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A nano-micro-continuum framework for liquid flow in multicomponent porous media: Impact of microporosity and microscale effects

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ABSTRACT

The multiscale features of shale, along with the inherent presence of microporosity due to current imaging limitations, pose significant challenges in accurately describing oil transport behavior. Microscale effects, such as adsorption and slip effects, further complicate the dynamic physical processes within nanoporous shale media. In this study, we present a multiscale modeling framework for confined shale oil flow that accounts for microporosity and microscale effects, including slip effects and heterogeneity in fluid density and viscosity. Sensitivity analyses are performed to quantify the impacts of unresolved pore radius, sub-resolution porosity, slip length, and total organic carbon (TOC). Two strategies are employed to represent multiple microporosities: (1) a homogeneous microporosity weighting based on TOC, and (2) an explicitly segmented organic and inorganic microporosity. Our findings reveal that microporosity and microscale effects have a significant impact on the single-phase flow of shale oil, even if microporosity exhibits extremely low permeability. The slip effect substantially enhances the overall permeability compared to the near-wall flow effects, and the contribution of microscale effects diminishes with the increase of sub-resolution porosity and unresolved pore radius. Furthermore, this work suggests that the spatial distribution of organic and inorganic microporosities critically affects the permeability of the rock sample, particularly when the two microporosities show distinct flow mobility. This work provides a novel multiscale modeling approach that integrates unresolved pores with confinement microscale effects, offering improved predictive capability for shale oil flow. Future work should focus on extending the model to multiphase flow conditions and improving the characterization of the microporosity distributions.

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1. Introduction

Shale oil and gas are now considered one of the most important resources, attracting considerable attention due to the growing global demand for energy resources, particularly in China and North America (Boak and Kleinberg, 2020; Yang et al., 2023; Zhao et al., 2025). The exploration and extraction of oil and gas resources from shale have been increasingly supported by well-developed

techniques, such as digital rock physics and field-scale numerical simulation (Yang et al., 2023; Blunt et al., 2013; Zhu et al., 2024; Liu et al., 2023). However, shale formation are known to us as a heterogeneous reservoir with an extremely complex pore structure and low to ultra-low porosity and permeability. A typical shale inherently spans several length scales with a pore size distribution from 2 nm to 200 nm (Javadpour, 2009; Wang et al., 2016b; Yang et al., 2022), comprising microscale intraparticle pores within organic matter and mineral matrix, macroscale interparticle pores, and natural microfractures (Loucks et al., 2012). In addition, the multiscale system is further complicated by horizontal drilling and multistage fracturing during development.

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Direct numerical simulation (DNS) offers an effective approach to understanding the dynamic processes in porous media at the pore scale (Blunt et al., 2013; Tahmasebi et al., 2020; Yang et al., 2023). However, DNS is critically dependent on the resolved pores, which are controlled by imaging resolutions. The multiscale pores in shale rock cannot be properly resolved by the current imaging techniques, such as micro-CT and focused ion beam scanning electron microscopy (FIB-SEM), which struggle to achieve high resolution and a large field of view (Liu et al., 2025). As a result, a substantial fraction of pores below the resolution threshold remains and cannot be explicitly captured. These unresolved pores are typically referred to as “microporosity” (Soulaine et al., 2016) or “sub-resolution porosity” (Carrillo et al., 2022), and are often treated as a distinct third phase in digital rock image segmentation, separate from the pore space and pure solid. Notably, even in relatively well-characterized rocks such as Berea sandstones, microporosity can account for 2% to 10% of the total volume (Soulaine et al., 2016). Previous studies have demonstrated that microporosity has a significant impact on flow and transport behaviors (Bultreys et al., 2015; Perez et al., 2022). Consequently, DNS cannot capture the precise properties of fluid flow and transport when ignoring the unresolved pores. Moreover, even when the resolution is sufficiently high, the image at a REV size would be much too large to run direct numerical simulations.

To address the aforementioned challenges, various multiscale models have been proposed, including two primary categories: the two-domain (or domain-decomposition) and single-domain approaches (Yang et al., 2021b; Soulaine, 2024). In the two-domain approaches, the dynamic processes are solved using distinct governing equations in different domains, e.g., the Navier-Stokes equation is used to describe the flow within resolved pores, while Darcy's law governs flow in microporosity (Molins et al., 2019). Meanwhile, the interaction between these domains is typically captured through a set of interfacial boundary conditions, such as Beavers-Joseph boundary conditions (Neale and Nader, 1974), to ensure the continuity of key physical variables, including velocity and shear stress. The pore-network-continuum models, a kind of two-domain approach, describe microporosity using “micro-links” between resolved pores (Bultreys et al. 2015, 2016; Ruspini et al., 2021; Shi et al., 2024). The pore network modeling (PNM) is applied to solve the free flow in resolved pores. Otherwise, single-domain approaches model the dynamic processes using a set of governing equations throughout the entire computational domain, eliminating the need for interfacial conditions. One such method is the multiscale pore network model, which captures flow and transport processes on multiscale physical network models (Mehmani and Prodanović, 2014; Song et al., 2016). In this framework, microporosity is described using a fine-scale network. The fine-scale pore networks are usually constructed based on the resolved pores at a higher resolution compared to the coarse-scale networks, which still lose a few unresolved pores. And it is also challenging to define the connectivity of microporosity within a pore network model (Yang et al., 2021b).

Micro-continuum method, another novel single-domain approach, applies a single set of cell-averaged fundamental equations (derived through volume-averaging over the control volumes) to solve the dynamic processes throughout the whole multiscale porous medium (resolved pores, microporosity, and pure solid), which is identified by a set of effective properties, such as porosity, permeability, specific surface area, and dispersivity (Soulaine and Tchelepi, 2016; Maes and Menke, 2024). For example, flow is solved using an extension of the Darcy-Brinkman-Stokes (DBS) (Brinkman, 1949), which tends to the Navier-Stokes equation in resolved pores and Darcy's law in unresolved pores,

as well as automatically satisfies the Beavers-Joseph boundary conditions between resolved and unresolved pore regions (Soulaine, 2024). The micro-continuum method can also be separately applied for pore-scale and continuum-scale modeling (Soulaine and Tchelepi, 2016). Moreover, the micro-continuum method shows effective and powerful capabilities in terms of multi physics modeling, including two-phase flow (Carrillo et al., 2020, 2022), heat transfer between fluid and solid (Maes and Menke, 2022), reactive transport processes (Maes and Geiger, 2018; Soulaine et al., 2021; Trinchero et al., 2021), Hydro-Bio-Geochemical processes (Kurz et al., 2022), as well as solid deformation, dissolution, and precipitation (Carrillo and Bourg, 2019; Yang et al., 2021a; Maes et al., 2022). For example, Zhou et al. (2025) have conducted multiscale shale oil flow simulations using a DBS approach based on multiscale digital rock samples.

It should be noted that shale matrix is a nanopore-dominated system, where the flow behavior of fluid is confined and quite different from that described by the Navier-Stokes equation and Darcy's law. In such confined environments, molecular interactions between fluid and solid result in spatial variations in density and viscosity (Wang et al., 2016b; Yang et al., 2020; Liu et al., 2022; Sun et al., 2023). These effects manifest as adsorption layers due to attractive forces and near-wall flow enhancement resulting from repulsive forces. The repulsive forces introduce a slip velocity at the interface, which depends on the strength of molecular interactions. Both molecular simulations and experimental studies have indicated that ignoring microscale effects, i.e., slip effect and heterogeneous density and viscosity, can significantly underestimate the flow capacity (Wang et al., 2016a; Wu et al., 2019; Xu et al., 2022). Nanoconfinement further amplifies the influence of microscale effects. In that case, the flow capability of confined water is 10^{-1} to 10^7 times greater than that calculated by the Hagen-Poiseuille equation with no-slip boundary conditions (Majumder et al., 2005; Wu et al., 2017). Unlike gas flow in nanochannels, the continuity assumption is still valid for liquid flow provided that microscale effects are properly incorporated (Yang et al., 2019). Many theoretical models have been proposed to characterize the liquid flow in nanopores, which strongly depend on the single nanopores and cannot reflect the heterogeneous nanoporous media (Zhang et al. 2017, 2018; Wang et al., 2019). Based on molecular simulations and theoretical models on single nanopores, PNM (Yang et al., 2019; Shi et al., 2024), DNS (Duan et al., 2022; Cha et al., 2023; Qin et al., 2024), and lattice Boltzmann methods (LBM) (Zhang et al., 2021; Wang et al. 2022a, 2022b) are widely developed to model liquid flow in nanoporous media to investigate the impact of microscale effects. Wang et al. developed a novel pore network modeling framework, which integrates liquid compressibility, pore deformation, and the interaction between organic and oil (Wang et al., 2026), as well as a two-phase flow PNM under mixed wetting conditions (Wang et al., 2025). However, understanding how these effects influence flow behavior at a larger scale remains limited due to the presence of microporosity. A key unresolved challenge remains in simultaneously accounting for unresolved microporosity and microscale effects within a unified multiscale modeling framework.

In this study, we proposed a nano-micro-continuum approach to model fluid flow in multicomponent shale formations, accounting for microporosity and associated microscale effects. An apparent permeability model is established to characterize flow behavior in nanoporous media, incorporating microscale effects, such as slippage and near-wall flow due to heterogeneous density and viscosity. The different flow properties in organic and inorganic pores are also considered, as shown in Section 2. Sensitivity analyses are carried out to assess the impact of sub-resolution porosity, average unresolved pore radius, slip length, and total

organic carbon (TOC). Two strategies are employed to represent the organic and inorganic microporosity: a TOC-controlled homogeneous microporosity and explicitly segmented organic and inorganic microporosity, as detailed in Sections 4.1 and 4.2. The overview of the proposed nano-micro-continuum modeling framework is illustrated in Fig. 1. To the best of our knowledge, this is the first application of the micro-continuum approach to simulate liquid flow in a shale image with nanoporous microporosity and the first investigation of how microscale effects influence flow behavior across larger-scale porous media.

2. Methodology and mathematical models

Micro-continuum approach (Soulaine and Tchelepi, 2016) is adopted to simulate the flow of shale oil in multiscale porous media, including resolved pores, unresolved pore regions, and no-flow solids. A single momentum equation combining the Navier-Stokes equations for fluid motion in resolved pores with Darcy's law for unresolved pore regions, where an apparent permeability model considering microscale effects is used, governs the flow behavior throughout the entire computational domain. We consider the fluid motion in resolved pores as a steady laminar flow of incompressible Newtonian fluid:

$$\nabla \cdot \mathbf{u} = 0 \quad (1)$$

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nu \nabla^2 \mathbf{u} \quad (2)$$

where ν is the kinematic viscosity, m^2/s ; $\mathbf{u}$ is the velocity, m/s ; p is the kinematic pressure, m^2/s^2 .

