Full Length Article

Liquid permeability of organic nanopores in shale: Calculation and analysis

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HIGHLIGHTS

- Liquid permeability of organic nanopores is studied by mathematical modelling.
- The effects of boundary slip and physical adsorption are incorporated and discussed.
- The shape of velocity profile is studied quantitatively and related to slip factor.

GRAPHICAL ABSTRACT
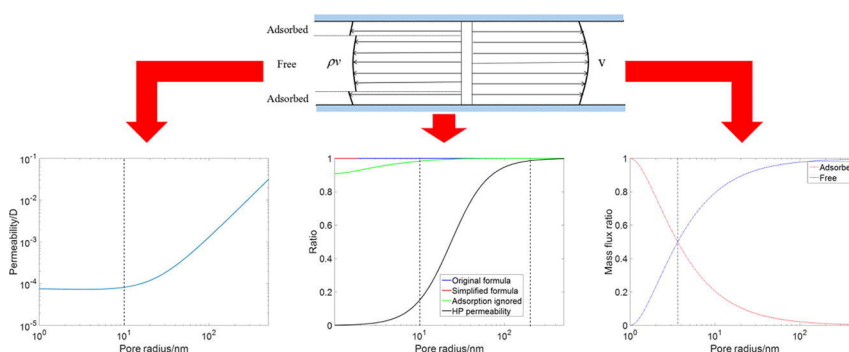
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ABSTRACT

The contribution of kerogen to oil flow in shale rock is not well understood but is crucial, and understanding the transport behaviors of oil through organic nanopores is important for shale oil reservoir development. Based on relevant MDS (molecular dynamics simulations), experimental and theoretical studies, a mathematical model was derived to calculate the liquid permeability of organic nanopores in shale. The model can incorporate the mechanisms of boundary slip and physical adsorption, and the complicated structural properties are included. The results show the following: (a) Flow enhancement or permeability is linearly related to the pore length. (b) For pore radii under 10 nm, the permeability changes slightly. The corresponding equivalent pore radius is 24 nm. (c) There is no need to consider the threshold pressure gradient or nonlinear flow characteristics for oil flow in kerogen. (d) For pore radii greater than 200 nm, slip is negligible. (e) Physical adsorption cannot obviously influence the permeability of the organic nanopores. (f) For pores larger than 500 nm, the mass flux of the physically adsorbed oil is negligible. By the definition of the normalized velocity, the shape of the velocity profile is studied quantitatively to show the dominance of a plug type velocity profile. The relationship between the slip factor and normalized velocity is also derived. As the normalized velocity approaches 1, the slip factor increases rapidly to infinity. This work can help in the understanding of the flow properties of kerogen and will shed light on the development of shale resources.

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Nomenclature

CNT	carbon nanotube(s)	W_A	adhesion work
MDS	molecular dynamics simulation(s)	τ	tortuosity
SEM	scanning electron microscope	λ_{eq}	the equivalent flow enhancement
TOC	total organic carbon	ρ_{ads}	density of the physically adsorbed oil
HP	Hagen-Poiseuille	ρ_{bulk}	density of the free oil
R^2	correlation coefficient	Q_{ads}	volume flux of the physically adsorbed oil
L	pore length/CNT thickness	Q_{bulk}	volume flux of the free oil
μ	viscosity	h	thickness of the adsorption region
C	slip velocity coefficient	M_{HP}	mass flux without slip and adsorption
R	pore radius	M	mass flux considering slip and adsorption
Δp	pressure difference	λ	flow enhancement
r	radial distance from the pore center	λ_C	slip factor
v_{HP}	velocity profile with the non-slip boundary condition	λ_{ads}	adsorption factor
v	velocity profile with the slip boundary condition	k_{tube}	permeability of a single tube
v_{slip}	slip velocity at the solid-liquid interface	R_{eq}	equivalent pore radius
v_r	normalized velocity		
D_s	surface diffusion		

1. Introduction

With the depletion of conventional resources, the efficient development of unconventional resources, such as shale oil reservoirs, has become a hot topic [1]. Shale oil reserves are abundant worldwide, and the US has seen a shale oil boom in recent years, attracting the attention of the whole world. However, owing to the extreme low permeability and poor connectivity in shale, a deeper understanding of the flow mechanisms in shale oil reservoirs is urgent and necessary for its efficient exploration and development. Rich organic matter [2] and nanoporosity are the main characteristics that distinguish shale oil reservoirs from other resources. However, only limited mature studies [3,4] have focused on kerogen, and up to now, the oil flow mechanism in nanoporous kerogen has remained a mystery.

