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Perspective

Micro- and nanoscale flow mechanisms in porous rocks based on pore-scale modeling

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Abstract:
Fluids flow within microporous and nanoporous rocks involves several industrial processes such as enhanced oil recovery, geological CO_2 sequestration, and hydraulic fracturing. However, the pore structure of subsurface rocks is complex, and fluid flow is influenced by strong fluid-fluid and fluid-solid interactions, including wettability, interfacial tension, and slip effects. Characterizing this flow processes is costly and challenging through experimental techniques. At meanwhile, pore-scale simulations have been widely employed to investigate complex flow behaviors within microporous and nanoporous media. This work investigates the applications of pore-scale simulation methods for characterizing flow processes in porous rocks considering microscale and nanoscale effects. Two mainstream simulation methods, pore network modeling and direct numerical simulation, are introduced. Their application scenarios encompass immiscible flow, as well as miscible and near-miscible flow involving CO_2 enhanced recovery. Additionally, some explorations of single-phase and multiphase flow processes within nanoporous media are described. Finally, future development of pore-scale simulations is discussed, with a focus on complex transport phenomena involving diffusion, reactions, and dissolution.

1. Introduction

The development of unconventional hydrocarbon resources has expanded significantly, particularly as conventional resources have depleted. The unconventional reservoirs contain numerous microscale and nanoscale pores (Bal et al., 2024), which serve as the main spaces for hydrocarbon migration and storage. However, the microscopic pore structure of subsurface porous rocks is highly complex, with diverse pore sizes and shapes, leading to significant heterogeneity (Wang et al., 2019). Fluid flow mechanisms are intricate in heterogeneous pore structures (Liu et al., 2022), influenced by the micro- and nanoscale effects. Accurately characterizing the fluid flow and transport mechanisms in microscale and nanoscale porous rocks presents a significant challenge.

Two-dimensional (2D) and three-dimensional (3D) imaging technologies have significantly enhanced the quantitative characterization of microscopic pore structures in unconventional reservoirs, allowing for accurate capture of the complex pore topology. Additionally, it is possible to construct digital rock models that represent real pore structures using micro-computed tomography (micro-CT) and scanning electron microscope (SEM) images (Singh et al., 2022; Zhao et al., 2022). However, describing flow processes in unconventional reservoirs is challenging due to the complex pore structure and the interplay of micro- and nanoscale effects (Qin et al., 2024). The fluid-fluid and fluid-solid interactions are significant in microscale and nanoscale pores, and the fluid flow is affected by wettability, interfacial tension, and boundary slip (Cai et

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al., 2024). In addition, the underground reservoir conditions are complicated, which may lead to miscible and immiscible flow forms. In recent years, pore-scale simulations considering microscale and nanoscale effects have made it possible to characterize flow behaviors in unconventional reservoirs. Compared with molecular dynamics simulations, complex pore topology can take into account in pore-scale simulations combined with image reconstruction technology. Consequently, pore-scale simulations serve as a bridge between molecular scale phenomena and continuum scale flow behaviors.

Researchers have successfully conducted simulations of microscale and nanoscale flows in porous media with complex pore topology, achieving substantial advancements. This work systematically describes the flow mechanisms in porous media based on pore-scale simulations (Fig. 1). First, the principles of two types of methods, pore network model (PNM) and direct numerical simulation (DNS), are introduced (Fig. 1 (a) and (b)). Then, broad application scenarios of pore-scale simulations are described in detail (Fig. 1(c)), including immiscible flow, miscible flow, nanoscale flow, etc. Finally, the challenges and suggestions for the development of pore-scale simulations are proposed.

2. Pore-scale modeling methods

DNS methods based on real pore topology and simplified PNM are two types of methods used in pore-scale simulations. These two methods have distinct characteristics and application scenarios. In terms of computational resources, PNM is efficient because it simplifies complex pore structures. Conversely, DNS methods is computationally expensive as it directly resolves the detailed fluid flow dynamics within complex pore structures. Regarding accuracy and application scenarios, DNS methods provide high-resolution simulations that capture intricate flow dynamics, such as pore-filling mechanisms, interface dynamics, and fluid distribution. In contrast, PNM focuses on macroscopic transport properties, such as relative permeability and capillary pressure curves.

