# Capillarity

### Current minireview

## Pore scale modeling of fluid transport in complex reservoirs: Multi-scale digital rock construction, flow experiments and simulation methods

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#### Abstract:

The heterogeneities of complex reservoirs are expressed in terms of multi-scale pore structure, different pore type and multiple occurrence mode. Fluid transport mechanisms notably differ from that in conventional sandstone reservoir. Conventional core scale experimental methods are not applicable to complex reservoirs because of nanoscale pore size and strong heterogeneity. Investigating pore scale fluid flow is the key to reveal flow mechanisms while the current pore scale modelling framework fails to consider the multi-scale structure, multiphase fluid-rock interaction and confined phase change. This work leverages the recent advances in pore scale modeling methods of fluid transport in complex reservoirs. The developing trend of multi-scale digital rock construction, flow experiments and simulation methods are elaborated in detail. The mentioned pore scale modeling methods in this work form the future research paradigm for understanding fluid transport mechanisms in complex reservoirs.

#### 1. Introduction

Traditional continuum mechanics of porous media flow typically deal with pore structure at the micron scale, whereas in complex reservoirs, the predominant pores are at the nanometer scale, with a diverse array of pore-fracture-vug systems and complex occurrence modes (Yao et al., 2018; Santos et al., 2022; Jia et al., 2023). Compared to fluid flow in micrometer-scale media, fluid flow within nano-scale and micro-scale media is extremely intricate, characterized by multiple transport mechanisms and scales (Zhang et al., 2019; Wang et al., 2020a; Cai et al., 2022). Flow mechanisms are governed by microscale effects, adsorption/desorption, and multiple flow modes interaction, rendering traditional continuum mechanics flow theories obsolete (Song et al., 2022a; Hu et al., 2023; Zhang et al., 2023b). The microscale effects are caused by the strong collision between fluid molecules and pore wall, which can be manifested in terms of fluid critical property change, slippage and Knudsen diffusion at different nano-micro pore size (Karniadakis et al., 2006). Investigating fluid flow in porous media at the pore scale is a crucial avenue for revealing flow mechanisms and gaining new insights. The extremely low permeability of complex reservoirs (shale, carbonate, tight sandstone, etc.) makes it difficult to conduct core flow experiments, and ensuring the accuracy of tests is challenging. At present, pore scale imaging and numerical simulation methods are the only viable approach to study

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Fig. 1. Deep learning-based super-resolution for multi-scale digital rock (Yang et al., 2022).

the microscopic flow mechanisms in complex reservoirs (Li et al., 2021; Zhu et al., 2021; Zhang et al., 2023a; Xu et al., 2024).

The aim of this work is to elucidate the recent advances in pore scale modeling of fluid transport in complex reservoirs. Section 2 evaluates two distinct types of multi-scale digital rock construction theories. In Section 3, the future direction of pore-scale experiments and the analysis of multiphase flow processes is illustrated. Section 4 not only assesses different pore-scale flow simulation methods for modeling fluid flow in complex reservoirs but also presents a future simulation framework. Two different types of multi-scale digital rock construction theory are evaluated in Section 2. The future direction of pore scale experiments and analysis on multiphase flow process is illustrated in Section 3. Different pore scale flow simulation methods are assessed in terms of modelling fluid flow in complex reservoirs and the future simulation framework is given in Section 4.

#### 2. Multi-scale digital rock construction theory

Most reconstruction methods only perform well for the digital rock with a single physical length scale, resulting in the trade-off between the field of view (FOV) and resolution is still an issue. Thus, researchers have put more effort into multiscale reconstruction methods. The basic and primary kind of these methods is hybrid superposition reconstruction method, which aims to fuse different single digital rocks with two or more length scales into a structure with a large FOV so that nano-pores to micro-pores can be reproduced in the ultimate 3D structure (Song et al., 2022b; Yang et al., 2023). The single digital rock can be stochastically reconstructed based on the statistical characteristics of rock images or directly obtained from such experimental methods as micro/nano- Computed Tomography (CT) and Focused Ion Beam Scanning Electron Microscopy (FIB-SEM). For instance, we can fuse a finescale digital rock, which is generated from SEM images using a Markov Chain Monte Carlo method, into a 3D micro-CT image (Zhang et al., 2020) or other stochastically reconstructed structures (Yang et al., 2015, 2019). Thus, the ultimate digital rock presents a high resolution and large field of view simultaneously. Another practical multi-scale method is pattern matching-based approaches (Yan et al., 2024), which utilizes templates to directly align high- and low-resolution patterns, or construct pattern dictionaries or sets to refine lowresolution images or 3D pore structures (Tahmasebi, 2018; Wu et al., 2019). Both the hybrid superposition method and pattern matching-based approach are biased by human factors, ignoring the spatial positions of fine-scale pores or introducing noise into the reconstruction structures.

