned a formation mechanism. Colors follow Figure 8. The wettability comparison is robust over the tested G_c – N_c ranges but should be interpreted comparatively rather than as a universal taxonomy.

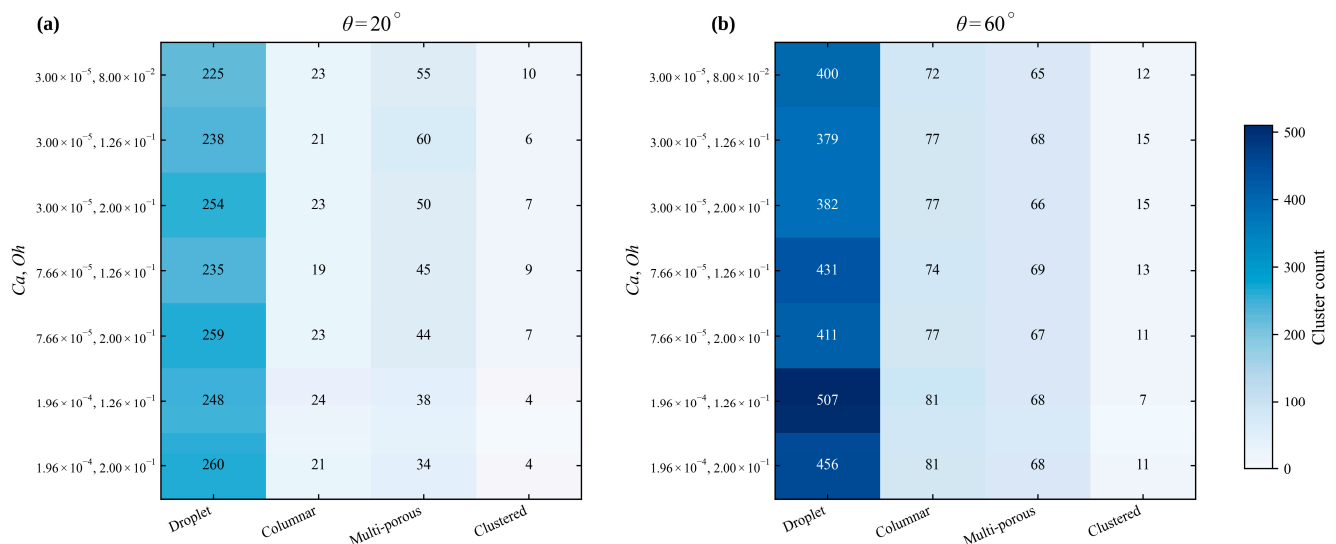


Figure 11. Number of residual-gas bodies in each classified occurrence type for the sampled $Ca-Oh-\theta$ conditions: (a) body counts for $\theta = 20^\circ$; (b) body counts for $\theta = 60^\circ$. Labels report counts that sum to 6306 classified bodies; 29 of the 6335 baseline bodies are retained as unclassified and omitted from the four-class panels. Droplets dominate by number, whereas clustered gas can remain important by volume despite occurring less frequently.

3.7. Implications, Applicability, and Remaining Uncertainty

For the present pore-space realization, the results suggest that upscaling descriptions may benefit from retaining three complementary state variables: total trapped-gas volume, the pore-size distribution of that volume, and ganglion connectivity. Saturation measures volume; pore-size occupancy identifies where the volume is located; and morphology distinguishes compact, elongated, several-pore, and spatially extended bodies. The threshold sensitivity analysis in Section 2.4 shows that these descriptors should be used comparatively rather than as universal taxonomic boundaries.

These descriptors may correspond to different remobilization or flow-blocking potentials. Droplet gas is numerous but small, columnar gas can occupy throat-scale connections, and multi-pore or clustered gas can retain larger volumes. However, the present simulations stop at the operational terminal state and do not apply a subsequent remobilization protocol. The proposed engineering implications are therefore hypotheses for future testing, not measured recovery outcomes.

The sampled wettability states also show different terminal signatures. Under $\theta = 20^\circ$, late gas is concentrated more strongly in large pores, and the morphology is consistent with a larger contribution from snap-off-related isolation. Under $\theta = 60^\circ$, small-pore gas is more persistent, and the morphology is consistent with incomplete access and bypassing-related retention. Two cases with similar saturation may therefore have different state descriptions. Upscaled models may benefit from distinguishing these signatures, but the present study does not establish a unique constitutive mapping from morphology to relative permeability or remobilization. At larger scales, sequence-to-sequence production models and sensor-based process-monitoring systems provide complementary frameworks for testing whether physically interpretable state descriptors improve forecasting and operational supervision [46,47].

