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Invited review

Numerical methods to simulate spontaneous imbibition in microscopic pore structures: A review

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Abstract:
Spontaneous imbibition, as a fundamental flow phenomenon, is widely utilized in fossil energy production, carbon dioxide and underground hydrogen storage. With the development of computing, the exploration of flow laws of spontaneous imbibition has evolved from macroscopic theoretical models to pore-scale numerical analysis. Currently, the solutions for multiphase flow in pore media mainly consider the volume of fluid and the phase field, and have been classed into level set methods based on macroscopic Navier-Stokes equations and the Shan-Chen, free energy, color gradient, and phase-field methods based on mesoscopic lattice Boltzmann equations. However, no comprehensive review article has summarized the strengths and limitations of these methods. Therefore, this work focuses on critically reviewing and commenting on the fundamentals and limitations of pore-scale models applied to spontaneous imbibition. In addition, recent works applying these methods are systematically reviewed. Our study aims to provide the scientific community with an expert opinion to understand the basic methods for solving the existing problems of spontaneous imbibition in porous media. Future research directions are suggested, namely, focusing on developing the reconstruction pore medium algorithms, establishing modeling methods for non-stationary states, exploring the flow laws in mixed wetting conditions, linking macroscopic and microscopic flow laws, and developing models for coupled multiphase flow numerical computation with machine learning. Overall, this review provides a comprehensive understanding of spontaneous imbibition simulation methods, promotes a thorough knowledge of spontaneous imbibition in porous media, provides guidance on exploring flow laws, and inspires researchers to give more credit to spontaneous imbibition studies.

1. Introduction

From the rising demand for conventional energy (oil, natural gas, coalbed methane) to the control of global warming (carbon dioxide sequestration and underground hydrogen storage), the development and utilization of underground reservoirs has reached new dimensions compared to several decades ago (Huppert and Neufeld, 2014; Caporin and Fontini, 2017; Raza et al., 2022; Aslannezhad et al., 2023; Hematpur et al., 2023). Reservoir production is based on spontaneous imbibition as a fundamental recovery mechanism, which involves a wetting fluid intruding into a porous medium through capillary forces and displacing non-wetting fluids (Morrow and Mason, 2001; Mason and Morrow, 2013; Cai et al., 2012a, 2014, 2020a). With the advancement of production technology from traditional water injection to hydraulic fracturing, the reservoir structure has changed significantly (Montgomery and Smith, 2010; Barati and Liang, 2014; Liu et al., 2017; Os-

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iptsov, 2017; Esene et al., 2019; Cai et al., 2017, 2020b; Chen et al., 2021; Abdelaziz et al., 2023; Almutairi et al., 2023). Moreover, the entensive discovery of shale reservoirs in large sedimentary basins, such as Bohai Bay, Songliao, Ordos, and Junggar, has led to a gradual transition of the detected reservoir characteristics from simple and homogeneous to highly fractured and double porosity, facilitating the research progress on spontaneous imbibition (Zhang and Zhu, 2008; Jia et al., 2012; Sun et al., 2013; Guo et al., 2019; Xin et al., 2021). In the study of spontaneous imbibition, the exploration of flow properties has been continuous, ranging from theoretical models to macroscopic laws and to pore-scale imbibition laws.

Regarding theoretical models, the exploration of imbibition theory commenced with the Lucas-Washburn model in the early 20th century, which was based on the spontaneous imbibition of water in a single capillary (Lucas, 1918; Washburn, 1921). Many theoretical analyses and experimental studies of spontaneous imbibition have taken this model as a basis. Similar theories of seepage include the Terzaghi model, Handy model, Mattax and Kyte factorless time scale model, and Aronofsky normalized recovery scale model (Aronofsky et al., 1958; Schembre et al., 1998; Li and Horne, 2000; Amico and Lekakou, 2002; Cai et al., 2012b). Cai and Yu (2012c) provided a detailed review of the strengths and weaknesses of these theoretical models and the development process. With the deepening of research, the model of imbibition theory has gradually developed from the initial capillary model to an irregular model (Ayyaswamy et al., 1974; Kim and Whitesides, 1997; Dong and Chatzis, 2003; Wang and Dong, 2011; Zhao et al., 2021). Cai et al. (2022) further reviewed the development of capillary imbibition and flow of wetting liquids in irregular capillaries covering the past century. During this period, the fractal theory was introduced, which integrates the structural information of porous media analytically into the models, enabling a more precise description of imbibition laws (Cai et al., 2010, 2012a; Wei et al., 2018; Liu et al., 2020b; Wu et al., 2021). The development of the theoretical model of imbibition and suction accelerated the understanding of the imbibition mechanism and also promoted the advancement of macro-scale experiments.

Regarding the macroscopic imbibition law, core scale experiments and Darcy-scale numerical simulations were used to investigate the effects of core geometric parameters (shape and size), physical properties (porosity, permeability), fluid properties (density, viscosity, surface tension), wettability (wetting angle, mixed wettability), and gravity on oil recovery in the process of spontaneous imbibition (Morrow and Mason, 2001; Hatiboglu and Babadagli, 2007; Meng et al., 2017, 2019; Yang, 2019). Gao et al. (2019) summarized spontaneous imbibition experiments for shale wettability. Owing to the complex fracture structure in the reservoir, different oil-water and matrix contact situations simultaneously exist. The different boundary conditions were also considered, including “one end open”, “two ends open”, “two ends open-free”, “two ends close”, and “all face open boundary” conditions (Yildiz et al., 2006; Lyu et al., 2019; Zhang et al., 2019). Meng and Cai (2018) summarized the research progress on spontaneous imbibition under different boundary conditions. As core-scale studies, these works have faced challenges regarding the consideration of microscale pore structure and internal flow details. Specifically, researchers had treated the permeability domain of porous medium as a “black-box” model and described the flow within the porous medium at the macroscopic scale by combining Darcy’s law and measuring parameters such as pressure difference, flow rate, etc.

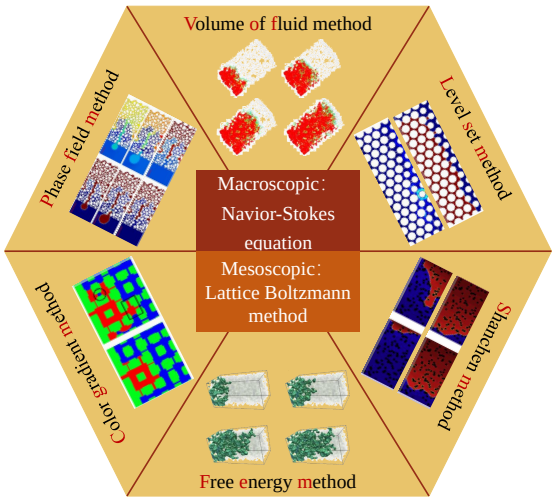


Fig. 1. Schematics of various multiphase flow models: Volume of fluid, phase field, level set, Shan-Chen, free energy, color gradient, and phase-field.

For pore-scale imbibition laws, the main method is to use pore-scale multiphase flow simulation to obtain the spatial distribution of velocity and pressure fields, and then to analyze the laws of fluid flow in the pore space (Golparvar et al., 2018; Ramstad and Berg, 2019; He et al., 2022a, 2023; Liang et al., 2023; Zou et al., 2023). This approach has become an important tool, in addition to laboratory physical experiments, in the study of microscopic seepage mechanism in reservoirs. Thus far, many pore-scale numerical simulation methods have been developed and matured, each with its own advantages in terms of computational speed, solution accuracy and computational domain scale. Commonly used multiphase flow models include the volume of fluid, phase-field, and level set methods, all being traditional computational fluid dynamics models based on the macroscopic Navier-Stokes equations (Wang et al., 2019), as shown in Fig. 1. In addition, relatively emerging multiphase flow models have been developed based on mesoscale lattice Boltzmann methods, such as the Shan-Chen, free energy, and color gradient models (Yang and Boek, 2013; Huang et al., 2015, Zhou et al., 2022). In recent years, numerous reviews have been published on the progress of pore-scale spontaneous imbibition studies. These include the mechanisms of fracturing fluid spontaneous imbibition behavior in shale reservoir (Hu et al., 2020), the phenomenon of counter-current spontaneous imbibition (Abd et al., 2019), spontaneous imbibition in shale (Li et al., 2019), and the wettability alteration by spontaneous imbibition using low-salinity water in naturally fractured reservoirs (Karimova et al., 2023). Nevertheless, all of the above reviews have solely commented on the development of a single aspect and

lacked a systematic organization and discussion of pore-scale spontaneous imbibition methods.

In order to facilitate the further exploration of spontaneous imbibition flow laws at the pore scale, the systematic review of recent research results is essential. This information is not only vital for understanding the flow laws of spontaneous imbibition but also it ultimately aids engineers in making better decisions with reduced uncertainties. The remaining sections of this study were organized as follows: Section 2 discusses the multiphase flow models based on macroscopic Navier-Stokes equations, along with the investigated problems. Section 3 focuses on the methodology and research issues of the multiphase flow model based on the mesoscopic lattice Boltzmann method. Finally, potential directions for future research are highlighted. This paper aims to provide readers with concise and reliable information about numerical simulations of multiphase flow at the pore scale.