2.1. Micro-continuum approach

In the micro-continuum framework, the model is discretized into control volumes, which are categorized into three computational domains: free-flow zones (resolved pores), nanoporous regions (unresolved pores, hereafter referred to as microporosity), and solid regions. The porosity field, ε , i.e., the volume fraction of pore space in a control volume, serves to distinguish different computational domains, as shown in Fig. 2. In free-flow zones, where no solid phase is

present in the control volume, $\varepsilon = 1$, and fluid motion is described by Navier-Stokes equation. Conversely, $\varepsilon = 0$ denotes solid regions instead, and there is no fluid flow. Within microporosity, ε varies from 0 to 1, where fluid flow is governed by Darcy's law.

The fluid flow of the micro-continuum system is solved in terms of volume-averaged velocity $\bar{\mathbf{u}}$ and pressure $\bar{p}$ over the control volume V . The pressure is averaged over the fluid volume V_f , defined as the intrinsic phase average (Eq. (3)). The volume-averaged velocity (Eq. (4)), being averaged over the control volume, is applied to agree with Darcy's law in porous regions.

$$\bar{p} = \frac{1}{V_f} \int_{V_f} p dV \quad (3)$$

$$\bar{\mathbf{u}} = \frac{1}{V} \int_V \mathbf{u} dV \quad (4)$$

where p and $\bar{p}$ are the pressure and phase-averaged pressure, Pa; $\mathbf{u}$ and $\bar{\mathbf{u}}$ represent the velocity and volume-averaged velocity, respectively, m/s ; V and V_f represent the control volume and fluid volume, respectively, m^3 . Note that the volume-averaged and phase-averaged velocities are the same in free-flow zones, which agrees with the Navier-Stokes equation.

2.2. Darcy-Brinkman-Stokes equation

The mass and momentum conservation equations for incompressible fluid based on averaged quantities can be derived using volume averaging, resulting in an extended Darcy-Brinkman-Stokes (DBS) equation (Soulaine and Tchelepi, 2016)

$$\nabla \cdot \bar{\mathbf{u}} = 0 \quad (5)$$

$$\frac{1}{\varepsilon} \left(\frac{\partial \bar{\mathbf{u}}}{\partial t} + \nabla \cdot \left(\frac{\bar{\mathbf{u}} \otimes \bar{\mathbf{u}}}{\varepsilon} \right) \right) = -\nabla \bar{p} + \frac{\nu}{\varepsilon} \nabla^2 \bar{\mathbf{u}} - \nu k^{-1} \bar{\mathbf{u}} \quad (6)$$

where k represents the permeability of the control volume in microporosity, m^2 . The momentum equation, Eq. (6), can describe the flow behavior throughout the entire computational domain without gravity involved. The left-hand terms correspond to the inertia effects, which can be neglected for fluid flow in shale

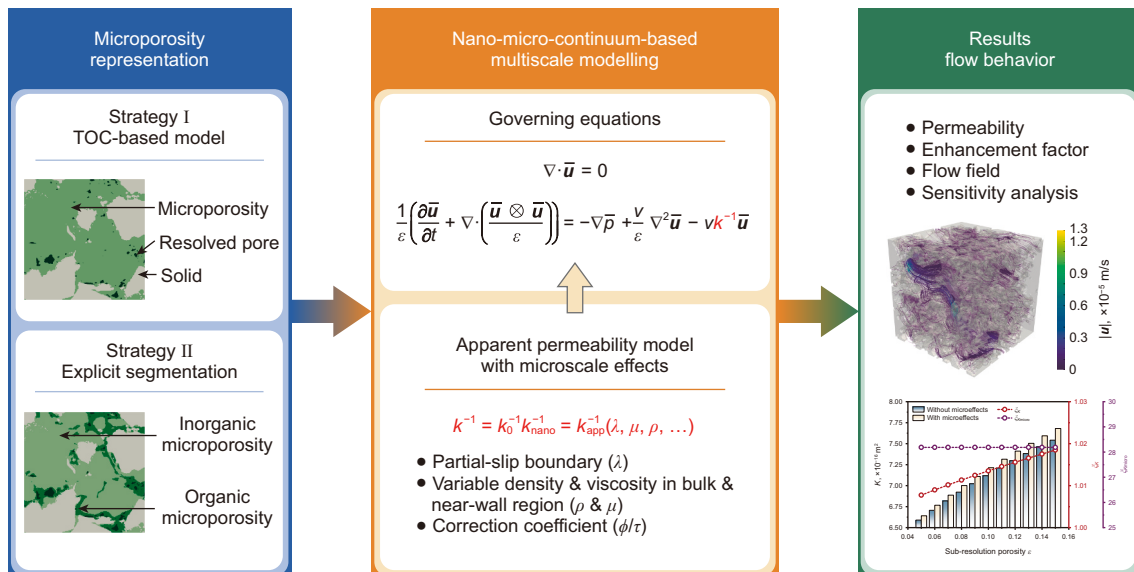


Fig. 1. Schematic illustration of the proposed nano-micro-continuum modeling framework for shale oil flow.

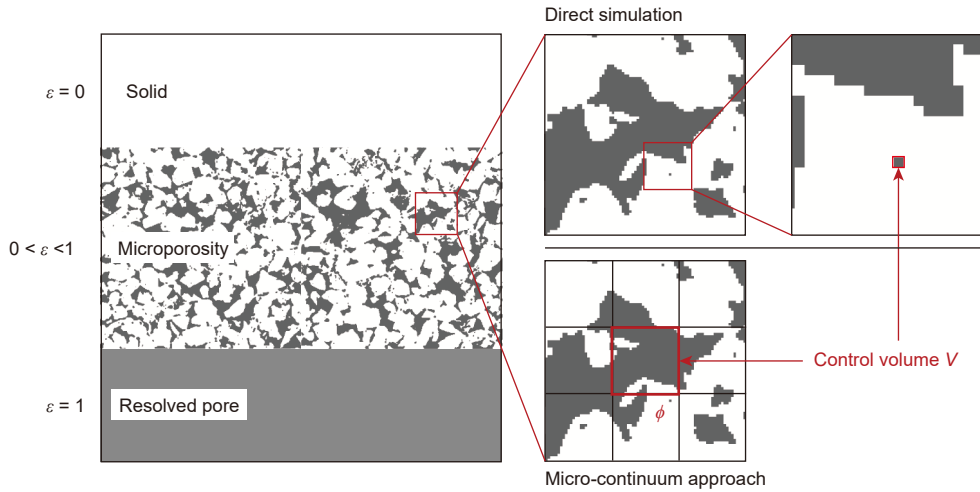


Fig. 2. Representation of multiscale porous media, cell grids, and the difference between direct numerical simulation and micro-continuum approach.

porous media. The first and second terms of the right-hand side are the pressure gradient and viscous dissipation terms, respectively. The term ν/ε , whose exact form remains unsolved, means effective viscosity in porous regions (Soulaine and Tchelepi, 2016; Maes and Menke, 2024; Golfer et al., 2015). The last term $\nu k^{-1} \bar{u}$ denotes the Darcy resistance, representing the momentum exchange between the fluid and solid, which is only dominant in microporosity and vanishes in free-flow zones, as there is no solid within the control volume. Thus, the extended DBS equation approximates Darcy's law $-\nabla \bar{p} = \nu k^{-1} \bar{u}$ in porous regions but tends toward the Navier-Stokes equation in free-flow zones.

The drag force $\nu k^{-1} \bar{u}$, assumed as a sub-grid model that represents the processes occurring below the grid size for continuum-scale modeling, has different forms depending on the underlying physical processes (Soulaine, 2024): a scalar k value for an isotropic medium (Soulaine and Tchelepi, 2016), an empirical function of porosity ε like the Kozeny-Carman model (Maes et al., 2022; Soulaine et al., 2016; Maes and Menke, 2022), or an advanced sub-grid model incorporating microstructure and nanoscale effects for shale gas (Soulaine et al., 2019). When we use the DBS framework for multiphase flow, the relative permeability model depending on the fluid saturation in cells is essentially involved (Carrillo et al., 2020). In this work, for nanoporous microporosity, we adopt an apparent permeability model that accounts for microscale effects, including slip flow and heterogeneous viscosity distribution in organic and inorganic pore space (see the following Section). It's supposed to be noted that the microscale effects are not considered in resolved pores in this work. Thereby, in solid regions, the permeability is assigned a sufficiently small scalar value to obtain a no-slip boundary condition at the fluid-solid interface.

2.3. Sub-grid model with microscale effects

The Darcy resistance coefficient k reflects the fluid mobility in porous media. To capture the Darcy resistance of nanoporous microporosity regions, we consider an apparent permeability of shale oil k_{app} , to present the comprehensive effects of microstructure and microscale effects for the sub-grid model. Given that shale is a nanopore-dominated porous medium, it cannot be neglected that the molecular interaction between fluid and solid results in slip

effect and heterogeneous viscosity distribution (Mattia and Calabrò, 2012; Wu et al., 2017). Flow enhancement occurs in water-wet inorganic pores due to the stronger interaction between oil molecules than that between oil and solid molecules, simultaneously leading to a lower viscosity near the wall than in the bulk region. In organic nanopores, which are generally oil-wet, the molecular simulation results found that the interaction between bulk oil molecules is weaker than that between oil and solid molecules, absorbing four oil layers near the wall (Yang et al., 2020, 2024; Wang et al., 2016a, 2016b). Zhang et al. (2017) developed a unified apparent permeability model for shale oil in nanoporous media, which takes flow enhancement, near-wall flow, and different types of pores into account. This model was derived based on the Hagen-Poiseuille (HP) equation with slip boundary conditions in a nanotube, which is divided into bulk and near-wall regions, e.g., the velocity in an inorganic nanopore can be expressed

$$u_b(r) = \frac{\Delta p}{L} \frac{R^2 - r^2}{4\mu_b} + c_1, 0 \leq r \leq R - \delta_{in} \quad (7)$$

$$u_w(r) = \frac{\Delta p}{L} \frac{R^2 - r^2}{4\mu_w} + c_2, R - \delta_{in} \leq r \leq R \quad (8)$$