It is experimentally difficult to isolate kerogen particles from shale samples [5,6], and knowledge about the characteristics of organic nanopores in shale oil rocks is still very limited. Thus, MDS might be the powerful tool needed for preliminary studies. For simplicity, kerogen is usually represented as graphene in the shale gas [7–9] or shale oil [10–12] studies. Wang et al. employed MDS to explore the multilayer adsorption behaviors [10,11] and flow behaviors [12] of oil in kerogen in underground conditions. Their results show that the velocity profile in nanoporous kerogen is pluglike, significantly different from inorganic pores [13]. The flow enhancement [14], which is the ratio of the actual flow rate to non-slip HP flow, was calculated to be 1–3 orders of magnitude. To characterize the flow behaviors, they employed slip length [14] and apparent viscosity [15] models. Empirical correlations were ultimately proposed. However, in the widely used ideal graphite pore model, structural properties such as mixed wettability [16], surface roughness [17–23], tortuous paths, and material disorder, are usually not considered, and ignoring these properties might lead to significant deviations from properties of the actual kerogen body [24]. On the other hand, MDS might not quantitatively describe the interfacial dynamics well [25], and it can be time consuming for calculations. Moreover, empirical correlations can hardly reflect internal flow mechanisms. Still, the shape of the velocity profile has not been studied quantitatively, and whether or not the velocity profile is always plug type remains to be answered. At last, the concepts of slip length and apparent viscosity are not the most appropriate for characterization.

In fact, the intrinsic viscosity of bulk liquid at the nanoscale is the same as that of a macroscale liquid, and employing the apparent viscosity model cannot reflect the actual velocity profile. Moreover, there is no satisfactory theoretical expression for the apparent viscosity. On the other hand, the slip length, an extrapolated length at which the tangential component of the velocity vector vanishes, appears physically unrealistic when it exceeds the dimension of the fluid [26].

Instead, flow enhancement resulting from boundary slip [27–32] in CNT is mostly employed to account for the deviation from non-slip HP flow. Both the hydrophobicity of the liquid [33] and wettability of the substrate [34] deeply influence the liquid flow at the nanoscale. This should be distinguished from the wettability dominated two-phase flow in microscale hydrodynamics or conventional reservoirs. Mattia and Calabro [35] derived an expression for the slip velocity of water flow in CNT. Based on this expression, a theoretical formula describing flow enhancement was achieved. The formula can incorporate the effects of solid-liquid interactions via surface diffusion [36–38] and the work of adhesion, as well as the geometric characteristics of the tubes. The effects of surface roughness and mixed wettability on the flow are included in the flow enhancement model [39], superior to the MDS method. However, fitness of the flow enhancement model to the experimental data is not very good, possibly resulting from the hydrogen bonding network between water molecules coupled with the surface roughness [22,38,40–43]. Ritos et al. [44] employed MDS to verify the application of Mattia's model to water flow in nanotubes of different materials. Mattia et al. [39] simplified his model and formulated the CNT permeability as a function of its solid-liquid molecular interactions. However, water is the most widely used in CNT studies [22,30,45–48], and until now, no study has validated the application of Mattia's model to oil flow in CNT.

Moreover, Mattia's model did not incorporate adsorption. It has been documented that the adsorption of polar components on mineral surfaces in reservoirs is irreversible [49]; thus, polar components can be regarded as rock matrix [50,51]. For simplicity, only physical adsorption induced by van der Waals [52] is considered here. In CNT studies, the contribution of physical adsorption [53] is negligible compared to boundary slip. Despite that, occurrence state of crude oil is of concern in petroleum reservoirs. The adsorption region is defined as the section in which its local density value deviates from that of the bulk [54–56]. Riewchotisakul and Akkutlu [57] developed a model of permeability for gas flow in the organic