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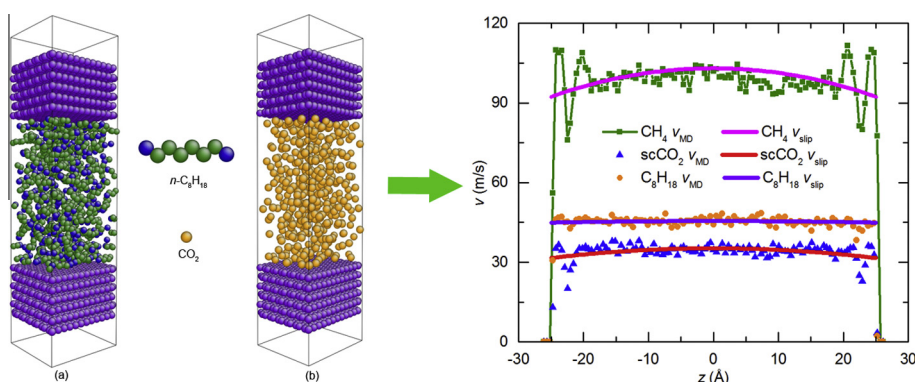
Fast mass transport of oil and supercritical carbon dioxide through organic nanopores in shale

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HIGHLIGHTS

- We studied oil and supercritical CO₂ flow through organic nanopores in shale.
- Velocity profile in an organic nanoslit deviates from parabolic to plugtype.
- Fluid flow exceeds the no-slip Poiseuille prediction by 1–3 orders of magnitude.
- We present two methods to correct liquid flow: slip length and apparent viscosity.
- Pore-scale models should differ oil flow in organic and inorganic pores.

GRAPHICAL ABSTRACT



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ABSTRACT

Hydrocarbon production from shale has grown dramatically in North America, and has the potential to do so globally. Nanoporous organic matter is probably the dominant mode of porosity occurrence in productive shale systems, but the physics of liquid transport through organic-hosted pores is still ambiguous. In the present work, molecular dynamics simulations were conducted to study the static properties and pressure-driven flow behavior of pure liquid hydrocarbons (octane) and supercritical carbon dioxide (scCO₂) confined in slit-shaped organic nanopores. Carbonaceous slits having apertures ranging from 1.5 to 11.2 nm were explored. A range of thermodynamic conditions, corresponding to the sedimentary reservoirs, were examined. Equilibrium molecular dynamics (EMD) enabled us to determine the density profile, from which we observed the layering structure of confined fluid and the preferential adsorption of scCO₂ relative to C₈H₁₈ and CH₄. As the pore size increases, the structure of the adsorbed phase transforms from a single-file chain to four and three dense monolayers for C₈H₁₈ and scCO₂, respectively. Then we calculated, using nonequilibrium molecular dynamics (NEMD), their velocity profiles and studied the hydrodynamics under a pressure gradient. We found that the velocity profiles in an organic slit tend to be pluglike, which deviates significantly from the parabolic profile in inorganic nanopores, and the flow exceeds predictions of the no-slip Poiseuille equation by 1–3 orders of magnitude. We proposed two models to characterize the flow behavior, each of which can be integrated into a bottom-up framework to mimic fluid transport in shale and estimate the apparent liquid permeability. The parameters in our models, slip length and apparent viscosity, are exponentially dependent on driving force, pore size, and temperature. Our results, which highlight the need for taking into account the different nature of organic matter and inorganic minerals in flow modeling, will shed light on the development of shale resources and, more generally, mass transfer in nanoporous materials.

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1. Introduction

With the advancement of less expensive fracking technology and large-scale industrial applications, both the extent of technically recoverable reserves and the production rate of hydrocarbons from shale have dramatically increased [1]. The proportion of U.S. shale gas production, which surged from 2% of its total gas production in 2000 to approximately 40% in 2013, has outweighed the share of other natural gas resources [2]. Most recently, we have witnessed a shale oil boom [3]: every day 3.22 million barrels of oil is being extracted from tight shale formations in the United States, representing 41% of its gross oil production [4]. The great success of exploiting oil and gas from fine-grained shale exhibits enormous potential to alleviate the impending energy crisis, leading to a worldwide “shale revolution” [5]. However, owing to the abundant presence of nanopores, developing greater knowledge of liquid transport through the shale matrix is essential. Understanding fluid flow mechanisms in shale nanopores is crucial because this fundamental information is the cornerstone of the mathematical models at both the core and the field scale, which play a significant role in numerical simulation, rate analysis, and production optimization. A new research frontier, therefore, has emerged: How do liquids transport through nanoporous geomaterials such as oil-rich shale kerogen [6]?