DNS methods enable accurate descriptions of complex displacement processes, fluids distribution, and interface dynamics. However, it is computationally expensive. DNS methods solve the Navier-Stokes equations directly to understand flow patterns and utilize specialized interface detecting algorithms to capture two-phase interfaces (Yang et al., 2023). Common numerical methods include finite volume and finite difference methods, while interface capturing techniques involve free surface models, volume of fluid (VOF) methods, micro-continuum Darcy-Brinkman-Stokes approach, level set (LS), and phase-field (PF) methods. Additionally, the Lattice Boltzmann method (LBM) uses particle-based approaches to solve equations (Wang et al., 2023b). LBM is a mesoscopic simulation method that has become a popular approach for studying micro- and nanoscale fluid flow due to its efficiency and effectiveness in handling complex pore structures. Color gradient models, pseudo-potential models, and free energy models have been widely applied in pore-scale simulations.

PNM simplifies the complex pore structure and improves the computational efficiency. According to the shape factor, irregular pore structures are equivalent to pores with circular, square and triangular cross-sectional shapes (El-Zehairy et al., 2019), which can consider the corner flow. The pores are connected by throats, and the throat size is equivalent to the size of the minimum cross-section between the connected pores. The network parameters such as coordination number, tortuosity, and pore-throat aspect ratio describe the structural properties of the pore network. The flow process can be solved by using the Hagen-Poiseuille equation. Quasi-static PNM and dynamic PNM are two commonly used methods to solve the flow behavior (Regaieg and Moncorgé, 2017). Gerke et al. (2020) modified the maximal ball algorithm and simulated the water-oil flow under the complete wetting condition based on quasi-static PNM to obtain relative permeability and capillary pressure curves. Qin et al. (2021) developed a dynamic PNM containing circular, triangular, and rectangular pores, taking into account the pore filling process of the main terminal meniscus movement and arc menisci filling. Therefore, the quasi-static method focuses on capillary-driven flow processes near equilibrium to obtain relative permeability and capillary pressure curves. Dynamic PNM considers the competition between viscous forces and capillary forces, enabling to capture displacement patterns such as viscous fingering and capillary fingering.

3. Microscopic multiphase multicomponent flow

The capillary force plays an important role in immiscible multiphase flow. The underlying flow mechanisms under different wettability and injection conditions can be reasonably explained based on pore-scale simulation methods (Joekar-Niasar et al., 2012; Chen et al., 2022). During the accumulation stage, hydrocarbon resources slowly invade the water-saturated pore networks. The invasion of non-wetting fluids is significantly affected by capillary resistance and is restricted in narrow throats (Ambekar et al., 2021). Consequently, higher pressure can facilitate the migration of hydrocarbons. During the development of hydrocarbon resources, the injected water invades into the pore system along the fractures, and the spontaneous imbibition under the action of capillary force and the forced imbibition driven by external force occur between matrix and fractures. Viscous and capillary forces influence the displacement process. The capillary number dimensionally quantifies the influence of viscous force and capillary force on displacement. A large number of studies have shown that the larger the capillary number, the better the displacement effect (Liu et al., 2022). The capillary effect is significant under low capillary numbers. Wetting fluid displaces the non-wetting fluid along the pore surface with significant interface dynamics. The convergence of the wetting fluid at the narrow throat leads to the trapping of the non-wetting fluid. This process is not conducive to hydrocarbon development but is beneficial for CO_2 storage. Under high capillary numbers, the effect of viscous force is significant, which effectively avoids the occurrence of snap-off events. Therefore, increasing the viscosity and injection rate of the invading fluid and reducing the interfacial tension are effective means for enhanced recovery.