2. CFD models based on Navier-Stokes equations

The multiphase flow simulation methods based on Navier-Stokes equations encompass various techniques, including the volume of fluid (VOF) method, phase-field method (PFM) and level-set method (LSM) (Broughton and Joshi, 2021; Chamakos et al., 2021). These aim to address the challenge of interface dynamics in multiphase fluids, involving the movement and interaction of fluid-fluid or fluid-solid interfaces. The VOF method describes fluid interfaces by tracking the volume fraction of different fluid phases (Welch and Wilson, 2019; Scapin et al., 2020). A scalar function represents the distribution of fluid phases at each spatial point. By calculating the volume fractions of different phases, the VOF can capture the position and shape of the fluid interface. This method is typically suitable for handling complex dynamic changes in the fluid interfaces, such as the motion of liquid-gas or liquid-solid interfaces. The PFM simulates the dynamic behavior of multiphase fluids by establishing a field representing the presence of each phase (Yue et al., 2006; Meakin and Tartakovsky, 2009). The distribution of different phases is tracked by solving the diffusion equation involving the phase field. The PFM combines the continuity equation and the Cahn-Hilliard equation, enabling the effective capture of phase transition phenomena and the motion of fluid interfaces. The LSM describes the evolution of interface position and shape by tracking the level set function surrounding the fluid interface (Ervik et al., 2014; Ning et al., 2023). It is based on an implicit function whose equivalent surface represents the fluid interface. This method demonstrates good performance in capturing changes in fluid interfaces and complex topological structures, providing an advantage in the dynamic handling of fluid-fluid or fluid-solid interfaces in complex multiphase fluids. Each of the above methods have advantages in solving interfacial evolution in multiphase fluids and a wide range of applications in their respective domains of applicability (Worner, 2012). The selection between them depends on the complexity of the particular problem, the availability of computational resources, and the required simulation accuracy (Santra et al., 2019).

2.1 Volume of fluid method

The VOF method can be traced back to the simple line interface calculation (SLIC) interface reconstruction algorithm proposed by Noh and Woodward (1976). Following decades of development, the VOF method has become one of the most widely used multiphase flow simulation methods. Its core idea is to define a volume fraction of the reference phase in a control cell. If the control cell is entirely occupied by the reference phase, the volume fraction is 1; if the control cell is entirely occupied by the other phase, the volume fraction is 0; at the interface, the volume fraction in the control cell ranges between 0 and 1 (Gueyffier, 1999; Renardy et al., 2001). Depending on the interface determination method, VOF methods can be divided into geometric reconstruction methods and interface compression (Tryggvason et al., 2006; Hu et al., 2017). Geometric reconstruction methods can be employed to reconstruct the interface by using line segments to represent the interface after solving to obtain the volume fraction in each control cell. On the other hand, interface compression obtains a thinner interface thickness by adding an interface compression term to the volume-fractional transport equation. The position of the interface is determined directly by solving the modified transport equation. This method is broadly used in open-source software such as OpenFOAM. Multiphase flow in porous media can be captured through the Navier-Stokes equation, namely:

$$\rho\frac{\partial \mathbf{u}}{\partial t}+\rho\left(\mathbf{u}\cdot\nabla\right)\mathbf{u}=-\nabla p+\nabla\left[\mu\left(\nabla\mathbf{u}+\nabla\mathbf{u}^{T}\right)\right]+\mathbf{f_s} \tag{1}$$

$$\nabla\mathbf{u}=0 \tag{2}$$

where p denotes the pressure; $\mathbf{u}$ denotes the velocity vector; ρ denotes the fluid density; μ denotes the fluid dynamic viscosity; t denotes the time; and $\mathbf{f_s}$ denotes the surface tension force:

$$\mathbf{f_s}=\sigma\kappa\mathbf{n} \tag{3}$$

where σ means surface tension, κ stands for the curvature, and $\mathbf{n}$ represents the normal vector of the interface. Therefore, $\mathbf{f_s}$ is nonzero at curved interfaces and represents the effect of Young-Laplace pressure.

The VOF is utilized to track the evolution of the muti-phase interface. A volume fraction α is introduced as an indicator function to represent the volume fraction of fluid within cells, as aforementioned:

$$\alpha=\begin{cases}0, \text{ in the nonwetting fluid}\\ 1, \text{ in the wetting fluid}\\ 0<\alpha<1, \text{ on the interface}\end{cases} \tag{4}$$

The evolution of α is given by an advection equation:

$$\frac{\partial\alpha}{\partial t}+\nabla\left(\alpha\mathbf{u}\right)+\nabla\left[\alpha\left(1-\alpha\right)\mathbf{u}_r\right]=0 \tag{5}$$

where $\mathbf{u}_r$ represents an artificial compression velocity to limit numerical diffusion (Rusche, 2003). Therefore, the viscosity μ and the density ρ in the whole domain can be expressed as:

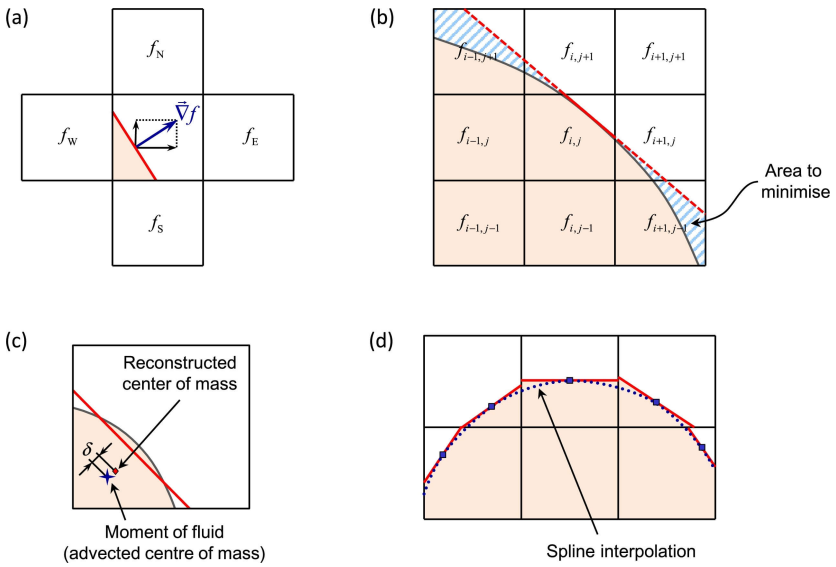


Fig. 2. Schematics of various PLIC interface reconstruction techniques: (a) gradient method, (b) least-square minimization error, (c) moment-of-fluid method and (d) spline interpolation, modified from Comminal et al. (2015).

$$\begin{aligned} \mu &= \alpha\mu_w + (1-\alpha)\,\mu_{nw} \\ \rho &= \alpha\rho_w + (1-\alpha)\,\rho_{nw} \end{aligned} \tag{6}$$

where μ_{nw} and ρ_{nw} represent the viscosity and density of non-wetting phase, respectively. Given that $\mathbf{n} = \nabla\alpha$, the source term $\mathbf{f_s}$ can be expressed in an alternative form (Brackbill et al., 1992):

$$\mathbf{f_s} = \sigma\kappa\nabla\alpha\delta\Gamma = -\sigma\kappa\nabla\left(\frac{\nabla\alpha}{\|\nabla\alpha\|}\right)\delta\alpha \tag{7}$$

Numerical simulation considers the wettability effect on the fluid flow by imposing an additional constraint at the intersection between the interface and solid surface (Ferrari and Lunati, 2013, 2015):

$$\frac{\nabla\alpha}{\|\nabla\alpha\|}\Big|_{x\in\text{wall}} := \mathbf{n}_s\cos\theta + \mathbf{n}_t\sin\theta \tag{8}$$

where θ denotes the contact angle; $\mathbf{n}_s$ represents the unit normal pointing into the solid, $\mathbf{n}_t$ is the unit tangent to solid points into the wetting phase; and the "wall" represents the wall surface in pore media.

From the earliest SLIC reconstruction technique to the method proposed by Hirt and Nichols (1981), followed by the flux line-segment and the piecewise linear interface calculation (PLIC) reconstruction method, the interfaces are becoming increasingly finer and the accuracy is also improving (Noh and Woodward, 1976; Hirt and Nichols, 1981; Ashgriz and Poo, 1991; Lopez et al., 2005). Among these techniques, PLIC is currently the most widely used interface reconstruction method, which is shown in Fig. 2. It conducts interface reconstruction in two steps: Firstly, it calculates the normal vector of the interface in the current control cell based on the volume fraction inside the current and the surrounding control cells, then it determines the equation of the interface line segments in the cell based on the normal vector. Although the reconstruction interface is not performed more accurately, the sharp corners are smoothed out. Furthermore, the actual two-phase interface is continuous but the reconstructed interface is discontinuous. However, as interface reconstruction techniques continue to improve, the degree of interface discontinuity is gradually decreasing (Tryggvason et al., 2006). The VOF method is effective in capturing significant interface topological deformations and ensuring mass conservation (Nguyen and Park, 2017). Its extension from two dimensions to three dimensions is relatively straightforward. Moreover, due to interface reconstruction being a local algorithm, VOF is amenable to parallelization. However, the VOF method does have certain limitations (Garoosi and Hooman, 2022). For instance, interface reconstruction in unstructured grids is generally challenging and curvature calculations are complex. Compared with methods like LSM, three-dimensional interface reconstruction is relatively intricate (Issakhov et al., 2018).