where $u_b(r)$ and $u_w(r)$ are the velocities, m/s, over radius r , m, in bulk and near-wall regions, respectively. μ_b and μ_w are bulk and near-wall oil viscosities, respectively, mPa·s. Δp is the pressure difference, Pa, along the nanotube with a length of L , m, and radius of R , m. δ_{in} represents the thickness of the near-wall region, m. Eq. (7) and Eq. (8) can be solved according to the following boundary conditions

$$\begin{aligned} \frac{\partial u_b}{\partial r} \Big|_{r=0} &= 0, u_b \Big|_{r=R-\delta_{in}} = u_w \Big|_{r=R-\delta_{in}}, \\ \mu_b \frac{\partial u_b}{\partial r} \Big|_{r=R-\delta_{in}} &= \mu_w \frac{\partial u_w}{\partial r} \Big|_{r=R-\delta_{in}}, -\lambda \frac{\partial u_w}{\partial r} \Big|_{r=R} = u_w \Big|_{r=R} \end{aligned} \quad (9)$$

to obtain the velocity equation

$$u_b(r) = \left[\frac{1}{4\mu_w} \left(R^2 - \frac{\mu_w}{\mu_b} r^2 \right) + \frac{(\mu_w - \mu_b)(R - \delta_{in})^2}{4\mu_w \cdot \mu_b} + \frac{\lambda R}{2\mu_w} \right] \frac{\Delta p}{L}, \quad 0 \leq r \leq R - \delta_{in} \quad (10)$$

$$u_w(r) = \left(\frac{R^2 - r^2}{4\mu_w} + \frac{\lambda R}{2\mu_w} \right) \frac{\Delta p}{L}, R - \delta_{in} \leq r \leq R \quad (11)$$

where λ is the slip length, m, which can be obtained from molecular simulation results. The integration of Eqs. (10) and (11) over the cross area of the nanotube results in the total mass flow rate

$$\begin{aligned} q_{in} &= \rho_b Q_b + \rho_w Q_w = \rho_b \int_0^{R-\delta_{in}} u_b(r) \cdot 2\pi r dr + \rho_w \int_{R-\delta_{in}}^R u_w(r) \cdot 2\pi r dr \\ &= \rho_b \frac{\pi \Delta p}{8L\mu_b} (R - \delta_{in})^2 \left[\frac{\mu_b}{\mu_{ads}} (4R\delta_{in} - 2\delta_{in}^2) + (R - \delta_{in})^2 + 4 \frac{\mu_b}{\mu_w} \lambda R \right] \\ &\quad + \rho_w \frac{\pi \Delta p}{8L\mu_w} (2R\delta_{in} - \delta_{in}^2) (2R\delta_{in} - \delta_{in}^2 + 4\lambda R) \end{aligned} \quad (12)$$

where Q_b and Q_w are volume flow rate across the bulk and near-wall regions, respectively, m^3/s . ρ_b and ρ_w are bulk and near-wall oil densities, respectively, kg/m^3 . Similarly, we can obtain the total mass flow rate in the organic pore

$$\begin{aligned} q_{or} &= \rho_b \frac{\pi \Delta p}{8L\mu_b} (R - \delta_{or})^2 \left[\frac{\mu_b}{\mu_{ads}} (4R\delta_{or} - 2\delta_{or}^2) + (R - \delta_{or})^2 \right] \\ &\quad + \rho_{ads} \frac{\pi \Delta p}{8L\mu_{ads}} (2R\delta_{or} - \delta_{or}^2) (2R\delta_{or} - \delta_{or}^2) \end{aligned} \quad (13)$$

where ρ_{ads} denotes oil density, kg/m^3 ; μ_{ads} is oil viscosity in the adsorption (near-wall) region, $mPa \cdot s$; δ_{or} is the thickness of adsorption layer in the organic pore, m. Note that only the adsorption effect is involved in organic pores due to the strong molecular interaction between the fluid and solid (Yang et al., 2020; Wang et al., 2016a). A correction factor ϕ_{eff}/τ based on effective tortuosity τ and porosity ϕ_{eff} is employed to expand Eqs. (12) and (13) into porous media (Zhang et al., 2017), yielding an upscaled mass flux

$$\begin{aligned} J_{in} &= \frac{\varepsilon}{\tau} \left(1 - \frac{\delta_{in}}{R} \right)^2 \rho_b \frac{\Delta p}{8L\mu_b} \left[\frac{\mu_b}{\mu_{ads}} (4R\delta_{in} - 2\delta_{in}^2) + (R - \delta_{in})^2 + 4 \frac{\mu_b}{\mu_w} \lambda R \right] \\ &\quad + \frac{\varepsilon}{\tau} \left[1 - \left(1 - \frac{\delta_{in}}{R} \right)^2 \right] \rho_w \frac{\Delta p}{8L\mu_w} (2R\delta_{in} - \delta_{in}^2 + 4\lambda R) \end{aligned} \quad (14)$$

$$\begin{aligned} J_{or} &= \frac{\varepsilon}{\tau} \left(1 - \frac{\delta_{or}}{R} \right)^2 \rho_b \frac{\Delta p}{8L\mu_b} \left[\frac{\mu_b}{\mu_{ads}} (4R\delta_{or} - 2\delta_{or}^2) + (R - \delta_{or})^2 \right] \\ &\quad + \frac{\varepsilon}{\tau} \left[1 - \left(1 - \frac{\delta_{or}}{R} \right)^2 \right] \rho_{ads} \frac{\Delta p}{8L\mu_{ads}} (2R\delta_{or} - \delta_{or}^2) \end{aligned} \quad (15)$$

According to Darcy's law, the apparent permeability of shale oil in inorganic and organic porous media can be given by

$$\begin{aligned} k_{in} &= J_{in} \frac{\mu_o L}{\rho_o \Delta p} = \frac{\varepsilon R^2}{8\tau} \\ &\left\{ \frac{\rho_b}{\rho_o} \left(1 - \frac{\delta_{in}}{R} \right)^2 \left[\frac{\mu_o}{\mu_w} \left(\frac{4\delta_{in}}{R} - 2 \left(\frac{\delta_{in}}{R} \right)^2 \right) + \frac{\mu_o}{\mu_b} \left(1 - \frac{\delta_{in}}{R} \right)^2 + 4 \frac{\mu_b}{\mu_w} \frac{\lambda}{R} \right] \right. \\ &\quad \left. + \frac{\rho_w}{\rho_o} \left[1 - \left(1 - \frac{\delta_{in}}{R} \right)^2 \right] \frac{\mu_o}{\mu_w} \left[\left(2 \frac{\delta_{in}}{R} - \left(\frac{\delta_{in}}{R} \right)^2 \right) + 4 \frac{\lambda}{R} \right] \right\} \end{aligned} \quad (16)$$

$$\begin{aligned} k_{or} &= J_{or} \frac{\mu_o L}{\rho_o \Delta p} = \frac{\varepsilon R^2}{8\tau} \\ &\left\{ \frac{\rho_b}{\rho_o} \left(1 - \frac{\delta_{or}}{R} \right)^2 \left[\frac{\mu_o}{\mu_{ads}} \left(\frac{4\delta_{or}}{R} - 2 \left(\frac{\delta_{or}}{R} \right)^2 \right) + \frac{\mu_o}{\mu_b} \left(1 - \frac{\delta_{or}}{R} \right)^2 \right] \right. \\ &\quad \left. + \frac{\rho_{ads}}{\rho_o} \left[1 - \left(1 - \frac{\delta_{or}}{R} \right)^2 \right] \frac{\mu_o}{\mu_{ads}} \left(2 \frac{\delta_{or}}{R} - \left(\frac{\delta_{or}}{R} \right)^2 \right) \right\} \end{aligned} \quad (17)$$

By introducing the total organic carbon (TOC) α , we have the unified apparent permeability model in shale porous media with both organic and inorganic pores:

$$\begin{aligned} k_{app} &= (1 - \alpha) k_{in} + \alpha k_{or} \\ &= (1 - \alpha) \frac{\varepsilon R^2}{8\tau} \left\{ \frac{\rho_b}{\rho_o} \eta_{in} \left[2 \frac{\mu_o}{\mu_w} (1 - \eta_{in}) + \frac{\mu_o}{\mu_b} \eta_{in} + 4 \frac{\mu_b}{\mu_w} \frac{\lambda}{R} \right] \right. \\ &\quad \left. + \frac{\rho_w}{\rho_o} \frac{\mu_o}{\mu_w} (1 - \eta_{in}) \left[(1 - \eta_{in}) + 4 \frac{\lambda}{R} \right] \right\} \\ &\quad + \alpha \frac{\varepsilon R^2}{8\tau} \left\{ \frac{\rho_b}{\rho_o} \eta_{or} \left[2 \frac{\mu_o}{\mu_{ads}} (1 - \eta_{or}) + \frac{\mu_o}{\mu_b} \eta_{or} \right] + \frac{\rho_{ads}}{\rho_o} \frac{\mu_o}{\mu_{ads}} (1 - \eta_{or})^2 \right\} \end{aligned} \quad (18)$$

where $\eta_{in} = (1 - \delta_{in}/R)^2$ and $\eta_{or} = (1 - \delta_{or}/R)^2$ represent the correction factors caused by near-wall and adsorption regions, respectively.

2.4. Numerical implementation and upscaling

The mathematical model formed by Eqs. (5), (6) and (18) is discretized using the finite volume method and numerically solved using simpleDBSfoam, a DBS-based solver implemented in GeoChemFoam (Maes and Menke, 2021, 2022; Maes et al., 2022), which is an open-source reactive transport toolbox based on OpenFOAM® (<https://www.openfoam.com>). This solver is developed based on SIMPLE algorithm and has been extensively validated (Carrillo et al., 2020; Soulaïne and Tchepeli, 2016). The sub-grid model is integrated into simpleDBSfoam as a porous media model to calculate the required effective permeability for nanoporous microporosity, which draws on another open-source toolbox, hybridPorousInterFoam (Carrillo et al., 2020).