The fluid-property assumptions further restrict applicability. Density matching ($\rho_w/\rho_g = 1$) removes the phase-density contrast from the inertial response. The separate omission of gravity eliminates buoyancy-driven segregation, while the constant-density weakly compressible lattice formulation does not represent real-gas compressibility. The water-based Reynolds numbers in Table 1 are 7.5×10^{-4} – 1.23×10^{-2} ; using the same

reference velocity and length, the corresponding gas-viscosity-based values in the matched-density model are $M Re_w \approx 0.020\text{--}0.321$. The simulations therefore address pressure-driven pore-scale capillary-viscous displacement with modest local inertial response inside the adopted model. They are not a quantitative representation of large-density-ratio, gravity-dominated, or compressible reservoir gas–water flow.

Two additional scope limitations are important. First, only one stochastic reconstruction was used. The study therefore quantifies within-structure trends but not structure-to-structure variability, an ensemble mean, or the statistical representativeness of the reported rankings. Different realizations may alter absolute capillary thresholds and the magnitude, or even the ordering, of some secondary trends. Second, the sparse, non-factorial parameter matrix precludes a continuous response surface or a formally separable Ca – Oh –wettability interaction. Numerical values and mechanistic rankings should therefore be generalized only with caution to pore networks having comparable statistics and to the sampled parameter ranges.

4. Conclusions

This study examined forced water invasion in an initially gas-saturated reconstructed tight pore space using a three-dimensional regularized color-gradient lattice Boltzmann model. Water was the invading phase, and gas was the defending phase. The viscosity ratio was fixed at $M = \mu_w/\mu_g = 26.11$, and the sampled variables were Ca , Oh , and the aqueous-phase contact angle. The conclusions below are comparative for one stochastic pore-space realization and the simulated parameter points.

- (1) A favorable viscosity ratio does not eliminate pore-scale trapping. The selected interface sequences directly show wall-associated precursor advance, abrupt pore-body filling, gas-neck closure, component splitting, and bypass-induced isolation. These observations establish that such events occur in the simulated pore space, but not their frequency or dominance across all conditions.
- (2) Among the sampled variables, Ca shows the strongest association with terminal displacement efficiency and front stabilization. Under $\theta = 60^\circ$, final efficiency changes little between the low and intermediate Ca points and rises from approximately 0.660 to 0.736 at the highest point. Under $\theta = 20^\circ$, the terminal trends are consistent with a reduced contribution from premature isolation and improved pore-body sweep as Ca increases. Three Ca values do not establish a sharp universal threshold or a cross- Ca event-suppression rate.
- (3) The sampled Oh dependence is weaker and conditional. Lower Oh at selected intermediate and high Ca values is associated with greater large-pore water occupancy, consistent with weaker damping and easier interface reconfiguration. Because diagnostics were obtained at one Oh , contain no local pressure or velocity fields, and the matrix is non-factorial, this remains a physical interpretation rather than a direct measurement or a general interaction law.
- (4) The two wettability states exhibit contrasting terminal trapping signatures rather than a demonstrated continuous transition. At $\theta = 20^\circ$, the selected event and terminal morphology are consistent with a larger contribution from snap-off-related fragmentation and large-pore isolation. At $\theta = 60^\circ$, small-pore gas is more persistent, and the terminal state is consistent with incomplete access and bypassing-related retention. The present data do not quantify mechanism frequencies or identify a transition contact angle.
- (5) Pore-size-resolved occupancy provides information not contained in total gas saturation. In this realization, terminal gas under $\theta = 20^\circ$ is concentrated more strongly in large pores, whereas under $\theta = 60^\circ$ it is more persistent in small pores. Increasing

Ca lowers gas occupancy in all pore classes at the sampled points, but the magnitude and location of the change depend on wettability.

- (6) The operational ganglion classification reveals a number–volume asymmetry and a robust comparative wettability contrast over the tested G_c – N_c ranges. Droplets are numerous but individually small, whereas a few multi-pore or clustered bodies can retain substantial volume. Morphological classes are not unique formation-mechanism labels, and their exact fractions remain threshold-dependent.
- (7) The grid-resolution assessment supports the adopted $300 \times 300 \times 400$ lattice for the global displacement-efficiency metric in the tested case. The $1.0\times$ and $1.5\times$ curves differ by no more than 0.58 percentage points over $0 \leq PV \leq 1.2$, with an RMSE of 0.43 percentage points and an endpoint relative difference of 0.50%. This evidence does not establish convergence of every local interfacial event. The sampled We range of 2.25×10^{-8} – 2.42×10^{-6} confirms a globally capillary-dominated forced-imbibition window. The broader scope remains limited by the single stochastic pore-space realization, the sparse non-factorial parameter matrix, density matching, omission of gravity, and absence of real-gas compressibility. The results do not establish a structure-independent response surface or a universal wettability transition. Additional pore-space realizations and event-resolved multi- Oh diagnostics are required to quantify those uncertainties.

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