In recent years, the VOF method has been widely applied for spontaneous imbibition in porous media. A chronological arrangement of relevant studies of spontaneous imbibition using the VOF model is presented in Table 1. Researchers have used this model to investigate the effects of injection velocity, interfacial tension, viscosity ratio, capillary number, contact angle, and wettability (Fig. 3) for spontaneous imbibition.

2.2 Phase-field method

The PFM is a type of diffusive interface model, whose idea can be traced back to the study of Van Der Waals (1979). From a thermodynamic perspective, a diffusive interface model can more naturally describe the two-phase distribution in the steady state than the sharp interface model (Cahn, 2004; Cahn and Hilliard, 2004a, 2004b). Subsequently, Cahn and Hilliard proposed the phase-field model, which has found widespread use. This method also applies Eqs. (1) and (2) to describe fluid flow within porous media. Therein, interface evolution and the dynamical behavior of the phase interface are described by the phase field equations:

Table 1. Summary of relevant studies on spontaneous imbibition using the volume of fluid method.

System	Object	Emphasis	Reference
Liquid, liquid	2D	Wettability	Rabbani et al. (2017)
Liquid, liquid	2D, pore network	Parasitic currents and dynamic capillary barriers	Pavuluri (2019)
Liquid, liquid	2D, fracture network	Capillary number, viscosity ratios	Mohammadi Alamooti et al. (2020)
Liquid, liquid	2D, heterogeneous, 3D	Capillary number, wettability	Zhu et al. (2021b)
Gas, liquid	2D	Wettability, interfacial tension	Xiao et al. (2021)
Water, oil	3D	Wettability, interfacial tension	Ambekar et al. (2021a)
Water, oil	2D	Wettability	Ghasemi et al. (2021)
Water, oil	3D	Injection velocity, interfacial tension, capillary number	Ambekar et al. (2021b)
Liquid, liquid	2D, heterogeneous	Wettability, injection velocity	Farhadzadeh and Nick (2022)
$ScCO_2$-brine	2D, homogeneous, pore network	Dynamics of immiscible displacement	Ranganathan (2022)
Gas, water	2D	Wettability, capillary numbers, geometry structure	Bagheri et al. (2023)
Water, oil	2D	Mesh geometry, contact angle	Derijani et al. (2023)

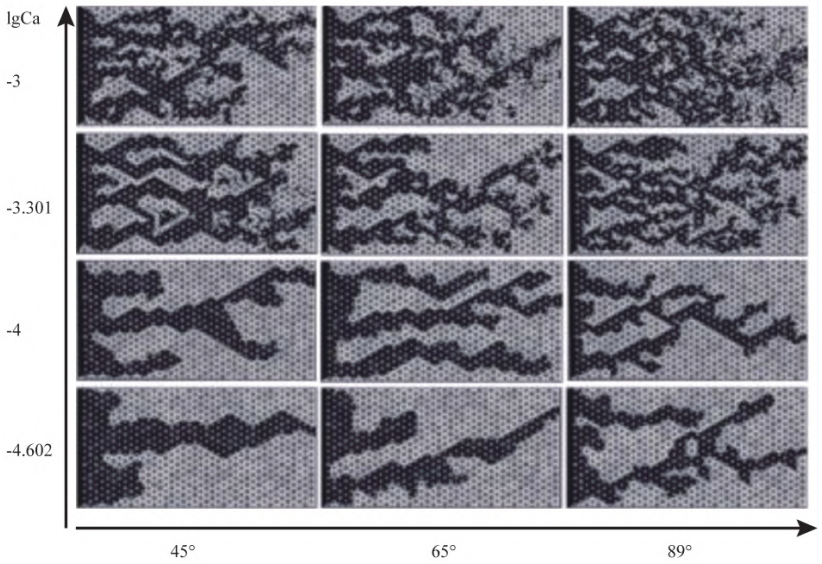


Fig. 3. Numerical simulations are conducted under different wettability conditions (from left to right: θ = 45°, 60° and 89°), where the black and white phases represent invading and defending fluid, respectively (Xiao et al., 2021).

$$\frac{\partial \phi}{\partial t} + \mathbf{u}\nabla\phi = \nabla\left(\frac{\gamma\lambda}{\varepsilon^2}\right)\nabla\psi \tag{9}$$

$$\psi = -\nabla\varepsilon^2\nabla\phi + \left(\phi^2 - 1\right)\phi \tag{10}$$

where $\gamma = \chi\varepsilon^2$ denotes the mobility, representing the migration speed of the interface in unit driving force; χ denotes the mobility tuning parameter; λ denotes the mixing energy density; and ε denotes the variable for controlling the interface thickness. Following the sensitivity study of Amiri (2014), χ was set to 1 m·s/kg to obtain a smaller volume shrinkage, while the value of ε was set to the maximum grid cell size at the location of the two-phase interface. The PFM uses the phase-field function ϕ, as a variable that describes the continuous variation of the phase interfaces from -1 to 1, blurring the phase interface into a continuous transition region. For the oil-water two-phase, fluid 1 represents the oil-phase, fluid 2 represents the water-phase, and the interval between -1 and 1 represents the oil-water interface:

$$\phi(x,t)\begin{cases} -1, \text{ Fluid 1} \\ \in (-1,1), \text{ Fhase interfrace} \\ 1, \text{ Fluid 2} \end{cases} \tag{11}$$

The mixing energy density λ, as a parameter in the phase field equation, is used to characterize surface tension

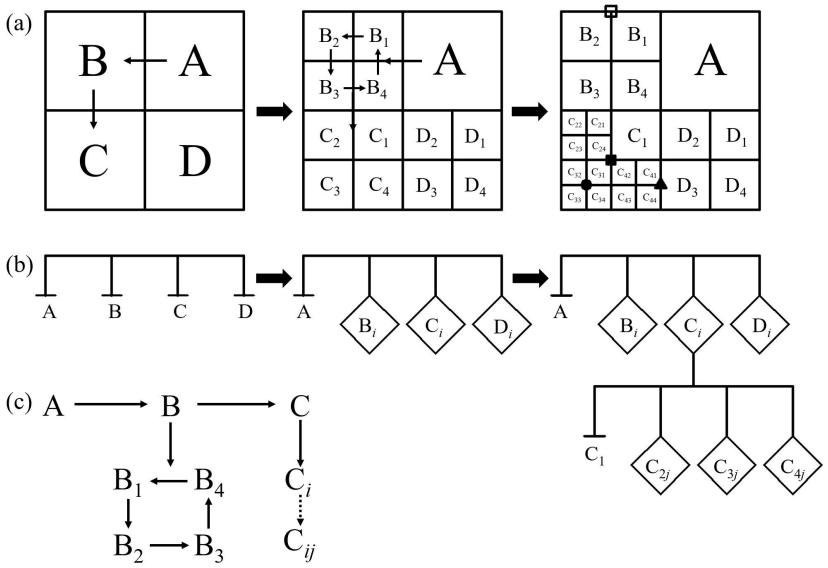


Fig. 4. Schematic diagrams of mesh refinement structure: (a) Typical sample mesh structure with three different sizes. Different node types during refinement, depicted by various symbols, are shown on the right, (b) Topological structure of a quadtree refinement and (c) Searching scheme of the data structure. The subscripts i and j denote the numbers 1, 2, 3 and 4 (Zhang et al., 2023).

coefficient σ between oil and water combined with parameter ε:

$$\sigma = \frac{2\sqrt{2}\lambda}{3\varepsilon} \tag{12}$$

The surface tension is obtained by combining the chemical potentials ψ and phase-field function ϕ in the system, thereby realizing the coupling of phase field equations and Navier-Stokes equations:

$$\mathbf{f_s} = \frac{\lambda}{\varepsilon^2}\psi\nabla\phi \tag{13}$$

Meanwhile, the wetting wall boundary acts as a key component of two-phase flow in the porous media. The detailed description is as follows:

$$\mathbf{n}\varepsilon^2\nabla\phi = \varepsilon^2\cos\theta\,|\nabla\phi| \tag{14}$$

$$\mathbf{n}\frac{\gamma\lambda}{\varepsilon^2}\nabla\psi = 0 \tag{15}$$

The PFM introduces a phase variable to track the two-phase interface, where the phase variable is a constant, such as 1 and -1, within the two phases. At the interface, the phase variable continuously changes between -1 and 1 (Takada et al., 2005, 2014; Ding et al., 2007; Gao et al., 2021). Consequently, the two-phase interface has a certain thickness and stores a specific amount of mixed free energy (Yue et al., 2004). The two-phase interface does not require explicit tracking or reconstruction. Only the Cahn-Hilliard equations containing the convection terms need to be solved, and they do not need to be reinitialized as in the LSM. Compared to other methods, the PFM has a clear physical interpretation and can be directly derived from thermodynamic laws. Therefore, the results obtained from the PFM are more reliable when the grid accuracy and time step are reasonable. Despite the fact that the phase-field model is simple, efficient and satisfies the law of mass conservation, it has certain drawbacks. When the system is in non-equilibrium, diffusion exists at the interface due to the chemical potential gradients. Consequently, even though the overall phase variable is conserved, individual phases are not. Thus, in practical simulations, small droplets are often found to disappear. Since the interface of the phase-field model has a certain thickness, the mesh size must be small to accurately describe the dynamics at the interface, leading to increased computational complexity. To address this issue, many researchers usually employ adaptive mesh techniques, as shown in Fig. 4, where a fine mesh is used at the interface and a coarse mesh is applied elsewhere (Li and Kim, 2012; Chen and Shen, 2016; Greenwood et al., 2018; Kim and Kim, 2021; Gupta et al., 2022). This approach enables the precise capture of interface evolutions while reducing computational costs.