The permeability of the sample is calculated from the simulation results using the GeoChemFoam utility processPoroPerm, which follows Darcy's law:

$$K = \mu \left(\frac{\Delta p}{L} \right)^{-1} \left(\frac{1}{V_{total} \int_{V_{total}} \bar{u} dV} \right) \quad (19)$$

where K is the permeability, m^2 ; $\Delta p/L$ is the pressure loss along the dominant flow direction (i.e., between inlet and outlet), Pa/m ; $\bar{u}$ is the velocity along the flow direction, m/s ; V_{total} is the sample volume, m^3 . The porosity ϕ of the sample can be easily calculated by integrating ε over the sample volume:

$$\phi = \frac{1}{V_{total}} \int_{V_{total}} \varepsilon dV \quad (20)$$

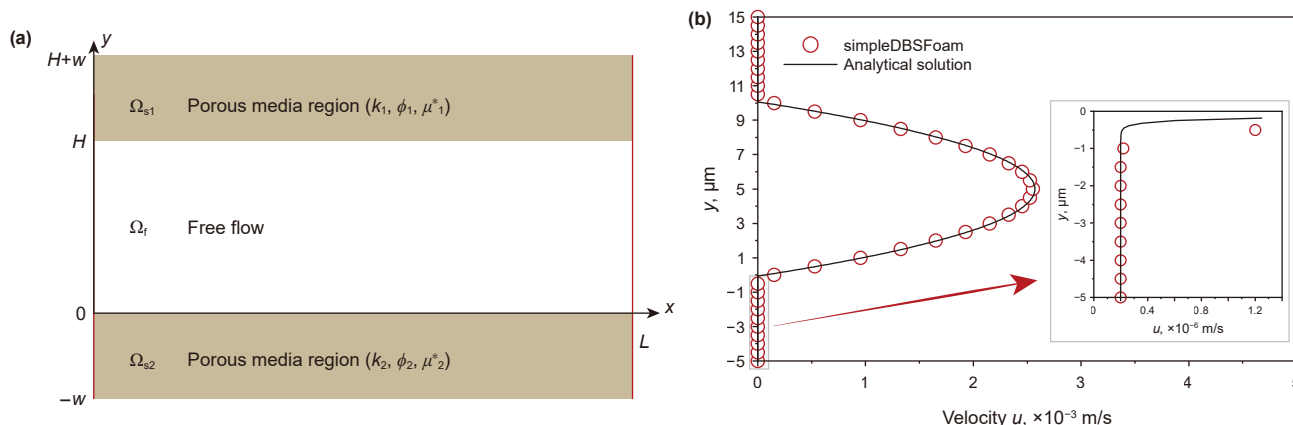


Fig. 3. The 2D channel with porous media (a) for validation and the comparison of velocity profiles between numerical and analytical solutions (b).

2.5. Model validation

To validate the proposed numerical model, a 2D channel model coupling a free-flow region and porous media was established, as shown in Fig. 3(a). The numerical simulation results were compared against the exact analytical solution of the Brinkman equation. The detailed derivation of the analytical solution can be found in previous studies by Youssef and Awotunde (2019) and Liu et al. (2024).

The porous regions Ω_{s1} and Ω_{s2} are assigned identical properties, including a permeability of $k_1 = k_2 = 1 \times 10^{-15} \text{ m}^2$, a porosity of $\phi_1 = \phi_2 = 0.2$, and a width of $w = 5 \mu\text{m}$. The width of the free-flow region Ω_f is $10 \mu\text{m}$, and the total length of the computational domain is $50 \mu\text{m}$. Water is the working fluid with a viscosity of $\mu = 1 \text{ mPa}\cdot\text{s}$ and a density of $\rho = 1000 \text{ kg/m}^3$, while the effective viscosity in the porous region is defined as $\mu^*_1 = \mu^*_2 = \mu/\phi = 5 \text{ mPa}\cdot\text{s}$. A constant pressure gradient is used by setting the inlet kinematic pressure to $0.01 \text{ m}^2/\text{s}^2$ and the outlet to zero. Impermeable boundary conditions are applied at the top and bottom boundaries.

Fig. 3(b) presents a comparison of the velocity profiles obtained from the simpleDBSFoam solver and the analytical solution of the Brinkman equation. The numerical results show excellent agreement with the analytical solution throughout the computational domain. Minor deviations are observed only near the interfaces between the porous media and the free-flow region, which can be attributed to numerical discretization and interface treatment. Overall, the consistency between the numerical and analytical solutions demonstrates the accuracy and reliability of the multiscale modeling framework.

3. Model generation and simulation setup

The following simulations are performed on 3D digital rock data reconstructed from high-resolution FIB-SEM images of Vaca Muerta, obtained from Andrew (Andrew, 2018, 2020) through the DigitalRockPortal. A Cartesian mesh with the same number of cells as the voxels of the original image is used in this study. Fig. 4 presents the creation process of the mesh model and porosity field. The segmented FIB-SEM image ($1024 \times 861 \times 606$ voxels) with a voxel size of $5 \text{ nm} \times 5 \text{ nm} \times 5 \text{ nm}$ comprises five phases: porosity, organic phases, quartz, calcite, and pyrite. The organic phases, quartz, and calcite are classified into a single computational domain, i.e., microporosity; thus, only three phases (porosity, microporosity, and pyrite) are used for simulation. To simulate the shale oil flow process in multiscale porous media, the voxel size

was increased to 100 nm , and a sub-volume with voxels of 200^3 , representing a physical volume of $20 \times 20 \times 20 \mu\text{m}^3$, was extracted. In that case, the microscale effects are only considered in the sub-porosity cells, where the sub-grid model is employed to calculate the permeability at resolutions below 100 nm/voxel according to the ε value and the basic parameters of shale oil and simulated shale rock. Note that we set ε as 0.0001 in solid regions to avoid division by zero during numerical computation. The ε equals 1 in free-flow regions and varies from 0 to 0.15 in the microporosity region (Table 1). Meanwhile, no-slip boundary conditions are used for the free-flow region.

The typical properties of shale image and shale oil, from experimental and molecular simulation results as reported in previous literature, are adopted to investigate the impact of microporosity properties on shale oil single-phase flow. Although the occurrence of slip flow in organic pores is uncertain, only adsorption effects are considered in this study, owing to the strong molecular interactions between shale oil and kerogen (Yang et al. 2020, 2024; Liu et al., 2022). Previous molecular simulation results indicate that the slip length becomes nearly constant when the pore size exceeds 5 nm (Thomas and McGaughey, 2008; Wang et al., 2016a). Moreover, four molecular layers are strongly affected by the pore walls, so that the thickness of the near-wall region for both organic and inorganic pores is assumed to be 1.92 nm (0.48 nm per molecular layer) (Wang et al., 2016a, 2016b). The density of adsorbed oil is set to 1.1 times that of bulk oil in organic pores, and it is opposite for near-wall oil and bulk oil in inorganic pores. In this work, the viscosity ratio between near-wall oil and bulk oil is assumed to match the density ratio, consistent with a previous study (Zhang et al., 2017). Additionally, the density and viscosity of bulk oil are consistent with that used in the free-flow region, i.e., $\rho_b = \rho_o$ and $\mu_b = \mu_o$. The basic parameters of shale oil and simulated shale rock are summarized in Table 1. During the simulation, a constant kinematic pressure drop of $1 \text{ m}^2/\text{s}^2$ ($p_{\text{inlet}} = 1 \text{ m}^2/\text{s}^2$ and $p_{\text{outlet}} = 0 \text{ m}^2/\text{s}^2$) is applied to force the flow.

4. Results and discussion

4.1. Multiscale simulation with TOC weight

This section presents the simulation results under different significant factors, including average unresolved pore radius R (average pore radius of microporosity), sub-resolution porosity ε (the porosity of microporosity cells), slip length λ , and TOC α . A series of basic multiscale simulations without microscale effects (hereafter referred to as “base” cases) was performed for

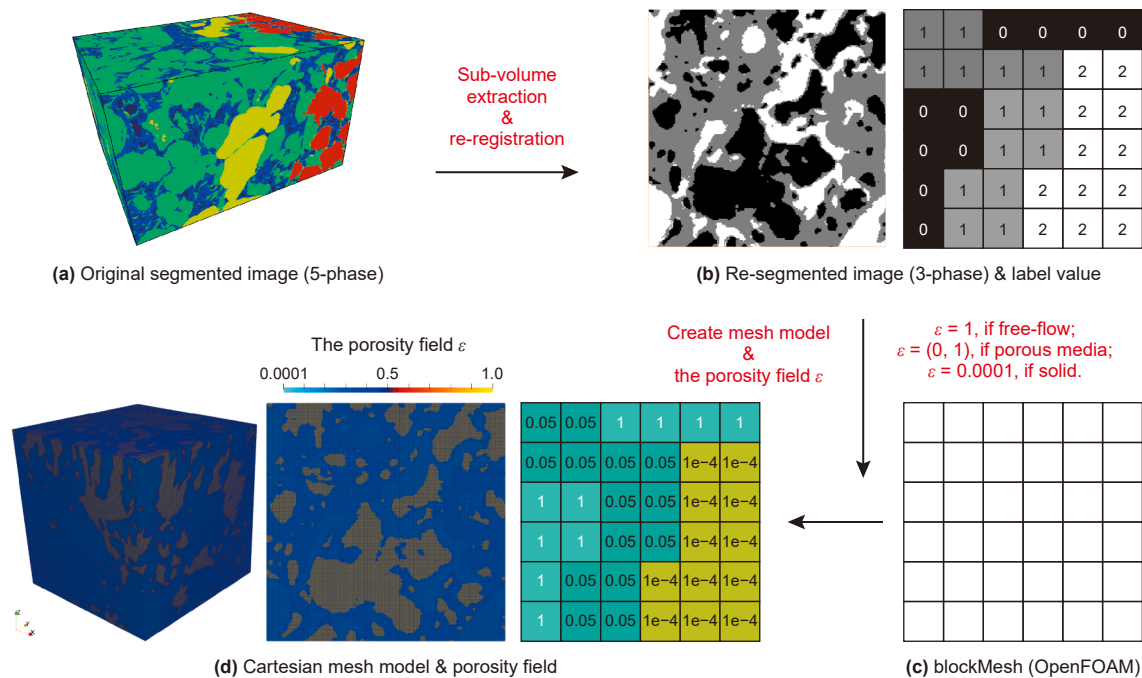


Fig. 4. The process of mesh model and porosity field creation: (a) original segmented FIB-SEM (5-phase); (b) re-segmented image (3-phase); (c) basic mesh model using blockMesh in OpenFOAM; (d) Cartesian mesh model and porosity field.