Booming deep learning algorithms provide promising ideas for multi-scale digital rock reconstruction, such as image super-resolution (Chen et al., 2020; Shan et al., 2022) and image-to-image translation (Liu et al., 2022). Image-to-image convolutional neural networks (CNN), i.e., super-resolution CNN, fast super-resolution CNN (Mirzaee et al., 2023), and conditional generative adversarial networks (GAN), i.e., superresolution GAN (Zhao et al., 2023), CycleGAN (Chen et al., 2020) and Cycle-in-Cycle GAN (Niu et al., 2020) are widely used to enhance the core images from the micro-CT to SEM-like quality (Yang et al., 2023). The paired lowresolution (LR) image and associated high-resolution (HR) image are used as training images to train the super-resolution network model, which can learn the LR-to-HR image mapping and was used to improve the LR image resolution (Dong et al., 2016; Wang et al., 2019). Shams et al. (2020) firstly coupled the GAN and auto-encoder networks to reconstruct multi-scale digital rock, in which GAN was used to generate large-scale structure and auto-encoder introduced intraparticle pores. The auto-encoder network performs in 2D slices, resulting in an ignoration of the spatial connectivity. Therefore, Yang et al. (2022) proposed a conditional GANbased method for multi-scale digital rock using the paired 3D LR digital rock and HR digital rock as training data (Fig. 1). Nevertheless, real-world paired LR and HR images are

often hard to obtain and the LR images are always limited in number. Thus, the cycle-consistent GAN-based methods (super-resolution cycle CNN (Chen et al., 2020) and Cycle-in-Cycle GAN (Niu et al., 2020) based on unpaired rock micro-CT images at different resolutions but belonging to related domains have been proposed. To address the issue of limited HR images, typical GANs (fastGAN, StyleGAN2-ADA, etc.) can be first trained using limited real-world data. The trained model is subsequently used to generate abundant HR images for CycleGAN training (Liu and Mukerji, 2022; Wu et al., 2023). Incorporating attention mechanisms is another design strategy to enhance the SR performance of neural networks. The Residual Channel Attention Network, which utilizes Residual in Residual modules and a channel attention mechanism, effectively exploits inter-channel features and simplifies the learning process. The Component Divide-and-Conquer Super-Resolution introduces a component attention mechanism, enabling the model to better restore the multiscale pore textures and details (Wei et al., 2020). Accurate restoration of the edges and textures of multiple components (micropores, microfractures, macropores, multiple minerals, etc.) is crucial for improving the accuracy of SR tasks (Wang et al., 2020b).

The success of Generative Pre-trained Transformer models has recently ignited growing interest in utilizing Transformer models for image processing tasks. Leveraging self-attention's ability to capture long-range dependencies, Transformer-based super-resolution models not only surpass state-of-the-art CNN models in performance but also achieve this with significantly fewer parameters. A transformer-based model called Efficient Attention Super-Resolution Transformer was proposed to effectively reconstruct high-quality 3D digital rocks (Xing et al., 2024). It integrates the self-attention and channel attention mechanisms, introduces multi-scale windows, and improves shifted windows. Deep learning-based methods can learn the features from real-world core images so that the realizations can reproduce the actual fine-scale structures. Whereas, the current challenges mainly include training data acquirement, the accuracy of the results, and the degree of super-resolution. Since the huge computation costs and high GPU memory requirement, the 3D application of deep learning-based methods is still an issue.