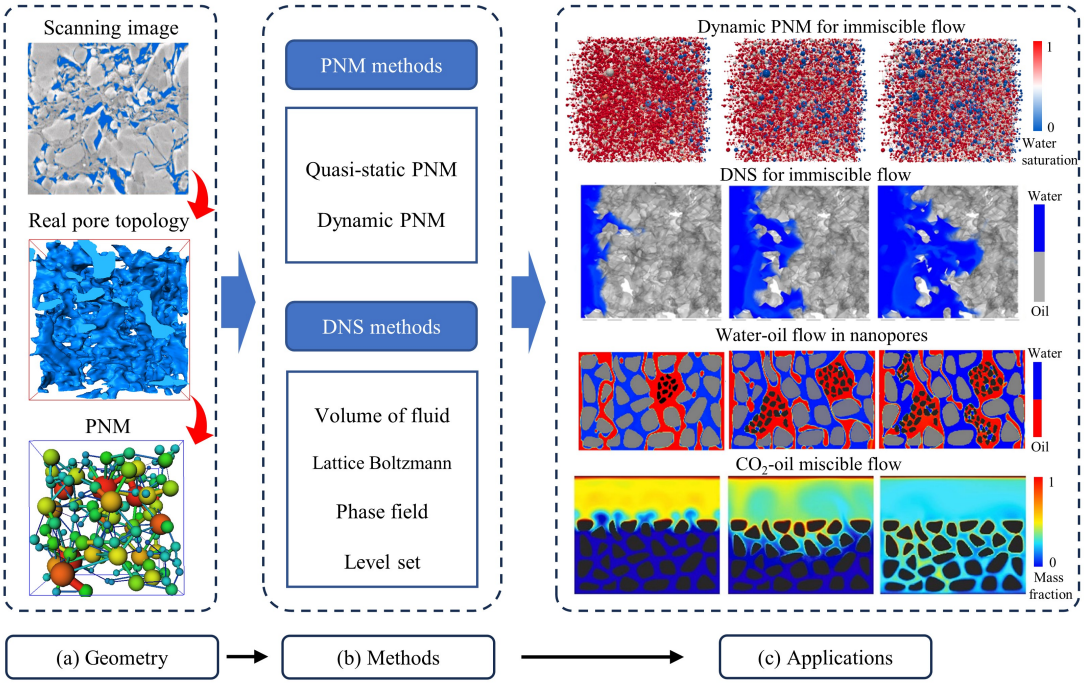

Fig. 1. Fluid flow in porous media based on pore-scale modeling. (a) Geometry of porous media, (b) simulation methos and (c) application scenarios of pore-scale simulations (Qin et al., 2022; Wang et al., 2022a; Wang et al., 2022b).

CO_2-oil miscible flow is an important means to improve oil recovery (Sharbatian et al., 2018; Behnoud et al., 2023; Zhu et al., 2024). Injecting CO_2 into the formation can reduce carbon emissions and protect the ecological environment. The temperature and pressure in deep unconventional reservoirs are extremely high, and CO_2 exists in a supercritical state. In addition, the interfacial tension between CO_2 and oil is extremely low or even non-existent under reservoir condition. During CO_2-oil miscible flow, CO_2 dissolved in oil reduces the density and viscosity of the oil and enhances the mobility. Adsorption, diffusion, and convection are important mechanisms of miscible flow. Wang et al. (2022a) simulated the CO_2-oil miscible flow considering adsorption and diffusion based on the LBM. They concluded that the proportion of adsorbed CO_2 increased, and the density of bulk CO_2 increased when CO_2 reached saturation. For CO_2-oil near-miscible flow involving interfacial tension, Yang et al. (2023) simulated the dissolution of CO_2 based on the VOF method, considering the interfacial mass transfer, and analyzed the effects of capillary number and wettability on CO_2 storage. Soulaine et al. (2018) adopted a micro-continuum approach to simulate the dissolution of solid minerals at the pore scale in the presence of multiple fluid phases. Behnoud et al. (2023) simulated the near-miscible CO_2-oil flow based on an improved PF method considering interfacial tension and Fick diffusion. Undoubtedly, pore-scale simulation has become an effective method for directly observing the dissolution characteristics of CO_2 in miscible and near-miscible flows.