Table 1		
Properties and parameters of shale oil and physical model used in this study.		
	Property parameters	Value or range
Physical model parameters	Tortuosity τ	2.54 (Song et al., 2016)
	Average unresolved pore radius R , nm	5–100 (Javadpour, 2009; Wang et al., 2016b)
	Slip length λ , nm	0–150 (Yang et al., 2019; Duan et al., 2022)
	Sub-resolution porosity ϵ	0–0.15
	Near-wall thickness δ_{in} , nm	1.92 (Wang et al., 2016a, 2016b)
	Adsorption thickness δ_{or} , nm	1.92 (Wang et al., 2016a, 2016b)
	TOC α	0–1
	Viscosity $\mu_o = \mu_b$, mPa·s	10.235 (Duan et al., 2022)
	Density $\rho_o = \rho_b$, kg/m ³	856 (Duan et al., 2022)
	Viscosity ratio $\mu_{ads}/\mu_b, \mu_b/\mu_w$	1.1 (Zhang et al., 2017)
Shale oil parameters	Density ratio $\rho_{ads}/\rho_b, \rho_b/\rho_w$	1.1 (Zhang et al., 2017)

comparison. In that case, the sub-grid model is converted into $k_{app} = \epsilon R^2/8\tau$ (Song et al., 2016). At the same time, a pore-scale simulation was conducted in resolved pores to calculate the permeability of the sample, excluding the influence of microporosity. The simpleDBSFoam is also used for solving the flow in resolved pores, whereby the ϵ is set to 0.0001 for both solid and microporosity, so-called Immersed Boundary Conditions (Soulaine et al., 2016).

The typical calculated overall permeabilities are summarized in Table 2, where K_{micro} refers to the computed permeability using the sub-grid model for microporosity cells and K is the overall permeability of the computational domain. For base cases, even the lowest calculated permeability from the multiscale simulation ($R = 5$ nm and $\epsilon = 0.05$), where the permeability of microporosity is only 6.15×10^{-20} m², is still 13.32% larger than that of the pore-scale case. As microporosity permeability increases to 7.38×10^{-17} m², the total permeability rises by up to 53.84%. This observation implies that the unresolved pores connect some isolated resolved pores as a bridge and improve the flow ability (Soulaine et al., 2016; Carrillo et al., 2022). The flow streamlines (Fig. 5) obviously show that new flow pathways for shale oil are formed in unresolved pore regions, and the pressures for base and

Table 2
Calculated permeabilities from simulations at different conditions.

Items	Pore-scale case	Base case		Microscale effect case	
		Minimum ($R = 5$ nm, $\epsilon = 0.05$)	Maximum ($R = 100$ nm, $\epsilon = 0.15$)	Minimum ($\alpha = 1$, $R = 5$ nm, $\epsilon = 0.05$)	Maximum ($\alpha = 0$, $R = 100$ nm, $\epsilon = 0.15$, $\lambda = 150$ nm)
$K_{micro}, \times 10^{-16}$ m ²	0	6.1516×10^{-4}	7.3819×10^{-1}	4.7574×10^{-4}	4.7739
$K, \times 10^{-16}$ m ²	5.8151	6.5896	8.9457	6.5891	13.5843
Relative difference D , %	/	13.32	53.84	13.31	133.60

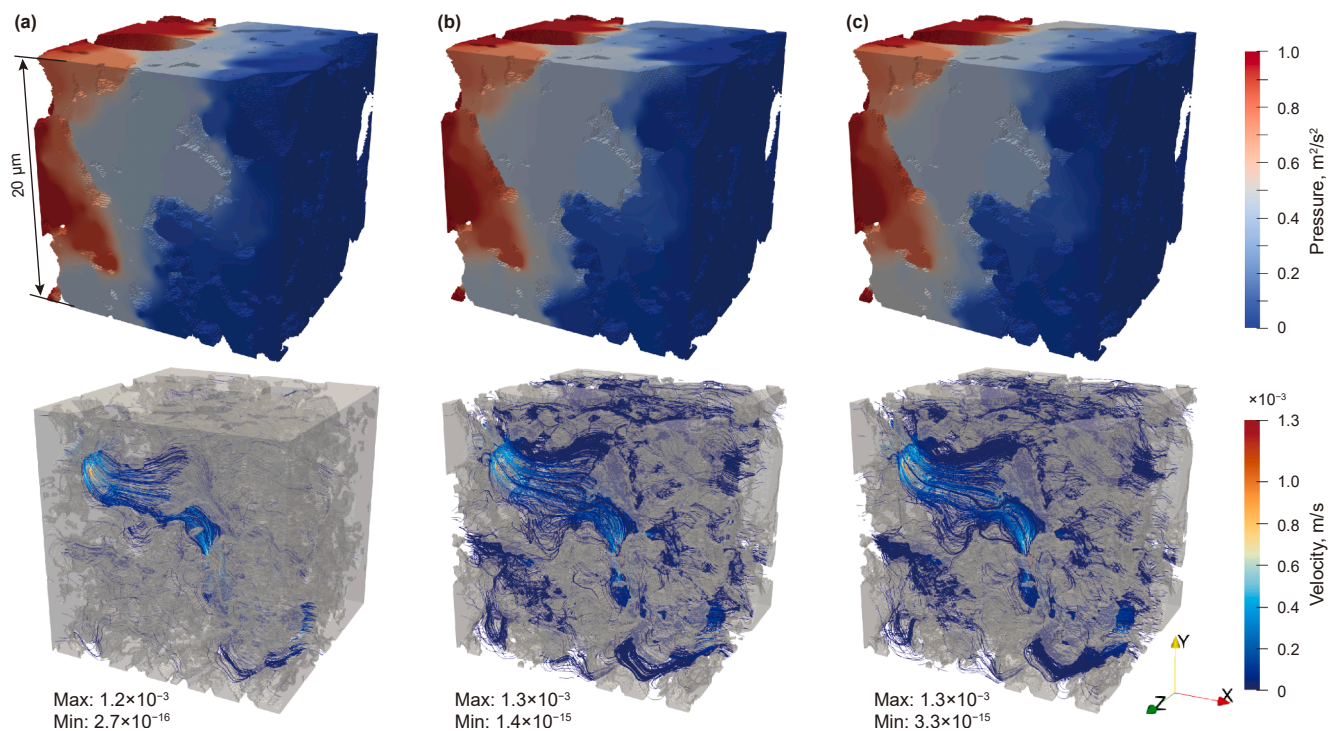


Fig. 5. The pressure distributions and flow streamlines for different scenarios: (a) pore-scale simulation only in resolved pores; (b) multiscale simulation without microscale effects ($R = 5$ nm); (c) multiscale simulation with microscale effects ($\epsilon = 0.15$, $\lambda = 100$ nm, $\alpha = 0.5$, and $R = 5$ nm).

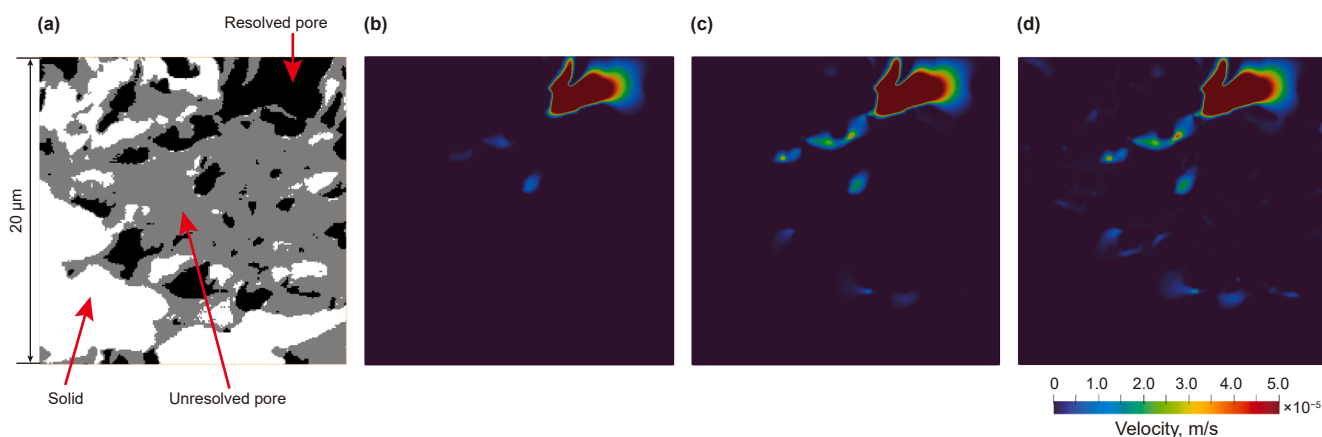


Fig. 6. The velocity distributions of y-z slice 110 along x direction: (a) segmented image slice corresponding to velocity distribution; (b) pore-scale simulation only in resolved pores; (c) multiscale simulation without microscale effects ($R = 5$ nm); (d) multiscale simulation with microscale effects ($\epsilon = 0.15$, $\lambda = 100$ nm, $\alpha = 0.5$, and $R = 5$ nm).

microeffect cases are redistributed. We can also observe that the velocities (minimum and maximum values) of the multiscale simulation are marginally larger than those of the pore-scale simulation. Fig. 6 shows the velocity-magnitude distribution of the y-z slice (No. 110 along the x direction). The higher velocity and more velocity distribution of base and microeffect cases are fairly intuitive compared to the pore-scale simulation. These visual observations further indicate that the unresolved pores can significantly improve the permeability through connecting isolated pores and new flow pathway formation. Despite the low permeability of microporosity, it substantially enhances the overall permeability.

Furthermore, when the microscale effects are included, the maximum improvement of the overall permeability can reach

133.60%, which suggests that the permeability is strongly underestimated by a huge percentage (more than double) due to neglecting the slip effect. On the other hand, the smallest permeability occurs in the case with $\epsilon = 0.05$, $\alpha = 1$, and $R = 5$ nm, which means that only the absorption effect is considered. This result is attributed to the fact that such pronounced intermolecular interactions suppress fluid motion near the wall. However, the minimum permeability (13.32% larger than that of the pore-scale case) of microscale effect cases is only slightly smaller than that of the base case, so that we can conclude that the adsorption effect in organic pores can be ignored when the pore radius exceeds 5 nm. More evidence will be provided in the subsequent analysis. To account for the uncertainty in microscale parameters, a systematic sensitivity analysis is conducted by varying key

parameters, such as average unresolved pore radius R , sub-resolution porosity ϕ , slip length λ , and TOC α , over physically meaningful ranges based on previous experimental and molecular simulation studies.