In recent years, the PFM has been widely applied in the spontaneous imbibition of porous media. A chronological arrangement of relevant studies on spontaneous imbibition using the VOF model is provided in Table 2. Researchers have employed this model to investigate the effects of injection velocity, interfacial tension, viscosity ratio, capillary number, contact angle, wettability, and fracture types (Fig. 5) for spontaneous imbibition.

2.3 Level set method

The concept of level set was first introduced by Olsson et al. (2007) to capture front motion and has since been widely applied in simulations of incompressible two-phase flows (Sussman et al., 1994). The core idea of the LSM is to introduce a level-set function, which is always zero at the interface, and the level-set functions within the two phases are greater than and less than zero, respectively. Unlike

Table 2. Summary of studies on spontaneous imbibition using the phase-field method.

System	Object	Emphasis	Reference
Water, oil	2D, heterogeneous, fracture	Wettability, interfacial tension, viscosity ratio	Rokhforouz and Akhlaghi (2017)
Water, oil	3D, rectangular prism-shaped	Wettability	Alpak et al. (2018)
Gas, oil	2D, straight, tapered, bifurcated tubes	Geometric structure	Xiao et al. (2019)
Water, oil	2D, heterogeneous	Wettability, interfacial tension, fracture size, injection rate	Jafari and Rokhforouz (2020)
Water, oil	3D, heterogeneous, fracture	Crack propagation	Nguyen et al. (2020)
Water, oil	2D, ideal heterogeneous model, real rock heterogeneous model	Temperature	Shi et al. (2021)
Water, oil	2D, straight capillary tube	Viscosity ratio, contact angle	Peng et al. (2021)
Water, oil	2D, heterogeneous, fracture	Fracture types	He et al. (2022b)
Water, oil	2D, fracture	Wettability, viscosity ratio, interfacial tension, fracture network	Wang et al. (2022)
Water, oil	2D, homogeneous, heterogeneous	Geometric structure	Meng et al. (2022)
Water, oil	2D	Viscosity ratio	Benson and Clarkson (2022)
Water, oil	2D	Geometric structure, fracture network, wettability	Chen et al. (2023)
Water, oil	2D, fracture network	Wettability	Liu et al. (2023a)
Water, oil	2D	Flow conditions, viscosity, contact angle, interfacial tension	Zhong et al. (2023)
Water, oil	2D	Fracture types	Zhou et al. (2023a)

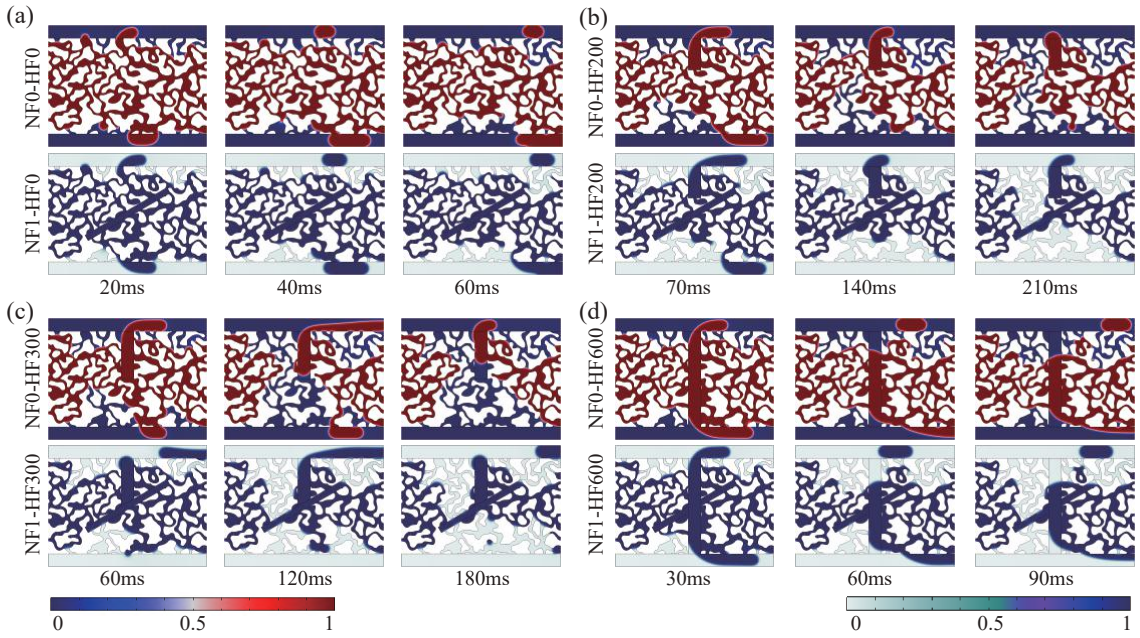


Fig. 5. Interface evolution differences between the same secondary hydraulic fracture propagation fractures and the same time, using the natural fracture as a differentiation criterion: (a) no secondary hydraulic fracture extension occurs, (b) secondary hydraulic fracture extends but does not reach the natural fracture, (c) secondary hydraulic fracture extends and touches the natural fracture, and turns at the end of the natural fracture and (d) secondary hydraulic fracture, which passes through the natural fracture and links the two primary fractures (Zhou et al., 2023a).

Table 3. Summary of studies on spontaneous imbibition using the level set method.

System	Object	Emphasis	Reference
Water, liquid	2D, random ball stacking, real rock, 3D	Fracture geometry	Prodanovic and Bryant (2006)
Water, liquid	2D, 3D	Interface evolution	Prodanovic and Bryant (2007)
Water, liquid	2D, 3D	Geometric structure, fracture network	Prodanovic and Bryant (2009)
Water, oil	2D, fracture	Fracture geometry	Prodanovic and Bryant (2009)
Water, oil	3D, heterogeneous, fracture	Geometric structure, connectivity	Rodriguez et al. (2012)
Gas, water	3D, straight capillary tube, sandstone	Geometric structure, contact angle	Jettestuen et al. (2013)
Water, oil	2D, fracture	Fracture types	Zhu et al. (2021d)
Water, oil	3D, capillary tube	Wettability, injection rate	Wang et al. (2022)

the VOF method, the level set function is smooth, thus the positions of the two-phase interfaces can be obtained directly by solving the transport equations for the level-set function. In the work of Olsson et al. (2007), the equation fails to conserve the volume due to the absence of a diffusion term in the equation. Therefore, when using numerical techniques, an artificial compression and diffusion are added to maintain the interface thickness (Olsson et al., 2007). The compression-diffusion equation is obtained as:

$$\frac{\partial \phi}{\partial t}+\mathbf{u}\nabla\phi=\xi\nabla\left[\varepsilon\nabla\phi-\phi\left(1-\phi\right)\frac{\nabla\phi}{|\nabla\phi|}\right] \tag{16}$$

where ξ is the re-initialization parameter, which ensures that the change in the level set function ϕ is within the range of the interface thickness. If the interface thickness ε is too small, the calculated fluid flow velocity will be distorted, while the interface will become blurred if the thickness ε is too large, affecting the accuracy of the results (Amiri and Hamouda, 2013). An excessively high ξ value will result in too small a time step and long calculations, while an excessively low ξ value will result in an incorrect oil-water interface (Olsson et al., 2007).

In the level-set method, the surface tension $\mathbf{f_s}$ is expressed as follows (Hernandez Cid et al., 2022):

$$\mathbf{f_s}=\sigma\delta\kappa\mathbf{n} \tag{17}$$

where δ denotes the delta function approximated by $\delta=6|\phi(1-\phi)||\nabla\phi|$; $\mathbf{n}=\nabla\phi/\phi$ (Olsson et al., 2007), $\kappa=-\nabla\mathbf{n}$.

