



Full Length Article

A molecular dynamics explanation for fast imbibition of oil in organic tight rocks

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ABSTRACT

Recent imbibition experiments show that the oil uptake of organic-rich tight rocks is significantly higher than their water uptake. The ratio, m , between oil and water imbibition rate from these experiments, m_{exp} , is significantly higher than that predicted by classical imbibition models which are based on Young-Laplace equation such as Handy model, m_{HD} ; i.e. $m_{exp} > m_{HD}$. We hypothesize that this discrepancy is due to fast imbibition of oil into organic nanopores of these tight rocks that are visualized by scanning electron microscope (SEM) images. We test this hypothesis by simulating the dynamics of octane and water molecules imbibition into graphite and quartz slits with the width, w , of 1, 1.5, and 2 nm. For quartz slits, the simulated ratio m_{sim-Q} is fairly close to m_{HD} . However, in graphite slits, $m_{sim-G} > m_{HD}$ and this observation is consistent with the results of the imbibition experiments on organic-rich tight rocks: $m_{exp} > m_{HD}$. The comparative analyses of simulated relative density profiles and calculated intermolecular potentials of octane and water in graphite and quartz slits indicate that this behavior is primarily due to the strong intermolecular interactions of octane and graphite at the nanopore wall compared with that of water molecules. These results are in favor of the proposed hypothesis and suggest that organic nanopores constitute a large fraction of the pore volume of the target tight rocks.

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1. Introduction

The soaring global demand for petroleum energy resources coupled with the quick depletion of conventional reservoirs have motivated the oil industry to shift the focus toward unconventional tight and shale reservoirs. It is challenging to understand and model the transport phenomena in micro- and nano-scale pores of organic-rich tight rocks due to their complex wettability and high values of surface to volume ratio. In particular, characterizing wettability of the pore system in tight rocks is significant for (a) selecting appropriate relative permeability and capillary pressure models, (b) investigating residual phase saturation and pore-scale distribution of the remaining oil, and (c) estimating the hydrocarbon reserve [2–4].

Recent oil and water imbibition experiments on organic-rich tight rocks and shales [3–5] suggest that the imbibed volume of oil is more than that of water, and this observation cannot be explained by classical imbibition models, such as Handy model, which are based on Young-Laplace equation: $P_c = \frac{2\sigma \cos \theta}{r}$. Based on

Handy model [6], $M = \sqrt{\frac{2S^2 \cos^2 \theta K \rho^2 S_{wf} P_c}{\mu}} t$, Habibi et al. [4] and Lan et al. [5] calculated the ratio between oil and water imbibition rate:

$$m_{HD} = \frac{\sqrt{\frac{2S^2 \cos^2 \theta K \rho^2 S_{wf} P_c}{H_0}}}{\sqrt{\frac{2S^2 \cos^2 \theta K_w \rho_w^2 S_{wf} P_{cw}}{H_w}}}$$

They compared m obtained from imbibition experiments (m_{exp}) with that predicted by Handy model (m_{HD}), and showed that $0.6 < m_{exp} < 2.5$ while $0.43 < m_{HD} < 0.55$. In general, their results show that $m_{exp} > m_{HD}$. The target tight rocks consist of nanoscale to microscale pores [3–5]. The imbibition experiments were aimed at describing the fluid flow in these nanoscale to microscale pores and throats. According to the pore-throat size distribution curves [3–5], the pore system of the target tight rock samples can be divided into nanoscale and microscale pores. Based on previous studies [1,7], the capillary flow in microscale pores can be explained by classical imbibition models. Therefore, the observed discrepancy between the experimental results [3–5] and the predictions of the classical imbibition models may be due to the flow behavior in organic nanopores.

The abundance of nanopores with the throat size in the order of the fluid molecular size invalidate the continuum approximation [7,8] which is the basis of Young-Laplace equation. As a result,

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Nomenclature

P_c	capillary pressure
K	permeability of core plug
M	imbibed mass
S_A	cross-section area of the core plug
S_{wf}	imbibition front saturation
t	imbibition time
ρ	density of the fluid
θ	contact angle
μ	viscosity
σ	surface tension
Φ	plug porosity

<i>Subscripts</i>	
exp	imbibition experiments
sim	MD simulation
HD	Handy model
o	octane
w	water
G	graphite
Q	quartz
vdw	van der Waals
el	electrostatic
ads	adsorbed layers

classical imbibition models fail to fully predict the fluid imbibition in tight rocks. Recent studies [9–48] using molecular dynamic (MD) simulation have made considerable progress in characterizing fluid flow at nanoscale. Based on previous studies [13–17], there is a significant difference between the filling rate of oil and water in carbon nanotubes. Supple and Quirke [13–15] presented MD simulations to investigate the imbibition of decane inside and outside of carbon nanotubes. They showed that the filling rates of decane in 0.584 nm and 1.398 nm diameter carbon nanotubes are 799 m/s and 155 m/s, respectively. Qin et al. [16] developed water filling MD simulations in carbon nanotubes and measured the filling rate of water using field effect transistors. Their results showed that the filling rate of water molecules in 0.81–1.59 nm diameter carbon nanotubes is less than 10^{-3} m/s. Evidently, both measured and modeled imbibition results report significantly higher filling rate of oil compared with that of water in carbon nanotubes. In this paper, we hypothesize that fast imbibition of oil into organic-rich tight rocks is due to fast imbibition of oil into nanoscale organic pores of such rocks.