## 3. Pore scale experiments and analysis on multiphase flow process

Pores, fractures, and vugs are typical pore structures in carbonate reservoirs. The ancient underground river vuggy carbonate is formed by the downward dissolution of surface rivers, with large vug size, and abundant reserves, which is an important area for oil production (Tan et al., 2022). However oil recovery of carbonates is typically lower compared to oil recovery of sandstone reservoirs with the same porosity and permeability (Alkhazmi et al., 2018). Applying visualization techniques to reservoir engineering allows observation of rock pore structure and fluid distribution. Medical or industrial CT can be used to carry out flooding and scanning experiments at the core scale. For example, Krevor et al. (2011) imaged the gas-water two-phase flow in homogeneous sandstones based on industrial CT and found that CO<sub>2</sub> upstream of the capillary barrier could not be displaced, and the residual CO<sub>2</sub> saturation was 2-5 times higher than the expected value. Seyyedi et al. (2022) performed gas-water injection and imaging experiments based on 1 m-long samples of the Bentheimer and Boise sandstones. The results showed that the migration of the CO<sub>2</sub> plume in the homogeneous sandstone was mainly controlled by buoyancy, whereas the migration of the CO<sub>2</sub> plume in the heterogeneous sandstone was mainly controlled by the pore structure. Al-Bayati et al. (2018, 2019) imaged the threephase distribution of oil, gas, and water in the layered porous media using medical CT, and found that the vertical change in permeability caused CO<sub>2</sub> to break through prematurely along the high permeability layer.

However, the low resolution of this technique does not allow for precise localization of the residual fluid distribution, and a great deal of information on fluid geometry is missing. Based on micro CT, the influence of micro pore geometry on fluid occurrence can be studied. The resolution of micro-CT is roughly distributed between 1-24  $\mu$ m, which can obtain a large amount of micro geometric topological information, but the scanning area is small. The pore scale displacement imaging experiment shows that capillary trapping is mainly controlled by pore throat radius, pore connectivity, and wall roughness (Oren et al., 2019; Tang et al., 2021; Geistlinger et al., 2024). Snap off is an important mechanism that leads to the formation of residual fluid. The fluid splits into two parts along the cross-section of the throat and then contracts into the pores connected to the other end of the throat (Abidoye et al., 2015; Harris et al., 2021; Algahtani et al., 2022). Ni et al. (2019) used 9 heterogeneous sandstones to search for the most favorable physical heterogeneity for CO<sub>2</sub> capillary storage in sandstone rocks. They found that 46%-97% of residual CO2 was caused by pore scale capture mechanisms, and 3%-54% of residual  $CO_2$  was caused by mesoscale capillary heterogeneity. Tanino and Blunt (2012) selected seven rock samples (four sandstone and three carbonate rocks) and finely characterized the pore geometry of each rock type through mercury intrusion, nuclear magnetic resonance, and X-ray microscopy imaging. They studied the relationship between residual fluid saturation and porosity, permeability, coordination number, and pore throat radius. Herring et al. (2019) further quantified the control effect of sandstone micro pore structure on CO<sub>2</sub> capillary capture at the micrometer scale. They used a new image analysis technique called "persistent homology", which quantifies the micro fluid structure from geometric, topological, and spatial distributions. Combining these factors, they proposed a new formula as a measure based on sustained homology, which has a good correlation with trapping efficiency. To make the characterization unit cell more representative of the whole sample, most pore-scale experiments are carried out based on porous media. Note that layered heterogeneity as well as porous-fractured-vuggy heterogeneity, as typical pore structures in reservoirs, are critical in their impact on oil and gas recovery and geological storage of CO<sub>2</sub>. There is an urgent need to clarify the effect of heterogeneity of complex pore structures on enhance oil recovery (EOR) at the pore scale



Fig. 2. Pore-scale fluid distribution in layered (a) and fractured-vuggy media (b) (Li et al., 2024).

(Fig. 2). The influence of microscopic pore geometry on the fluid transport distribution in the same type of media has been basically clarified. However, the variation of EOR key parameters needs to be further investigated in different types of media (e.g., layered heterogeneous media and pore-fractured-vuggy heterogeneous media).