The density ρ_{if} and viscosity μ_{if} of the oil-water interface are respectively defined as:

$$\rho_{if}=\rho_o+\left(\rho_w-\rho_o\right)\phi_1 \tag{18}$$

$$\mu_{if}=\mu_o+\left(\mu_w-\mu_o\right)\phi_1 \tag{19}$$

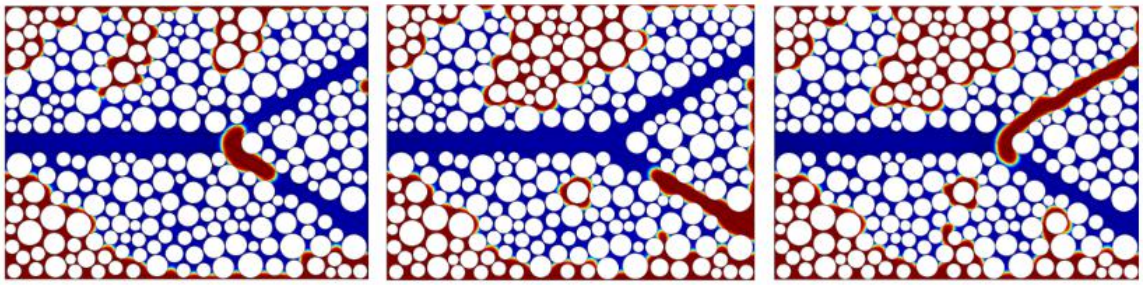
where ϕ_1 denotes the volume fractions of the oil and water phases, respectively; ρ_o and ρ_w denote the fluid densities of the oil and water phases, respectively; and μ_o and μ_w denote the viscosities of oil and water, respectively.

In the LSM, the thickness of the two-phase interface depends on the distribution of the level-set function at the interface. To maintain a constant interface thickness, the distribution of the level set function at the interface must remain consistent. Therefore, the level-set function needs to be corrected using a reinitialization process at each time step. To improve the computational efficiency, the reinitialization can be conducted at intervals when the interface motion is relatively slow, but it must be performed at every time step when the interface motion is faster. Compared to the VOF method, the LSM does not require explicit tracking of the interface or interface reconstruction. The extension of LSM from two to three dimensions is straightforward, making the method simpler and more efficient (Cortazar et al., 2008; Burfeindt and Alqadah, 2023). However, the reinitialization process in the LSM can result in artificial interface motion, leading to mass non-conservation. In response to this drawback, a series of improvement methods have been proposed (Olsson and Kreiss, 2005, 2007).

In recent years, the PFM has been widely applied in the spontaneous imbibition of porous media. A chronological arrangement of relevant studies of spontaneous imbibition using the VOF model is presented in Table 3. Researchers have used this model to investigate the effects of injection velocity, interfacial tension, viscosity ratio, capillary number, contact angle, wettability, and fracture types (Fig. 6) for spontaneous imbibition.

3. CFD models based on the lattice Boltzmann method

Since 1989, the lattice Boltzmann method (LBM) has evolved into an effective numerical simulation tool that is widely used nowadays for simulating and studying various complex physical phenomena, including multiphase flow, turbulence, heat transfer, phase change, and flow in porous media (Grunau et al., 1993; He et al., 1997; Lallemand and Luo, 2000). The LBM is based on the dynamical theory from Boltzmann equation and utilizes a microscopic particle model to obtain the macroscopic flow characteristics through particle distribution functions. Due to the foundation established by the LBM, it can describe the interactions between particles at the mesoscale and reflect the macroscopic flow field. The advantages of the LBM lie in the complete linearization of discrete lattice Boltzmann equations, whereas traditional methods often require handling the nonlinear convective term in solving the Navier-Stokes equation. In solving the traditional Navier-



(a) (b) (c)

Fig. 6. Distribution of oil and water in the bifurcated fracture under different boundary conditions at $t = 50$ s: (a) both outlet 1 and outlet 2 are open, (b) outlet 2 is closed and (c) outlet 1 is closed (Zhu et al., 2021d).

Stokes equations, a huge amount of computational effort is needed to process the Poisson equation to obtain the pressure field, whereas in LBM, the pressure field can be obtained by the computation of fluid state equation. Furthermore, compared with traditional numerical simulation methods, LBM is more adept at handling complex boundaries, facilitating the simulation of complex interface variations. The LBM exhibits high computational efficiency and complete parallelism (Chen et al., 2014). Based on the traditional molecular dynamic theory, it can simulate multiphase flow systems characterized by dramatic changes in liquid surfaces without the need for interface tracking, distinguishing it from conventional numerical simulation methods. Unsurprisingly, various LBM multiphase flow models have been developed and applied for the simulation of multiphase flow phenomena, which can be classified into three main categories: Shan-Chen, free energy, color models (Yu and Fan, 2010; Sudhakar and Das, 2020; Petersen and Brinkerhoff, 2021).

3.1 Shan-Chen method

Shan and Chen (1993, 1994) established a simple pseudopotential model integrated with a simple pseudopotential to simulate the interactions between particles, reflecting the difference in the average molecular forces exerted on either side of the interface. Owing to the simplicity and applicability of this model, it is now widely used in multiphase flow simulation. It has the following formula:

$$f_\alpha(\mathbf{x}+\mathbf{e}_\alpha\Delta t, t+\Delta t) - f_\alpha(\mathbf{x},t) = -\frac{1}{\tau}\left[f_\alpha(\mathbf{x},t) - f_\alpha^{eq}(\rho,\mathbf{u}^{eq})\right] \tag{20}$$

where f_α, $\mathbf{x}$, $\mathbf{e}_\alpha$, and t represent the probability distribution function of fluid particle in direction α, space position, microscopic velocity, and time, respectively; τ represents the relaxation time; $\mathbf{u}^{eq}$ represents the equilibrium distribution velocity; and $f_\alpha^{eq}(\rho,\mathbf{u}^{eq})$ is the local equilibrium distribution function.

Shan and Chen (1993, 1994) introduced a special pseudopotential to simulate the interactions between particles at the interface, where the external force term $\mathbf{F}(\mathbf{x},t)$ is defined as:

$$\mathbf{F}(\mathbf{x},t) = -G\psi(\mathbf{x},t)\sum_\alpha \omega_\alpha \psi(\mathbf{x})\psi(\mathbf{x}+\mathbf{e}_\alpha\Delta t,t)\mathbf{e}_\alpha \tag{21}$$

where G is a constant controlling the interaction force between nodes; ψ denotes the effective density associated with each component; and ω_α denotes the weights. Notably, the interaction forces of the pseudopotential model depend solely on neighboring nodes. The ψ is defined as follows:

$$\psi(\rho) = \psi_0\left[-\exp\left(-\frac{\rho_0}{\rho}\right)\right] \tag{22}$$

where ψ_0 and ρ_0 are arbitrary constants. Sbragaglia et al. (2006) improved the external force term to enable the separate adjustment of surface tension and density ratio:

$$\begin{aligned}\mathbf{F}(\mathbf{x},t) = &-\psi(\mathbf{x},t)\sum_\alpha \omega_\alpha[G_1\psi(\mathbf{x})\psi(\mathbf{x}+\mathbf{e}_\alpha\Delta t,t)\\ &+G_2\psi(\mathbf{x})\psi(\mathbf{x}+2\mathbf{e}_\alpha\Delta t,t)]\mathbf{e}_\alpha\end{aligned} \tag{23}$$

where G_1 and G_2 represent parameters that control the strength of the interaction between neighboring and sub-neighboring particles.

For the pseudopotential model, the selection of appropriate external force terms can increase the numerical stability and computational accuracy of the calculations. The commonly used external force terms can usually be summarized into three formats, including the original Shan-Chen model external force format, the extra difference method format, and Guo's force scheme.

In the original Shan-Chen model, the external force term is incorporated into the computation of the equilibrium state equation, namely (Shan and Chen, 1994):

$$\mathbf{u}^{eq} = \mathbf{u} + \frac{\tau}{\rho}\mathbf{F}\Delta t \tag{24}$$

where $\mathbf{u} = \sum e_\alpha f_\alpha$.

Taking into account the lattice effects and momentum exchange, Guo et al. (2002) constructed a discrete external force format F_α incorporated into the particle distribution equation. It is expressed as:

$$F_\alpha = \omega_\alpha\left(1-\frac{1}{2\tau}\right)\left(\frac{\mathbf{e}_\alpha-\mathbf{u}}{c_s^2}+\frac{\mathbf{e}_\alpha\mathbf{u}}{c_s^4}\right)\mathbf{F} \tag{25}$$

where c_s is the lattice sound speed.

The external force term of the extra difference method format proposed by Kupershtokh et al. (2009):

$$F_\alpha = f_\alpha^{eq}\left(\rho,\mathbf{u}+\frac{\mathbf{F}\Delta t}{\rho}\right) - f_\alpha^{eq}(\rho,\mathbf{u}) \tag{26}$$

Table 4. Summary of studies on spontaneous imbibition using the Shan-Chen method.