Recent experimental studies using scanning electron microscopy (SEM), low-pressure gas adsorption, and mercury intrusion capillary pressure (MICP) suggest that the size of pores in a shale matrix ranges from a few micrometers down to the scale of nanometers (~ 2 nm) [7,8]. Fig. 1 presents an SEM image of an Eagle Ford Shale sample. The darkest spots in the black areas correspond to the nanopores located within organic matter (OM). Although numerous studies have been conducted to address gas transport through tight porous media [9–12], only a few studies deal with mass transfer of liquids in shale nanopores. Wu et al. [13] proposed a lab-on-a-chip approach by combining an epi-fluorescence microscopy technique with fabricated nanofluidic chips to directly visualize single- and two-phase flow in nanochannels. They reported that water flow through 100-nm-depth slits fabricated from silicon wafers fits closely into the Poiseuille equation. Dehghanpour and his coworkers [14,15] measured the spontaneous imbibition rates of oil and water into the crushed packs and intact samples of shales and suggested that the connected pore network of an intact shale is hydrophilic, whereas the poorly connected pores are hydrophobic. Using an atomic force microscope (AFM), Javadpour et al. [16] developed a method to determine the slip length (250 nm) of brine flowing over shale organic surfaces and evaluated the apparent permeability. These contributions, although remarkable, may be insufficient to provide a whole view of the physics of liquid flow in shale nanopores because several factors, e.g., materials, surface roughness, and experimental temperature, affect flow measurements. Molecular dynamics (MD) serves as an efficient tool to mimic the dynamic evolution of a system at the conditions hardly accessible in experiments. In this work, we present a detailed molecular study of oil flow through shale organic nanopores. As one of the specialties and major components of shale nanoscale transport systems, the nanopores within organic-hosted porosity are crucial in the determination of fluid accumulation as well as pore network conductivity [7].

A multilayer graphene slab has been extensively used to represent OM substrate in shale [17–19]. On the basis of this model, Ambrose et al. [17] explored the density distributions of CH_4 confined in shale organic pores. Later, Mosher et al. [18] used an asymptotic model to estimate the CH_4 adsorption isotherms across a wide range of pore sizes. Most recently, Wang et al. [19] extended this model to study oil adsorption in shale nanopores and examined its effect on the estimation of recoverable oil in place. To

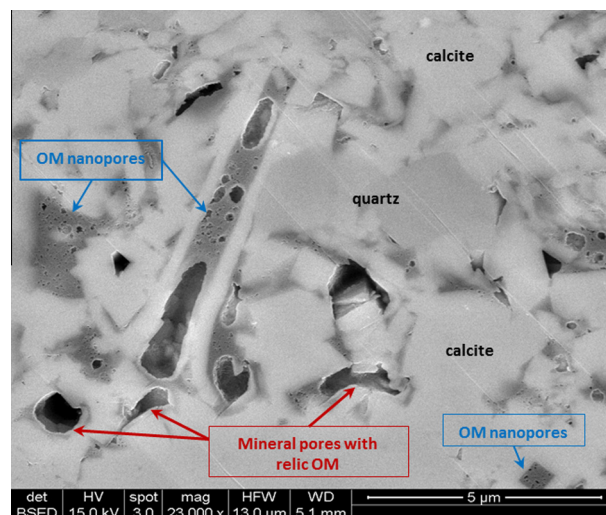


Fig. 1. SEM image of an Eagle Ford Shale sample showing nanopores in OM and interparticle pores in inorganic matter (IM) composed of quartz and calcite. The black areas correspond to OM, in which the darkest spots represent pores.

get a thorough understanding of the graphene–alkane system, prior to our MD simulations, we briefly review the works focusing on the dynamic behavior of this system.

A few studies dealing with the adsorption and static properties of confined hydrocarbon liquid films have been reported [20–23]; however, there is only limited research on the mass transfer of alkanes inside the carbonaceous substrate, in spite of its immediate relevance to applications. The MD simulations conducted by Supple and Quirke [24] show a rapid decane imbibition (≤ 445 m/s) along the inner surface of a (13, 13) carbon nanotube (CNT) at 298 K, and the penetration length is linearly dependent on time. They attributed the discrepancy from the Washburn equation to the nanosecond time scale of the filling process and the ultrasmoothness of graphitic surfaces [25]. Majumder et al. [26] measured the flow of several liquids through a freshly fabricated membrane constituted by 7-nm aligned multiwalled CNTs. They reported that the flux is 4–5 orders of magnitude greater than that predicted from the conventional Poiseuille equation. In particular, the enhancement factor, E , defined as the ratio of the actual flux to the no-slip Poiseuille prediction, is $\sim 1 \times 10^4$, $\sim 4 \times 10^3$, and $\sim 3.2 \times 10^4$ for hexane, decane, and ethanol, respectively. Whitby et al. [27] performed an experimental study on amorphous carbon nanopipes having large inner diameters (~ 44 nm) and found an enhancement of ~ 45 times for decane. In order to demonstrate that the molecular origin of fast liquid transport through CNTs correlates with their perfectly ordered structure and frictionless surface instead of the depletion length or wettability, Falk et al. [28], using MD simulations, calculated the friction coefficients for liquid flow in graphitic nanopores of various sizes and geometries at 300 K, 0.1 MPa. They reported an enhanced transport of 10– 10^3 times above continuum hydrodynamics coupled with the no-slip boundary condition (BC). They also found that the friction coefficient is primarily determined by the wall curvature and interfacial structure; for decane confined within a graphene slab, the friction is insensitive to the aperture, whereas if the slab size is smaller than 3 nm, the confinement effect will become prominent. The main results of these works are summarized in Table 1.

These findings, although fundamentally important to broaden our knowledge of liquid alkane flow through carbonaceous materials, have two key deficiencies: (1) all of the above studies were conducted at standard ambient temperature and pressure, which cannot represent the conditions in a realistic shale; and (2) there

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