4. Nanoconfined flow in porous structures

Nanoscale flows are subject to strong fluid-fluid and fluid-solid interactions, and their flow mechanisms are significantly different from those of microscale and continuous-scale flows (Wang et al., 2023a). Adsorption layer and slip effect are key factors to be considered in nanoscale flows, and they are both related to the contact angle (Zhao et al., 2018). When the contact angle is small, fluid-solid interactions are significant, causing the fluid flow to be constrained by the solid surface, with minimal slip distance. As the contact angle increases, the fluid becomes less constrained by pore surfaces, leading to increased slip effect and a substantial enhancement in fluid flow. Additionally, the near-wall viscosity is inversely related to the contact angle, a diminished effect of the resulting in a diminished effect of the adsorption layer as the contact angle increases. Although molecular dynamics simulations have been widely used in nanoscale flow, this method is limited within a single nanopore and cannot consider complex pore topology. Based on pore-scale simulation methods, the simulation scale is improved by considering micro- and nanoscale effects. Zhao et al. (2018) used LBM to study the nanoconfined flow based on the slip distance and effective viscosity obtained from molecular dynamics simulations. They concluded that the end effect has a significant impact on the flow. Song et al. (2022) constructed a multicomponent hydrocarbon mass transport model based on PNM, considering mixed wetting, adsorption layer and slip effects. They analyzed the effects of pressure, pore structure, and organic content on hydrocarbon permeability.

For nanoscale multiphase flow, fluid-fluid and fluid-solid interactions are significant (Hilaire et al., 2023). Due to differ-

ences in wettability, wetting and non-wetting fluids exhibit inconsistent slip effects at the pore surface. Usually, the wetting fluid is constrained by the pore surface and generally exhibits a no-slip flow, while the interaction between the non-wetting fluid and the pore surface is weak and the mobility is enhanced (Yu et al., 2020). In addition, liquid-liquid slip may occur at the two-phase interface, which corresponds to the interfacial momentum transfer. No slip means that the flow of two-phase fluids is consistent and shares a velocity field. Partial slip means there is a loss of momentum between the two-phase interface, while no slip means there is no momentum transfer between the two-phase fluids (Cui et al., 2022). Currently, only a limited amount of research has explored nanoscale multiphase flow through pore-scale simulations, in comparison to single-phase flow. Wang et al. (2022b) simulated water-oil flow based on the improved LBM, considering liquid-liquid slip, liquid-solid slip and heterogeneous viscosity. They found that liquid-solid slip can improve the flow capacity, and liquid-liquid slip can enhance the relative permeability of non-wetting fluids. Zhang et al. (2022) simulated water-oil flow in shale based on PNM considering slip effect and dual wettability. They concluded that increased organic content results in a higher volume of oil being trapped. Pore-scale simulations considering nanoscale effects provide new insights into fluid flow in complex pore systems of unconventional reservoirs. This helps in accurately predicting the flow capacity of hydrocarbons, offering a foundation for precise yield estimation and effective production planning.

5. Conclusion and prospect

Pore-scale simulation has been widely used to reveal microscopic flow mechanisms due to its visualization and quantification advantages. It provides a new method for characterizing complex flow behaviors that are difficult to obtain experimentally. Since DNS methods retain the complex pore topology, it has advantages in describing the interface dynamics, pore filling mechanisms, and fluids distribution under complex wettability and pore structure conditions. In contrast, PNM simplifies complex pore topology and can consider local pore filling mechanisms to simulate the flow process in large-scale heterogeneous pore structures, which has advantages in characterizing global properties such as relative permeability and capillary pressure. Furthermore, pore-scale simulation has also been applied to nanoscale flows corresponding to shale oil and gas development, taking into account adsorption layer and slip effects, revealing the single-phase and multiphase fluid flow mechanisms within shale nanopores.

In the future, it is necessary to focus on complex transport mechanisms as computing power increases. Considering the impact of interfacial tension, diffusion, and slip on the flow processes, attention should be given to the immiscible, near-miscible, and miscible flow processes associated with CO_2. This will provide an in-depth understanding of microscale and nanoscale flow mechanisms and improve the recovery of hydrocarbon resources in unconventional reservoirs. In order to realistically simulate the complex flow process in reservoirs, ion-related flows, low-salinity water flooding, reactive flows, etc. have also gradually gained attention. In addition, pore-scale models that consider multi-field coupling such as stress and heat transfer need to be further developed to expand application scenarios. It is worth noting that pore-scale simulation has scale limitations. Pore-scale simulation can be combined with large-scale models (such as fracture and reservoir scales) to form a multi-scale modeling framework to effectively predict and analyze flow processes.

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Conflict of interest

The authors declare no competing interest.

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