System	Research object	Research emphasis	References
Water, oil	3D, tight sandstone	Geometric structure	Zheng et al. (2021)
Gas, water	3D, shale	Geometric structure, wettability	Zheng et al. (2018a)
Water, liquid	2D, sinusoidal, wedge, bifurcated channels	Tortuosity, channel shape	Zheng et al. (2018b)
Gas, water	2D, slit-type channel	Wettability	Sheng et al. (2022)
Water, oil	2D	Pore size, fluid-surface slip, water film, oil-water interfacial slip, water bridge, pore structures	Wang et al. (2023)
Water, oil	2D	Pore dimensions, pore shapes, nanoscale effects, dynamic contact angle	Wang et al. (2021)

The equilibrium distribution velocity is:

$$\mathbf{u}^{eq} = \mathbf{u} + \frac{1}{(\tau - 0.5)\psi^2}\mathbf{F}\Delta t \tag{27}$$

The expressions for the physical velocity $\mathbf{u}_p$ of the aforementioned three external force terms are listed as follows:

$$\mathbf{u}_p = \mathbf{u} + \frac{1}{2\rho}\mathbf{F}\Delta t \tag{28}$$

For isothermal LBM models, many boundary treatments have been devised. Based on the isothermal LB model proposed by He et al. (1998), Chai and Zhao (2013) devised an improved LBM model by introducing an additional term into the equilibrium temperature distribution function as well as a source term into the thermal LBM equation. Yuan and Schaefer (2006) presented the details of phase separation. Li et al. (2013) extended the pseudopotential LBM model to simulate multiphase flows under large density ratio and relatively high Reynolds number. The Shan-Chen model can directly describe the interaction force between microscopic particles, reflect the essence of multi-component and multi-phase fluid dynamics, and automatically track the interface evolution. In contrast to the color gradient method, this model avoids the process of manually calibrating colors and can achieve phase separation phenomena automatically when the interactions between particles are chosen appropriately. However, it also has some drawbacks: the spurious velocities at the interface are high, and the model is consistent with the thermodynamic principles only when the effective density function in the interaction takes the exponential form (Eq. (22)). This stringent requirement significantly limits the application of such multiphase flow models.

In response to the above issues, numerous improvements have been made to the Shan-Chen model. A chronological arrangement of relevant studies of spontaneous imbibition using the Shan-Chen model is included in Table 4. Researchers have used this model to investigate the effects of geometric structure, tortuosity, wettability, contact angle, and so on, for spontaneous imbibition (Fig. 7).

3.2 Free energy method

In 1995, Swift constructed a multi-phase and multi-component LBM consistent with the thermodynamic principles on the basis of the theory of multi-phase flow free energy (Swift et al., 1995, 1996). By introducing the correct non-ideal fluid stress tensor to rewrite the equilibrium distribution function, the collision term in the lattice Boltzmann equation was modified to ensure that the ultimate equilibrium state in the system corresponds to the selected free energy. Compared to other models, this model incorporates greater physical realism, reducing the occurrence of discretization unphysical effects.

For a one-component non-ideal fluid system containing a phase interface, the free energy generalization $\Psi(\mathbf{x})$ is given by:

$$\Psi(\mathbf{x}) = \int \left[\psi_1(\rho(\mathbf{x}), T(\mathbf{x})) + \frac{\kappa}{2}|\nabla\rho(\mathbf{x})|^2\right] \mathrm{d}\mathbf{x} \tag{29}$$

where $\psi_1(\rho(\mathbf{x}), T(\mathbf{x}))$ represents free energy density function in the phase region, and $\kappa|\nabla\rho(\mathbf{x})|^2/2$ is the contribution pressure of surface tension to free energy. The relationship between pressure and free energy functional $P(\mathbf{x})$ is as follows:

$$P(\mathbf{x}) = \rho\frac{\delta\Psi}{\delta\rho} - \Psi = P_0 - \kappa\rho\nabla^2\rho - \rho\frac{\kappa}{2}|\nabla\rho|^2 \tag{30}$$

where $P_0 = \rho\psi_1'(\rho) - \psi_1(\rho)$ represents state equation whereby the pressure tensor $P'_{\alpha\beta}$ including interface contributions can be obtained:

$$P'_{\alpha\beta} = P\delta_{\alpha\beta} + \kappa\frac{\partial\rho}{\partial x_\alpha}\frac{\partial\rho}{\partial x_\beta} \tag{31}$$

In order to construct an LBM that can conform to the thermodynamic theory described above, the free energy model employs an equilibrium distribution function that includes a density gradient:

$$f_\alpha(\mathbf{x} + \mathbf{e}_\alpha, t+1) - f_\alpha(\mathbf{x}, t) = -\frac{1}{\tau}[f_\alpha(\mathbf{x}, t) - f_\alpha^{eq}(\rho, \mathbf{u}, \nabla\rho)] \tag{32}$$

whereby the equilibrium distribution function f_α^{eq} is satisfied:

$$\sum_\alpha f_\alpha^{eq} = \rho, \sum_\alpha e_\alpha f_\alpha^{eq} = \rho\mathbf{u}, \sum_\alpha e_\alpha e_\alpha f_\alpha^{eq} = \mathbf{P}' + \rho\mathbf{u}\mathbf{u} \tag{33}$$

Notably, Xu et al. (2003) improved the definition of the partial moment relationship and the equilibrium distribution function formula in the above free energy model, and their improved model is more consistent with the rules of ther-

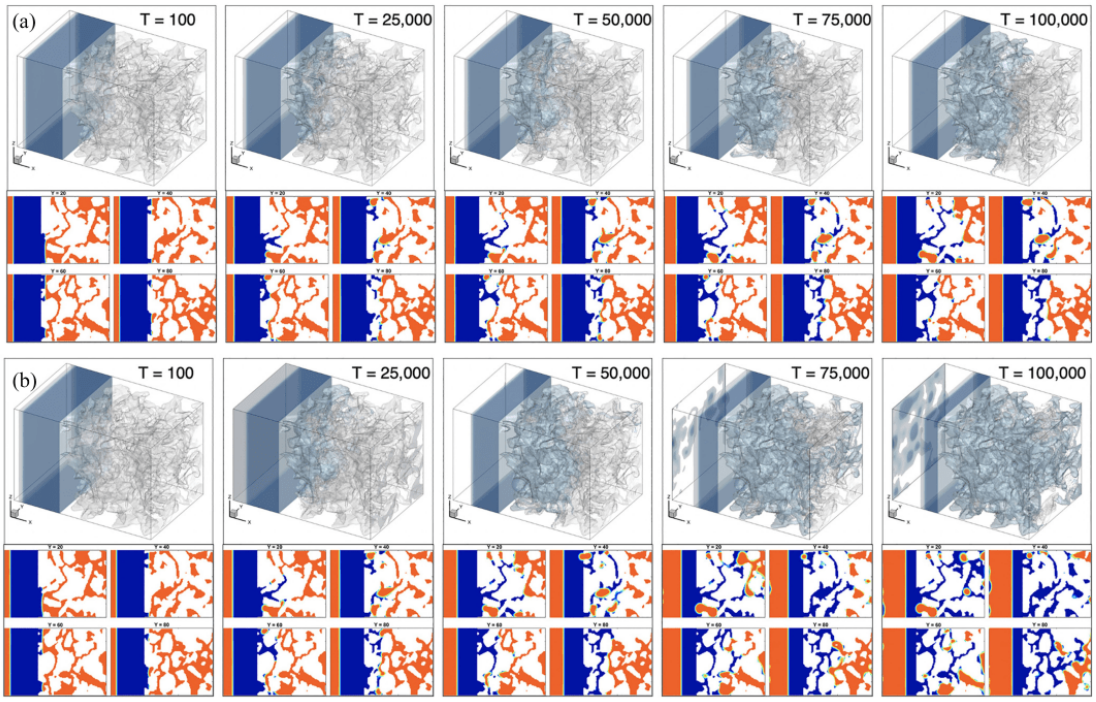


Fig. 7. Visualization of spontaneous imbibition behaviors in the representative porous model at the time steps of 100, 25,000, 50,000, 75,000, and 100,000 s under (a) the ambient condition and (b) the reservoir condition. The upper row of each figure displays the 3D wetting phase morphology in the porous model, with the blue indicating the water phase and the gray indicating the pore space. The lower row displays the distribution of two phases in the slices of Y = 20, 40, 60, and 80 of the porous model, with the blue indicating the water phase and the red indicating the oil phase (Zheng et al., 2021).