## 4. Pore scale fluid flow simulation with phase change and rock-fluid interaction

The simulation of flow at the pore scale serves as a bridge between macroscopic production simulation and the microscale flow processes of confined fluids (Cui et al., 2022; Foroughi et al., 2024; Landry et al., 2024). The classic methods mainly include direct Monte Carlo simulation, lattice Boltzmann method, and pore network model. Direct Monte Carlo simulation uses an appropriate number of simulation particles to represent a large number of real gas molecules, simulating the physical processes of momentum and energy transport and exchange caused by the motion and collision of gas molecules, thereby producing macroscopic aerodynamic thermal effects

(Christou and Dadzie, 2016). Direct Monte Carlo simulation is only suitable for rarefied gas flow and is not suitable for high-pressure conditions with high gas density flow and lowspeed flow. The lattice Boltzmann method is derived from a simplified model of the Boltzmann equation-the Boltzmann-BGK equation (Eshghinejadfard et al., 2016). Simulating fluid flow in nano-porous media requires consideration of the varying mean free path and boundary slippage caused by nanoscale pore sizes (Wang et al., 2016, 2023). Scholars mainly study the flow patterns of single-component fluid in nano-porous media by establishing lattice Boltzmann methods considering microscale effects (Chen et al., 2015; Zhao et al., 2016). However, the lattice Boltzmann method requires enormous computational resources. The pore network model extracts the complex pore space of porous media into a network composed of large voids and narrow throats (Yao et al., 2019). This method has a fast computation speed and is widely used (Giudici et al., 2023).

However, the classic pore-scale flow simulation methods are not suitable for modelling pore scale multiphase and



Fig. 3. Pore-scale fluid distribution in layered and fractured-vuggy media (Song et al., 2023).

multicomponent fluid transport process in complex reservoirs. The main reasons can be attributed into three aspects. First, the current studies fail to model the flow of non-Newtonian multiphase multi-component fluids with confined phase change. Cueto-Felgueroso et al. (2018) developed a diffuse-interface model of single-component two-phase flow (a van der Waals fluid) and studied the dynamics of vaporization-condensation fronts in conceptual 2D porous media. Fei et al. (2023) developed pseudopotential multiphase lattice Boltzmann model to study the isothermal two-component evaporation in conceptual 2D porous media. Second, the multiphase flow theory only considers the interfacial capillary force and ignores the interaction forces between nano-pore walls and fluid molecules (van der Waals force, electrostatic force, structural force), which notably affect the confined fluid occurrence state. Microfluidic experiments and molecular simulation results found that the interaction force between the wall and fluid molecules leads to more wetting phase fluids remaining in the nano-pores (Sedghi et al., 2014; Liu et al., 2018; Wang et al., 2021). Mahady et al. (2016) and Abu-Al-Saud et al. (2017) considered the van der Waals force and developed the improved volume of fluid method and level-set method to study wetting film influence on immiscible two-phase flow. Song et al. (2022c, 2023) recently developed multi-phase multi-component pore network-based transport models that capable of predict non-Newtonian shale oil threshold pressure gradient and shale condensate gas mobility considering phase change and rock-fluid interaction (Fig. 3). Third, Efficient hybrid models of multiscale digital rocks that can accurately capture the multiphase flow processes across different scales of pore structures with varying wettabilities are currently absent. Shi et al. (2024) recently combined coarsened microporosity grids with the pore network of resolved macropores and developed a porenetwork-continuum hybrid model to study single phase fluid flow patterns in complex reservoirs. However, the influences of temperature changes and stress changes during production on fluid flow are notable in complex reservoirs, especially in deep oil and gas reservoirs. Currently, there are still significant challenges in establishing a pore-scale numerical simulation method to study the microscopic flow mechanisms of multiphase multicomponent fluids in complex reservoirs under thermal-fluid-solid coupling conditions. The multiphysicscoupling flow simulation approach based on lattice Boltzmann method or pore network model should be an optimal method to solve this problem in the future.

#### **5.** Conclusions

In this paper, the recent advances in pore scale modeling of fluid transport in complex reservoirs were reviewed. The future research paradigms of multi-scale digital rock construction, flow experiments and simulation methods were elaborated in detail. Deep learning-based methods are anticipated to become a more favorable option for the construction of multi-scale digital rocks, though the issue of 3D training data remains to be addressed in the future.. In addition, the pore scale flow experiments should focus on the variation of EOR key parameters in different types of heterogeneous media. Finally, multiphase multi-component fluid flow simulation with confined phase change and rock-fluid interaction is still a big challenge and pore network modelling should be an optimal way to solve this problem compared with other methods.

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#### **Conflict of interest**

The authors declare no competing interest.

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