4.1.1. Impact of average unresolved pore radius

In order to investigate the effects of average unresolved pore radius R , the sub-resolution porosity $\varepsilon = 0.05$ and the slip length $\lambda = 100$ nm are kept constant during the simulations. The TOC α is set to 0, 0.5, and 1 to investigate the radius effects of purely inorganic, mixed, and purely organic porous media regions, respectively. The enhancement factor ξ , defined as the ratio of permeability with and without microscale effects, is used to measure the influence of microscale effects on flow capability, as detailed in Eqs. (21) and (22).

$$\xi_K = \frac{K}{K^*} \quad (21)$$

$$\xi_{K_{\text{micro}}} = \frac{K_{\text{micro}}}{K_{\text{micro}}^*} \quad (22)$$

where ξ_K and $\xi_{K_{\text{micro}}}$ represent the enhancement factor of the entire computational domain and microporosity, respectively. K (m^2) and K^* (m^2) are the permeability of the entire computational domain from the multiscale simulation with and without microscale effects, respectively. K_{micro} (m^2) and K_{micro}^* (m^2) are the permeabilities of the microporosity from the multiscale simulation with and without microscale effects, respectively.

As expected, the calculated permeabilities for all three α scenarios increase with increasing average unresolved pore radius R due to the decreasing flow resistance, as shown in Fig. 7(a). Even with extremely low permeability (K_{micro}), the multiscale permeability (K) remains at least 13.32% higher than the pore-scale simulation results (K_∞). This indicates that microporosity acts as a bridge connecting isolated resolved pores, significantly enhancing the overall flow capacity. The overall permeability remains slightly lower than that obtained without considering microscale effects at $\alpha = 1$, which indicates that the adsorption of shale oil in organic pores exerts a negligible effect on permeability. This is because the small slip length in organic pores leads to a balance between slip enhancement and resistance caused by the adsorption layer, as reflected by the trends of ξ_K and $\xi_{K_{\text{micro}}}$ for $\alpha = 1$ in Fig. 7(b). Zhang et al. (2017) have reported that adsorbed oil transport dominates the total apparent permeability only when

the pore radius is less than 2 nm. In this study, the scenario with a pore radius less than 5 nm was not considered, as the slip length significantly increases with decreasing pore radius.

Furthermore, the permeability difference under different α increases with R (Fig. 7(a)), suggesting that the influence of microscale effects becomes more significant at larger R , which is more clearly reflected by the increasing enhancement factor ξ_K with R (Fig. 7(b)). This trend is counterintuitive, as local microscale effects typically diminish in larger pores, as reflected by the decreasing $\xi_{K_{\text{micro}}}$ in Fig. 7(b). This observation is because the intrinsic permeability of microporosity is too low to contribute meaningfully to the overall flow, despite the strong enhancement of microscale effects at a small R . As R increases, the intrinsic permeability of microporosity rises. Consequently, the relatively weakened microscale effects act on a higher baseline permeability (K_{micro}), thereby making a greater absolute contribution to the overall flow, until the microscale effects eventually diminish at larger R . The impact of TOC α on permeability will be discussed in the following Section 4.1.4.

4.1.2. Impact of sub-resolution porosity

In this section, each simulation case is identified by the sub-resolution porosity ε varying from 0.05 to 0.15, while the other variables remain constant, i.e., $\alpha = 0.5$, $R = 5$ nm, and $\lambda = 100$ nm. It should be noted that $\varepsilon = 0.0001$ in microporosity means unresolved pore regions are recognized as solid, resulting in no flow in unresolved pores (pore-scale case mentioned above). Fig. 8 clearly

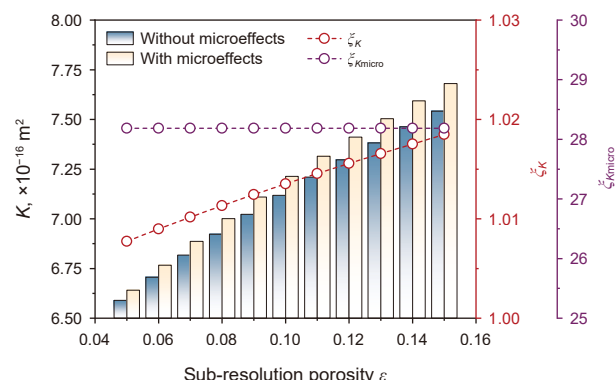


Fig. 8. The evolution of permeabilities and enhancement factors for different sub-resolution porosities.

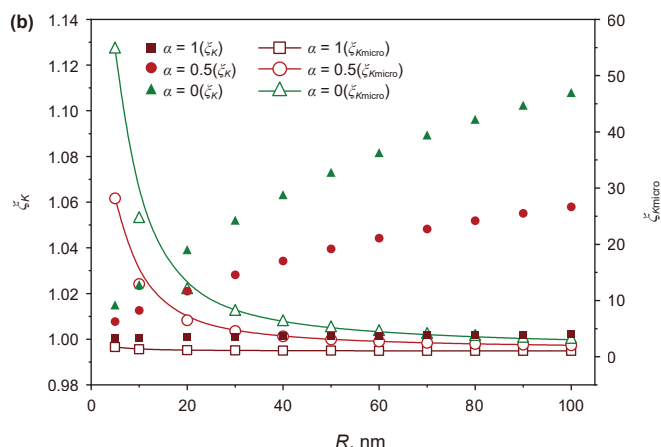
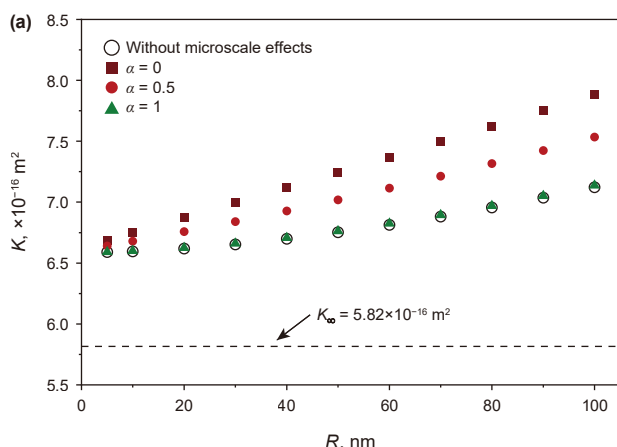


Fig. 7. The evolution of permeabilities and enhancement factors for different average radii R of unresolved pores: (a) permeability vs. R ; (b) enhancement factors vs. R .

shows that the overall permeabilities increase with sub-resolution porosity ε for both cases with and without microscale effects. Specifically, as ε increases from 0.05 to 0.15, K improves by 16% when microscale effects are considered, compared to a 14% increase when they are ignored. This improvement is attributed to that a higher porosity effectively enhances the permeability of microporosity, promoting overall multiscale flow.

Notably, a higher K can be observed when microscale effects are considered. The discrepancy between the two scenarios with and without microscale effects becomes apparent as ε increases, demonstrating that microscale effects exert a more pronounced influence on the multiscale flow capacity at higher sub-resolution porosity. The increasing enhancement factor ξ_K further indicates that conclusion, as shown in Fig. 8. Interestingly, the enhancement factor of microporosity $\xi_{K\text{micro}}$ remains constant at a high value of 28.19, suggesting that the influence of microscale effects on microporosity is independent of sub-resolution porosity. However, sub-resolution porosity can indirectly determine the contribution of microscale effects to the overall permeability through dictating how effectively microporosity connects resolved pores and participates in multiscale flow.

4.1.3. Impact of slip length

In this study, the slip effect is only considered in inorganic unresolved pore regions. Given that the slip length remains almost unchanged with the pore size as the pore radius is larger than 5 nm, we assume the slip length is a constant in each simulation. Fig. 9(a) shows the overall trend of permeability: The calculated permeabilities for $\varepsilon = 0.05$, 0.10, and 0.15 are all gradually increasing with the slip length varying from 0 to 150 nm with the fixed TOC (0.5) and average unresolved pore radius (5 nm). The fastest increase in permeability is identified as $\varepsilon = 0.15$, and $\varepsilon = 0.05$ is the slowest, which further indicates that the slip length has a stronger impact on the overall permeability with a higher sub-resolution porosity. In the scenario with $\alpha = 0.5$ and $\varepsilon = 0.15$, the permeability of the model with a 150 nm slip length involved is 4% higher than that without the slip effect and 35% higher than the permeability calculated from the pore-scale simulation. Moreover, we obtained an almost identical permeability to the base case ($R = 5$ nm and $\varepsilon = 0.05$) when the slip length is zero, redemonstrating that the influence of the near-wall fluid flow can be neglected when the unresolved pore radius exceeds 5 nm. The possible reason for this observation is that the difference in viscosity and density between the bulk and near-wall fluid is too slight to influence the total flow in the channel. And it is also

attributed to the thickness of the near-wall region and the adsorption layer.

4.1.4. Impact of TOC

Fig. 9(b) presents the variation of permeability with different TOC α at $\varepsilon = 0.05$, $\lambda = 150$ nm, and $R = 5$ nm. As α increases, the permeability decreases almost linearly from $6.73102 \times 10^{-16} \text{ m}^2$ to $6.58944 \times 10^{-16} \text{ m}^2$, slightly below the permeability of the base case ($6.58952 \times 10^{-16} \text{ m}^2$). While the absorption effect is less significant than the slip effect, the negative impact of the adsorption layer can still be observed at $\alpha = 1$. A TOC increase means that the amount of inorganic unresolved pores is reduced, resulting in the decline of the slip effect since it is only considered in inorganic pores. Thus, we can conclude that the decrease in permeability with α is mainly attributed to the slip effect.