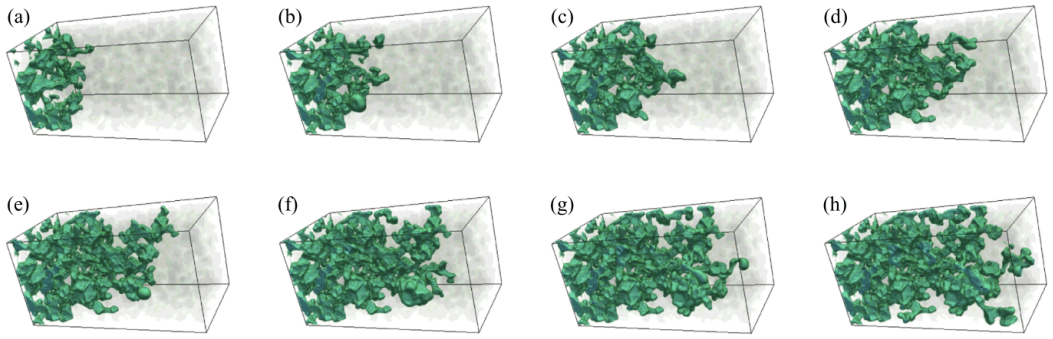


Fig. 8. Sequence of snapshots from the free energy model during the drainage of Bentheimer sandstone at time intervals of $dt = 5 \times 10^4$ lu, initial time is 5×10^4 lu (Zacharoudiou and Boek, 2016).

modynamics and has better numerical stability. Holdych et al. (1998) modified the Galilean invariance of the model by adding density gradient-related terms. Zheng et al. (2006) proposed a free energy model that satisfies Galilean invariance under the limited density ratio. Hao and Cheng (2010) used the free energy model to simulate gas-liquid two-phase flow in porous media. Zacharoudiou and Boek (2016) numerically investigated the dynamics of capillary filling and Haines jump events using free energy model, as shown in Fig. 8. Their work focuses on capillary filling and demonstrate that the numerical method can capture the correct dynamics in the limit of long times for both high and low viscosity ratios, i.e., it gives the correct scaling for the length of the penetrating fluid column as a function of time. In addition, they observed that the Haines jump events are cooperative, non-local and associated with both drainage and imbibition dynamics. Zacharoudiou et al. (2017) investigated the role of pore body shape on fluid displacement during drainage and imbibition via quasi-static and spontaneous experiments under ambient conditions.

3.3 Color gradient method

Building on the lattice gas automata non-mixing model by Rothman and Keller (1988), the color model was proposed by Gunstensen et al. (1991, 1992, 1993) using red and blue particles to represent different phases of the fluid. In this model, the interaction between different fluids is achieved by

Table 5. Summary of studies on spontaneous imbibition using the color gradient model.

System	Object	Emphasis	Reference
Water, oil	2D, heterogeneous	Injection velocity, interfacial tension, viscosity ratio	Gu et al. (2019)
Water, oil	2D, microfractures in media	Fracture types	Liu et al. (2020a)
Water, oil	2D, fourth-order Sierpinski carpet	Surface roughness	Liu et al. (2021b)
Anhydrous ethanol, air	3D, homogeneous	Viscosity ratio, contact angle, wettability	Liu et al. (2021a)
Water, oil	3D, tight sandstone	Wettability	Lin et al. (2021)
Gas, liquid	3D, capillary bundle model	Fluid viscosity, surface tension, contact angle, gravity	Zhao et al. (2021)
Wetting, non-wetting	2D, heterogeneous	Viscosity ratio, tortuosity, mixed wettability	Diao et al. (2021)
Water, oil, and gas	3D, cylindrical tube model	Gas injection after water displacement	Li et al. (2021)
Water, oil	3D, heterogeneous	Grain shape, geometric structure, boundary conditions	Liu et al. (2022b)
Water, oil	2D, random ball stacking	Geometric structure, capillary number	Wu et al. (2022)
Water, liquid	2D	Geometric structure, flow conditions, gravitational acceleration, viscosity ratio	Li et al. (2022)
Water, oil	2D	Viscosity ratio	Cheng et al. (2022)
Water, oil	3D, real core	Interfacial tension	Gong et al. (2023)

introducing a color gradient, which facilitates the mixing or separation of fluids. The collision consists of the conventional BGK operator, which is (1) related to the viscosity of the fluid and (2) reflects the dynamics of the interface, related to surface tension. The computation process in this model is divided into three steps: Streaming, collision and coloring. Latva and Rothman (2005) further divided the collision step into two parts, represented as:

$$f_\alpha^k(\mathbf{x},t) = f_\alpha^{k^*}(\mathbf{x},t) + (\Omega_\alpha^k)^1 + (\Omega_\alpha^k)^2 \tag{34}$$

where $f_\alpha^{k^*}(\mathbf{x},t)$ represents the post-collision distribution function; $f_\alpha^k(\mathbf{x},t)$ represents the pre-collision distribution function; $(\Omega_\alpha^k)^1$ denotes the first collision phase; $(\Omega_\alpha^k)^2$ denotes the second collision phase. One of the first collision phases is expressed as:

$$(\Omega_\alpha^k)^1 = -\frac{1}{\tau}[f_\alpha^k(\mathbf{x},t) - f_\alpha^{k,eq}(\mathbf{x},t)] \tag{35}$$

The second collision phase has different formats. Gunstensen et al. (1991) determined the second collision phase as:

$$(\Omega_\alpha^k)^2 = -\frac{A_k}{2}|\mathbf{f}|[2\cos^2(\lambda_\alpha) - 1] \tag{36}$$

where A_k represents the parameter for adjusting surface tension; $\mathbf{f}$ denotes the color gradient; λ_α denotes the angle between color gradient and discrete velocity. As proposed by Latva and Rothman (2005):

$$\cos(\lambda_\alpha) = \frac{\mathbf{e}_\alpha \mathbf{f}}{|\mathbf{e}_\alpha||\mathbf{f}|} \tag{37}$$

Reis and Phillips (2007) determined the second collision phase to obtain the correct surface tension in the Navier-Stokes equation:

$$(\Omega_\alpha^k)^2 = \frac{A_k}{2}|\mathbf{f}|\left[\omega_\alpha \frac{(\mathbf{e}_\alpha \mathbf{f})^2}{|\mathbf{f}|^2} - B_i\right] \tag{38}$$

where B_i is a constant. In addition, Latva and Rothman (2005) determined the recoloring step expression as:

$$f_\alpha^{1+} = \frac{\rho_1}{\rho} f_\alpha^* + \beta \frac{\rho_1 \rho_2}{\rho^2} f_\alpha^{eq}(\rho, \mathbf{u} = 0)\cos(\lambda_\alpha) \tag{39}$$

$$f_\alpha^{2+} = \frac{\rho_2}{\rho} f_\alpha^* + \beta \frac{\rho_1 \rho_2}{\rho^2} f_\alpha^{eq}(\rho, \mathbf{u} = 0)\cos(\lambda_\alpha) \tag{40}$$

This model has been verified by the law of Laplace and applied to the study of complex problems such as phase separation and flows in porous media (Golparvar et al., 2018; Zhu et al., 2021c; Wei et al., 2022; Mora et al., 2023). A chronological arrangement of relevant studies of spontaneous imbibition using the color gradient model is presented in Table 5. Researchers have used this model to investigate the effects of injection velocity, interfacial tension, viscosity ratio, capillary number, contact angle, wettability, tortuosity, fracture types, gravitational acceleration, boundary conditions (Fig. 9), and geometric structure (Fig. 10) for spontaneous imbibition. However, this model is phenomenological and have significant limitations, such as the correlation of surface tension with the orientation of the interface, spurious velocities near the interface, difficulties in considering the thermodynamic effects, and substantial computational cost in the recoloring process.

3.4 Phase-field method

He et al. (1999) proposed an LBM based on the PFM involving dual distribution equations, where one distribution equation corresponds to an irreducible N-S equation and the

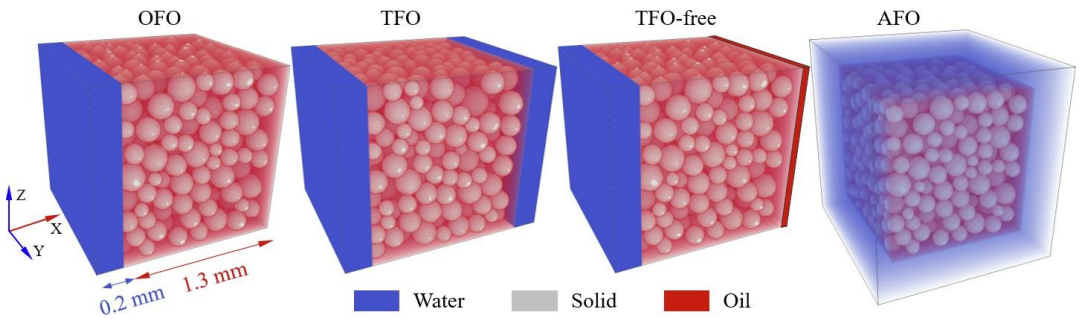


Fig. 9. Realization of the various considered imbibition boundary conditions (Liu et al., 2022b).