We performed MD simulations to compare water and octane imbibition into graphite and quartz slits representing nanoscale pores identified by mercury injection capillary pressure (MICP) data and observed in high-resolution SEM images of the target tight rocks [3,5]. The rest of this paper is composed of the following sections. In Section 2, organic and inorganic slit-like pores are represented by graphite and quartz slits, respectively, based on previous results of focused ion-beam/scanning electron microscope (FIB/SEM) images and MICP data of the target tight rocks [3,5]. In Section 3, we compare the simulated rate of octane and water imbibition in quartz and graphite slits. We compare the ratio of octane to water imbibition rate predicted by MD simulations (m_{sim}) and Handy model (m_{HD}). Similarly, we compare such ratio calculated by the measured data of oil and water imbibition in organic-rich tight rocks (m_{exp}) [4,5] and Handy model. In addition, we compare the relative density profiles of octane and water in graphite and quartz slits. In Section 4, we calculate the ratio of octane to water pressure gradient in graphite and quartz slits calculated by the average relative density results. In addition, we compare this ratio with that predicted by Handy model. Finally, we compare the difference between fluid/wall and fluid/fluid intermolecular potentials of octane and water in graphite and quartz slits.

2. Methodology

2.1. Slit structure and model unit

We build MD models to compare oil and water imbibition in quartz and graphite slits, representing inorganic and organic pores of tight rocks, respectively. Fig. 1 shows the FIB/SEM images [3,5]

of the target samples. We observe the existence of (a) inorganic materials, such as quartz and clay particles, (b) organic materials, such as pyrobitumen, and (c) organic and inorganic pores of different shapes, such as slit-like pores. Based on the XRD (X-ray diffraction) results of the target samples [5], more than 50 wt.% of the total minerals is quartz. Thus, quartz slit is selected to represent inorganic pores in our simulations. Graphite slit is selected as the simplest representative of organic pores. Fig. 2 shows pore-throat size distribution (PSD) curves of the target tight rocks [4,5]. In general, the pore-throats are smaller than 10 nm. Also the PSD curves show that 40–60% of the pores have throats smaller than 2 nm, and cannot be accessed by mercury even at high pressures. The analysis of SEM images and thin sections of the rock samples suggests that such small nanopores are primarily within or coated by degraded bitumen [5]. In this paper, we analyze water and oil imbibition into pores smaller than 2 nm.

We select two parallel graphite substrates to represent the organic slit based on previous reports [10–12]. Fig. 3a and b shows the model of graphite slit. Each substrate consists of three parallel sheets of graphene. The distance between the two sheets is 0.335 nm. The thickness of one single graphite substrate is 0.67 nm. The most stable polymorph of silica at ambient conditions, α -quartz [44–46], is selected as the inorganic slit. Since sedimentary formations are initially water saturated, we build the quartz surface according to previous reports [44–47] by cleaving the α -quartz at (1 0 0) surface and adding hydroxyl groups to incomplete silicon dangling bonds. This quartz surface has been obtained from previous XRD measurements [49]. The surface density of silanol group in α -quartz is 7.55 sites/nm², which is consistent with the calculation of crystal chemistry (5.9–18.8 sites/nm²) [49]. Fig. 3c and d shows the model of quartz slit. The thickness of the single-layer quartz substrate is 2.5 nm. The length of –OH bond is initially set to 0.1 nm.

We build MD models for octane and water molecules imbibition in graphite and quartz slits to simulate the oil and water imbibition into organic and inorganic nanopores, respectively. Fig. 4 shows the model, which consists of a fluid reservoir and a slit pore. The size of the model is $5 \times 50 \times 100$ nm. The size of the fluid reservoir is $5 \times 50 \times 50$ nm, and the length of the slit pore is 30 nm. The reservoir is initially filled with octane or water molecules with bulk densities of 0.8 g/cm³ and 0.987 g/cm³, respectively. The distance between two substrates is the slit width, w . The periodic condition is applied at the boundaries of the model in all directions (the system unit repeats in all directions).

2.2. Governing equations

The total energy of a system containing fluid molecules and slit atoms consists of the intramolecular and intermolecular energy. The intramolecular energy describes the energy of connected

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