4.2. Multiscale simulation in a multi-component image

In the current model, the unresolved pore region is treated as a homogeneous mixture of organic and inorganic matter. The sub-grid apparent permeability contributions of each component are weighted by TOC α , enabling multiscale single-phase flow simulation of shale oil under varying TOC conditions. However, this assumption does not fully reflect realistic conditions, as the spatial distribution of organic and inorganic matter can also significantly affect the overall permeability. According to the sub-grid model (Eq. (18)), the impact of organic and inorganic unresolved pores on permeability is opposite, which can alter the entire flow field of the computational model, resulting in different overall permeability. Thus, we redevelop the porous media model in the simpleDBSFoam solver to identify the different components and separately calculate the apparent permeability of organic and inorganic porous media regions. In this case, compared to the homogeneous mixture of microporosity (see Fig. 10(a)) employed in the previous sections, the computational model for the revised model includes four phases: resolved pore, organic microporosity, inorganic microporosity, and solid, as shown in Fig. 10(b). In the following sections, to further investigate the influence of microporosity and microscale effects on overall permeability, we carry out multiscale single-phase flow simulations on the new four-phase model (referred to as the 2-phase case), where the permeability for both organic and inorganic microporosity is explicitly calculated. Additionally, for comparison, we also conduct a series of simulations under the same situations using the same geometric model but with microporosity treated as a single phase

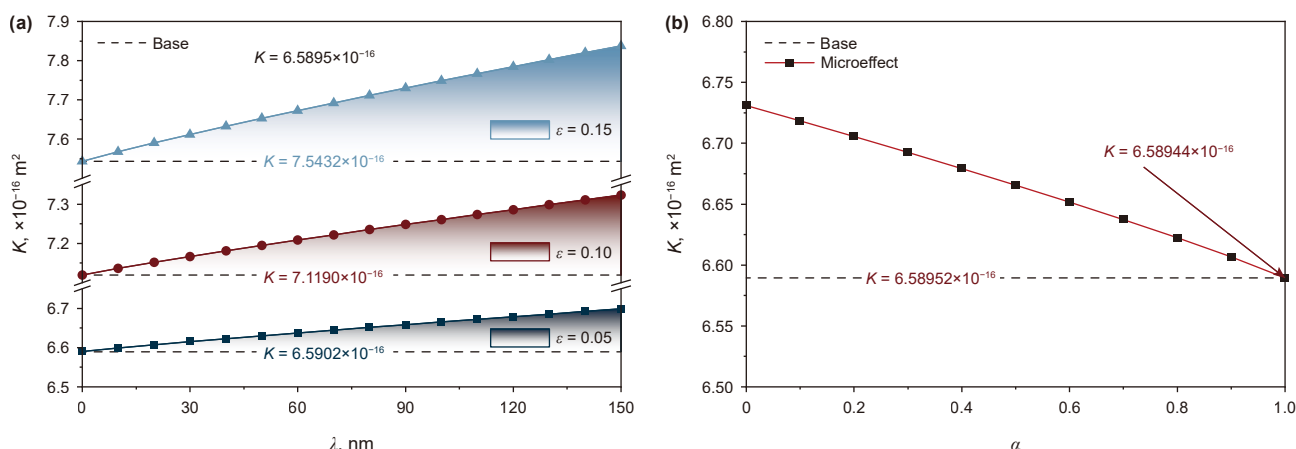


Fig. 9. Calculated permeabilities for different slip lengths and TOC: (a) permeability vs. slip length λ ; (b) permeability vs. TOC α .

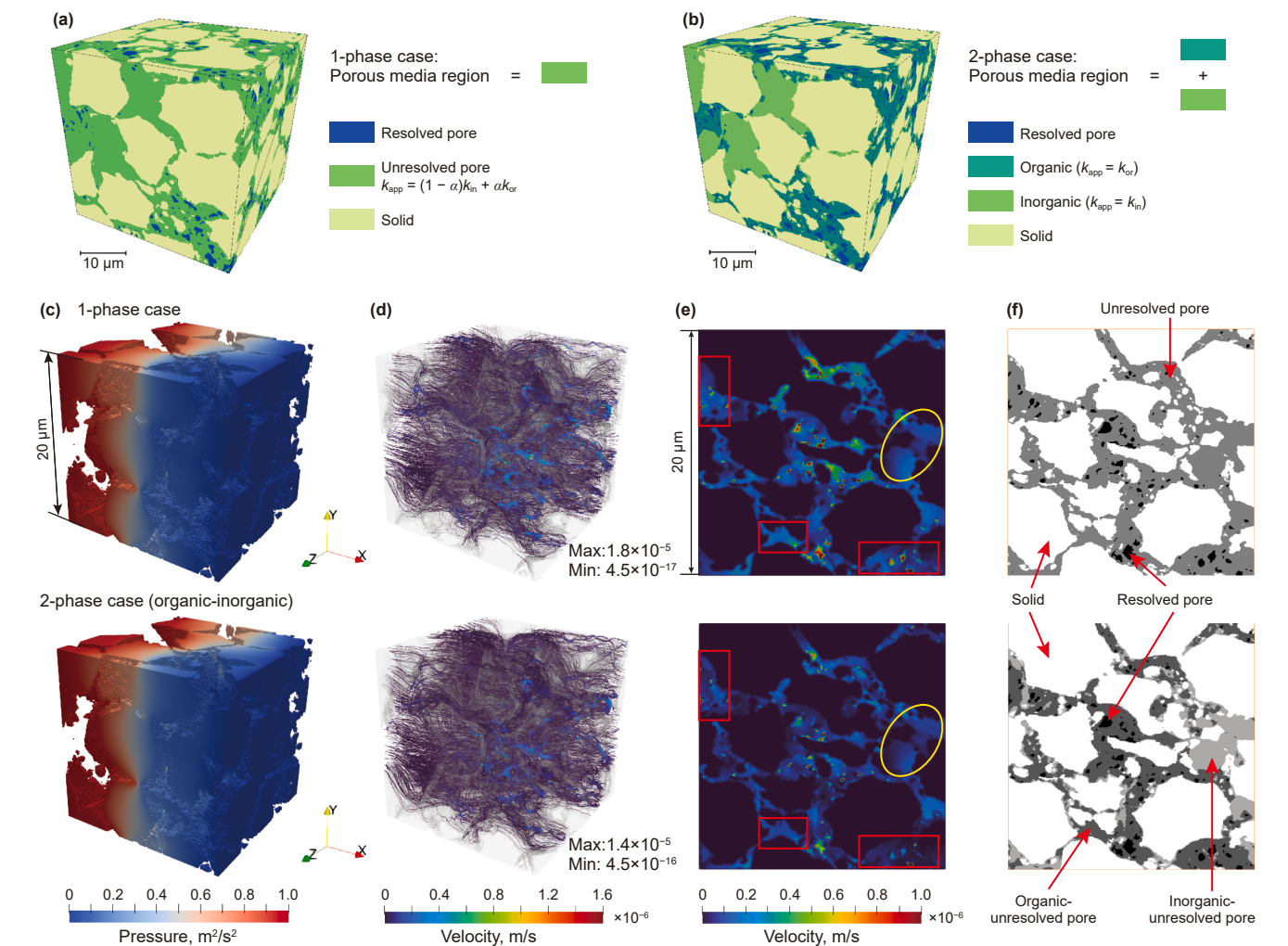


Fig. 10. 3D segmented image and simulation results at the case of $R = 100 \text{ nm}$, $\lambda = 100 \text{ nm}$, and $\varepsilon = 0.05$: (a) 3D segmented images with 1 phase in porous media region; (b) 3D segmented image with 2 phases in porous media region; (c) pressure distribution in resolved pores and microporosity; (d) streamlines; (e) velocity distribution of y–z slice 170 along x direction; (f) 2D segmented images corresponding to velocity distribution.

Table 3
Structure parameters and fluid properties used for multiscale simulation in the multi-component image.

	Model size	Component	Volume fraction	Simulation parameters
1-phase case	400 ³ voxels 100 nm/voxel	Resolved pores	0.03	$\alpha = 0.5476$, $R = 5\text{--}100 \text{ nm}$, $\varepsilon = 0.05$, $\lambda = 0\text{--}150 \text{ nm}$, $R = 5\text{--}100 \text{ nm}$, $\varepsilon = 0.05$, $\lambda = 0\text{--}150 \text{ nm}$.
		Unresolved pores	0.42	
		Solid	0.55	
2-phase case	400 ³ voxels 100 nm/voxel	Resolved pores	0.03	
		Unresolved pores	0.23	
		Organic	0.19	
		Inorganic	0.19	
		Solid	0.55	

combining organic and inorganic microporosity (1-phase case). In the 1-phase case, the TOC ($\alpha = 0.5476$) is calculated based on the volume of organic (0.23) and the total volume of microporosity (Table 3), ensuring TOC consistency with these two scenarios. The geometric models for the two scenarios are also extracted from the segmented Vaca Muerta FIB-SEM image, which has a size of 400³ voxels and a voxel size of 100 nm. And the detailed parameters for multiscale simulation are summarized in Table 3. Since the resolved pores are completely unconnected, we didn't perform the pore-scale simulation for comparison in this section.

In general, these two scenarios show absolutely different permeabilities under the same settings. The smallest permeability of the 1-phase and 2-phase cases is $3.19389 \times 10^{-20} \text{ m}^2$ and $3.07923 \times 10^{-20} \text{ m}^2$ ($\varepsilon = 0.05$, $R = 5 \text{ nm}$, and $\lambda = 0 \text{ nm}$), while the highest permeability is $6.42687 \times 10^{-17} \text{ m}^2$ and $3.06206 \times 10^{-17} \text{ m}^2$ ($\varepsilon = 0.5$, $R = 100 \text{ nm}$, and $\lambda = 150 \text{ nm}$), respectively. The difference in permeability between 1-phase and 2-phase cases is negligible when the slip effect is not considered. Otherwise, the permeability is overestimated by up to 109.89% ($\lambda = 100 \text{ nm}$) when the spatial distribution of organic and inorganic microporosity is

not taken into account. The observations are due to the fact that all microporosity can effectively connect the isolated resolved pores in the 1-phase case, even to the point of forming main flow pathways, given the stronger mobility compared to pure organic microporosity, especially when considering the slip effect. Although the impacts of the flow in near-wall and adsorption regions are relatively small compared to the slip effect, the permeability is also slightly overestimated by at least 3.72% in the 1-phase case.

Fig. 10(c)–(e) display the pressure distribution, flow streamlines, and velocity distribution at $\varepsilon = 0.05$ and $\lambda = 100$ nm, and $R = 100$ nm. It visually indicates that the higher flow capacity of shale oil occurs in the 1-phase case. The pressure distributions for the two cases show almost consistent results. From the flow streamlines (Fig. 10(d)), we can obviously observe that the shale oil indeed flows through the geometric model, even though the resolved pores are absolutely unconnected, thanks to the new pathways created by microporosity. The highest velocity still occurs in resolved pores (Fig. 10(e)), as expected (Soulaire et al., 2016). Simultaneously, it is particularly intuitive that the velocity in the 1-phase case is overall higher compared to the 2-phase case. Specifically, the maximum velocity of the 1-phase case exceeds that of the 2-phase case, while the minimum velocity is lower in the 1-phase case. The cross-sectional velocity distributions (Fig. 10(e) and (f), y - z slice at $x = 17$ μm) provide further evidence that the microporosity of the 1-phase case has a stronger flow capacity compared to the pure organic microporosity of the 2-phase case, as highlighted in the red box. Unlike the homogeneous microporosity in the 1-phase case, shale oil tends to flow through the inorganic microporosity, where the slip effect significantly enhances fluid mobility, resulting in a relatively lower resistance than the pure organic microporosity. In addition, we know that 54.76% of homogeneous microporosity is organic microporosity, so the flow ability of the pure inorganic microporosity should be stronger than that of homogeneous microporosity. However, we observed a counter-intuitive result that the velocity in homogeneous microporosity is slightly higher than in pure inorganic microporosity (highlighted in yellow circles in Fig. 10(e)). The possible reason is, as noted above, that the explicitly identified microporosity redistributes the entire flow field. Furthermore, the connectivity of organic microporosity is better than that of inorganic microporosity (Fig. 10(b)), making the organic microporosity the main flow pathway. We conclude that the distribution of inorganic and organic microporosity has a considerable impact on the single-phase flow of shale oil.