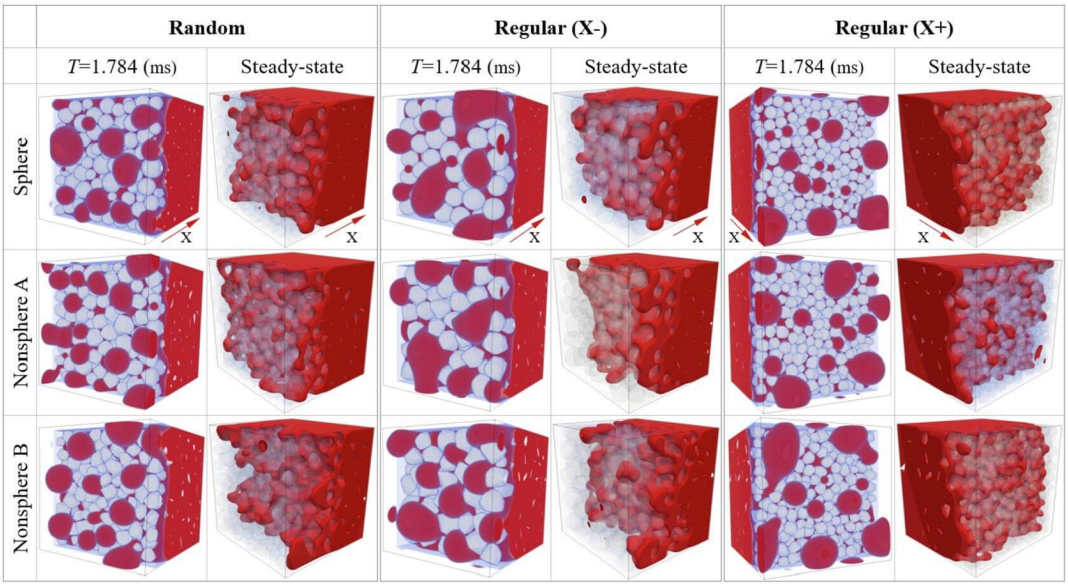


Fig. 10. Oil distribution (red color) and steady-state for different geometric structure models under the "one end open" boundary condition (Liu et al., 2022b).

other distribution equation corresponds to a macroscopic phase field equation:

$$\begin{aligned}&\bar{f}_\alpha(\mathbf{x}+\mathbf{e}_\alpha\Delta t,t+\Delta t)=\bar{f}_\alpha(\mathbf{x},t)-\frac{1}{\tau}[\bar{f}_\alpha(\mathbf{x},t)-\bar{f}_\alpha^{eq}(x,t)]\\&+F_\alpha(\mathbf{x},t)\Delta t\\&\bar{g}_\alpha(\mathbf{x}+e_i\Delta t,t+\Delta t)=\bar{g}_\alpha(\mathbf{x},t)-\frac{1}{\tau}[\bar{g}_\alpha(\mathbf{x},t)-\bar{g}_\alpha^{eq}(\mathbf{x},t)]\\&+F_\alpha^{'}(\mathbf{x},t)\Delta t\end{aligned}\tag{41}$$

The expressions for the external force terms F_α and $F_\alpha{}'$ are:

$$\begin{aligned}F_\alpha&=\left(1-\frac{1}{2\tau}\right)\frac{\Gamma_\alpha(\mathbf{u})}{c_s^2}(\mathbf{e}_\alpha-\mathbf{u})\nabla\varphi(\phi)\\F_\alpha^{'}&=\left(1-\frac{1}{2\tau}\right)(\mathbf{e}_\alpha-\mathbf{u})\Phi\end{aligned}\tag{42}$$

where $\varphi(\phi)=P(\phi)-\phi c_s^2$ and $\Phi=\Gamma_\alpha(\mathbf{u})(F_s+F_g)-[\Gamma_\alpha(\mathbf{u})-\Gamma_\alpha(0)]\nabla\varphi(\rho)$, in which F_s denotes the surface tension force, F_g denotes the gravity force, and $\phi(\rho)$ and $\Gamma_\alpha(\mathbf{u})$ are given by Eqs. (43) and (44), respectively:

$$\varphi(\rho)=P-\rho c_s^2\tag{43}$$

$$\Gamma_\alpha(\mathbf{u})=\omega_\alpha\left[1+\frac{\mathbf{e}_\alpha\mathbf{u}}{c_s^2}+\frac{(\mathbf{e}_\alpha\mathbf{u})^2}{c_s^4}-\frac{|\mathbf{u}|^2}{2c_s^2}\right]\tag{44}$$

where P represents the hydrodynamic pressure. The variable ϕ in $\varphi(\phi)$ is an order parameter and is calculated $\phi=\sum_\alpha f_\alpha$.

Relying on the LBM model based on the PFM mentioned above, Zheng et al. (2005, 2006) proposed an improved LBM model for interface capturing that introduces spatial difference terms of distribution functions. Based on a similar idea, Zu and He (2013) developed another LBM that utilizes spatial differences of balanced distribution functions instead of distribution functions. Liang et al. (2014) proposed an LBM model in which the time derivative term is introduced into the evolution function. However, from a theoretical perspective, Cahn-Hilliard equations comprise a fourth-order partial differential equation and cannot be directly recovered from the LBM model through Chapman Enskog analysis (Wang et al., 2016). From a numerical perspective, due to the need for non-local finite difference schemes to calculate the spatial derivatives of order parameters, the locality of the collision process cannot be preserved in the above models. To solve this problem, a second-order Allen-Cahn equation of LBM model is needed. Geier et al. (2015) first developed a center

moment LBM model for local Allen-Cahn equation. Subsequently, Ren et al. (2016) pointed out that this LBM model cannot provide the correct local Allen-Cahn equation, so they proposed an improved LBM model for the same Allen-Cahn equation. Under the framework of LBM, Chai et al. (2018) first developed an LBM model for the non-local Allen-Cahn equation that ignores advection. Liu et al. (2022a) constructed a new diffuse-domain LBM for two-phase flows in complex geometries. Thereafter, Liu et al. (2023b) developed an improved LBM based on phase-field, in which a hybrid Allen-Cahn equation with a flexible weight instead of a global weight is used to suppress the numerical dispersion and eliminate the coarsening phenomenon. Within the phase-field framework, Liang et al. (2019) presented an accurate and robust LBM for simulating the contact-line motion of immiscible binary fluids on the solid substrate. A detailed review of these models was provided by Wang et al. (2019).

One of the greatest challenges is multiphase flow simulation at high density ratio, for which a lot of work has been carried out. Premnath and Abraham (2005) proposed an axisymmetric phase-field model based on the PFM. McCracken and Abraham (2005) incorporated the multiple-relaxation-time collision operator into the axisymmetric phase-field model. Amaya and Lee (2010) and Lee and Lin (2005, 2010) improved the PFM to obtain a phase-field model that can simulate high density ratios. The numerical results showed that the model proposed by Lee and Lin (2005) is capable of simulating multiphase flows at the density ratio 1000. Nevertheless, Chiappini et al. (2010) analytically demonstrated that the different discretization of the streaming operator along the directions of molecular versus fluid motion is non-conservative in principle. Lou et al. (2012) also found that the second-order mixed difference scheme, which plays a critical role as proposed by Lee and Lin (2005) for enhancing the numerical stability at large density ratios, is non-Galilean invariant and does not conserve the total mass of the system.

4. Conclusions and outlook

Spontaneous imbibition, as a fundamental phenomenon of fluid flow in porous media, is of great significance in guiding reservoir development through exploring the fluid flow law from a pore-scale perspective. This study presents a systematic and comprehensive review of the operational principles and limitations of commonly applied computational models, including the volume of fluid, phase-field, and level set methods based on macroscopic Navier-Stokes equations, and the Shan-Chen, free energy, color gradient, and phase-field methods based on mesoscopic lattice Boltzmann equations. Additionally, it provides further statistics on related work in recent years. By combining the summaries and comparisons of this study, future research directions are recommended, that is, more focused investigations, as outlined below, should be conducted to lay the foundation of flow laws in the spontaneous imbibition of porous media. More specifically:

1) For complex pore space structures, the main acquisition methods are imaging techniques such as CT scanning; however, these methods are burdened by high cost and the unavailability of large data sets, limiting the exploration of universal flow laws. Despite previous efforts regarding reconstruction pore medium algorithms (Hyman and Winter, 2014; Mosser et al., 2017; Zhou et al., 2023b), there is still much room for improvement.
2) The snap-off of wetting fluid in porous media greatly influence the flow dynamics. The fluid distribution under unsteady-state in porous media should be studied, especially for the unsteady-state front-end during corner flow. It is critical to develop an advanced modeling approach to capture the complete physical mechanisms of multiphase flows in complex solid domains.
3) Considering the diagenetic law of the reservoir and the adsorption characteristics of minerals, the reservoir is in a mixed wetting state. Although previous research has been conducted on mixed wetting (Akbarabadi et al., 2017; AlRatrout et al., 2018; Liu et al., 2023a), the mechanisms of flow laws in mixed wetting conditions still remain unclear.
4) For the problem of linking microscopic and macroscopic flow laws, establishing multiscale mathematical relationships by parameters with microscopic and macroscopic properties, such as fractal dimensions, is likely an effective approach.
5) The data mining problem in exploring the universal flow laws needs to be solved. Machine learning promises to be a promising solution via utilizing the large amount of data provided by the numerical computation of multiphase flows.

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Conflict of interest

The authors declare no competing interest.

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