Moreover, we subsequently quantify the overall permeability of both scenarios across various average unresolved pore radii and slip lengths. The overall permeability K obtained from different models increases with the unresolved pore radius R , as shown in Fig. 11. Notably, the permeabilities of 1-phase and 2-phase cases consistently outperform those of the case without microscale effects. The permeability difference between 1-phase and 2-phase cases at an identical TOC α further highlights that the spatial distribution of organic and inorganic microporosity critically influences the multiscale flow of shale oil. Notably, the resolved pores in the model used in this section are entirely isolated. Thus, the baseline permeability without microporosity is zero ($K_\infty = 0$), and the overall multiscale flow is entirely governed by microporosity, making the influence of unresolved pore radius R and microscale effects on the overall permeability more pronounced.

Fig. 12(a) depicts the permeability under the conditions of $\varepsilon = 0.05$ and $\lambda = 100$ nm ($\alpha = 0.5476$ in the 1-phase case). For the 1-phase case, the permeability increases linearly with the average unresolved pore radius, which is in agreement with the sensitivity

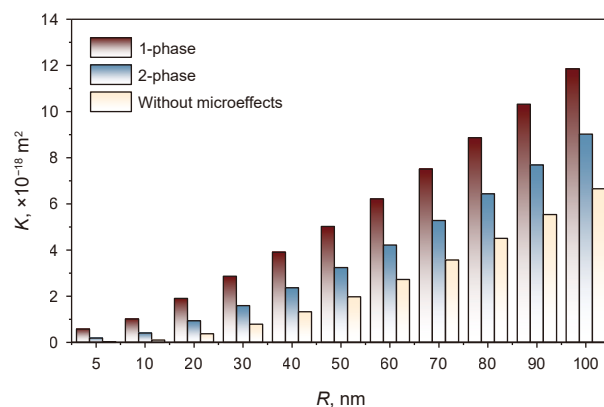


Fig. 11. The evolution of permeabilities for varying unresolved pore radius based on different models.

analysis above. However, the increasing trend of permeability in the 2-phase case accelerates with the average unresolved pore radius. We speculate that the negative impact of adsorption in organic microporosity is becoming weaker as the average unresolved pore radius increases. Additionally, organic microporosity is the primary flow pathway in the 2-phase case, finally leading to a faster rise in permeability across the average unresolved pore radius. The permeability is overestimated by up to 72.48% at a larger unresolved pore radius if the spatial distribution of inorganic and organic microporosity is ignored.

With a constant sub-resolution porosity ($\varepsilon = 0.05$) and average unresolved pore radius ($R = 5$ nm), we vary the slip length from 0 to 150 nm to figure out the impact of slip length when the organic and inorganic microporosities are separately considered, as shown in Fig. 12(b). The slip length has a common positive impact on the variation of the permeability for the 1-phase case: as the slip length increases, the permeability increases linearly in the 1-phase case. But for the 2-phase case, the permeability slowly grows until reaching a stable value, likely because of the well-connected inorganic microporosity. On the one hand, the increasing slip length definitely enhances the fluid mobility in pure inorganic microporosity, leading to slow increase of permeability. On the other hand, the contribution of pure inorganic microporosity to overall permeability is limited by its connectivity. Once the flow mobility of pure inorganic microporosity exceeds a critical threshold, further increase results in only marginal improvement, or even no further enhancement, in the overall permeability. Due to the different responses to the slip length, the permeability difference between the two scenarios reaches a maximum of 484.82% when the slip length varies from 0 to 150 nm. In the absence of slip effect, the permeabilities of these two scenarios are nearly identical. This can be attributed to the limited influence of adsorption layers and near-wall flow in this study. Consequently, the flow capabilities are comparable in both pure organic and inorganic microporosities, closely resembling that in the homogeneous microporosity in the 1-phase case.

Overall, the spatial distribution of organic and inorganic microporosities can significantly affect the permeability of the rock sample, especially when the two microporosities show extremely different flow mobility. In this study, the slip effect is only considered in organic microporosity, while the absorption layer and near-wall flow have a negligible influence due to the slight difference in viscosity and density. Consequently, the overall permeability of the sample can be overestimated by up to 484.82% at $\varepsilon = 0.05$, $R = 5$ nm, and $\lambda = 150$ nm.

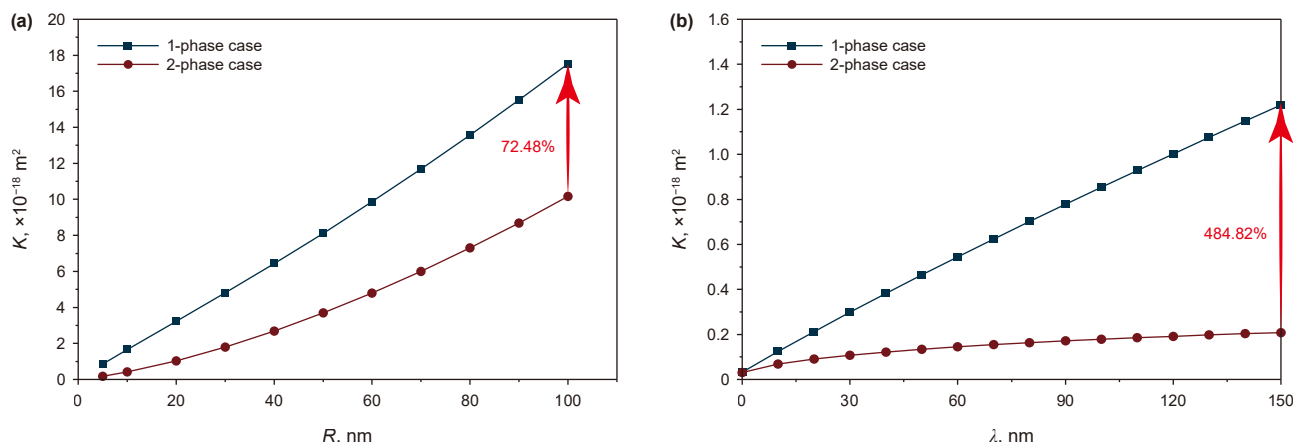


Fig. 12. Calculated permeabilities for different unresolved pore radius and slip length: (a) permeability vs. unresolved pore radius R ; (b) permeability vs. slip length λ .

4.3. Discussion

The findings and results in our work are not limited to the specific shale sample considered in this study but are broadly applicable to multiscale porous media systems with unresolved pore structures. The proposed nano-micro-continuum framework provides a general modeling approach to incorporate sub-resolution porosity and microscale effects. To the best of our knowledge, this is the first application of the micro-continuum approach to simulate liquid flow in a shale image with nanoporous microporosity and the first investigation of how microscale effects influence flow behavior across larger-scale porous media. The framework can also be extended to single-phase simulation in a fracture-matrix system, where the matrix (a kind of microporosity) properties can be obtained from a finer-scale micro-continuum simulation, i.e., what we did in this study, resulting in upscaling research integrating machine learning methods.

The results and sensitivity analysis provide general insights into how microporosity and microscale effects affect shale oil flow behavior in multiscale and multicomponent porous media. These insights are relevant not only for shale oil but also to other unconventional resources and porous materials with multiscale multicomponent heterogeneity and widely developed nanoscale pores.

Overall, this work contributes to a more general understanding of flow and transport in complex porous media and provides a basis for improving permeability prediction and multiscale modeling in a wide range of applications.

5. Conclusions

In this work, we presented a multiscale modeling framework to investigate the effects of microporosity and microscale effects on single-phase flow of shale oil using the micro-continuum approach. This framework was validated against the analytical solution of Brinkman equation based on a 2D channel coupling a free-flow region and porous media. Sensitivity analyses were performed to study the impact of unresolved pore radius, sub-resolution porosity, slip length, and total organic carbon on the overall permeability of the rock sample.

The visual and quantitative results further demonstrate that microporosity and microscale effects make a considerable contribution to the single-phase flow of shale oil. Despite microporosity having extremely low permeability, it can connect the resolved pores and even form the primary flow pathways when the

resolved pores are poorly connected. One notable finding is that the slip effect substantially enhances the overall permeability compared to the near-wall flow, which has a slight impact due to the large pore size and small difference in density and viscosity. The contribution of microscale effects to the overall permeability weakens as the sub-resolution porosity and unresolved pore radius increase. Additionally, the spatial distribution of organic and inorganic microporosities significantly affects the permeability of the rock sample, especially when the two microporosities show distinct flow mobility. The overall permeability can be overestimated by up to 484.82% at $\varepsilon = 0.05$, $R = 5$ nm, and $\lambda = 150$ nm in this study using homogeneous microporosity instead of separate organic and inorganic microporosities.

This framework can be adopted for multiscale modeling of liquid single-phase flow considering microscale effects, for both single homogeneous microporosity and multiple microporosities, which are explicitly segmented. It can also be extended to single-phase simulation in a fracture-matrix system, where the matrix (a kind of microporosity) properties can be obtained from a finer-scale micro-continuum simulation, i.e., what we did in this study, resulting in upscaling research integrating machine learning methods (Maes and Menke, 2024; Menke et al., 2021). Moreover, further improvements to this work include simulations with microscale effects in the entire computational domain, as the current model only accounts for microscale effects in microporosity, and the development of a sub-grid model for oil-water or oil-gas two-phase flow.

CRediT authorship contribution statement

Fu-Gui Liu: Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Resources, Methodology, Investigation, Formal analysis, Conceptualization. **Julien Maes:** Supervision, Software, Resources, Conceptualization. **Yong-Fei Yang:** Supervision, Resources, Project administration, Funding acquisition, Conceptualization. **Huai-Sen Song:** Writing – review & editing, Methodology, Formal analysis, Conceptualization. **Jun Yao:** Supervision, Resources, Project administration, Funding acquisition.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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