Contribution ID: **167**

Type: **Poster Presentation**

Molecular investigation on sorption-induced kerogen deformation and its impact on gas transport

Monday, 30 May 2022 09:40 (1h 10m)

Shale gas is becoming an increasingly important source in the global energy sector. The shale reservoir is characterized by the small porosity and ultra-low permeability, and the shale gas production decays rapidly with time. In the process of gas production, shale is expected to deform in response to gas adsorption and desorption, similar to many other nanoporous materials. Despite the potential effects on gas permeability and transport, the sorption-induced deformation remains poorly understood and is often overlooked in large-scale simulations.

In this study, we first use a hybrid Monte Carlo and molecular dynamics method to investigate methane adsorption and desorption in a flexible kerogen matrix (i.e., shale's primary organic matter). The volume of the simulation box is monitored during the process, and the volumetric strain is calculated at each pressure. Using a surface energy approach, a non-linear adsorption-strain model is derived to describe the relationship between the methane adsorption amount and the volumetric strain by taking the methane adsorption and deformation coupling into consideration. Furthermore, methane flow is simulated by non-equilibrium molecular dynamics in both rigid and flexible kerogen slit pores with sizes ranging from 10 to 40 Å. The total gas flux and the apparent gas permeability are calculated and analyzed separately as a function of pore pressure. In addition, a diffusive-viscous gas flow model is proposed by coupling the adsorption-strain relationship to provide predictions for gas flux in realistic kerogen nanopores.

It is found that methane adsorption can induce a swelling volumetric strain up to 5.1% in the kerogen matrix, which narrows the 10 Å slit pore by 30% under the constant volume condition. The sorption-induced swelling dominates over the mechanical compression within 50 MPa. The decrease of the main flow path significantly reduces viscous gas flux in the confined environment. Compared with the rigid structure, the flexible kerogen slit pore results in less mass flux under the same pressure. This discrepancy is insignificant at low pressure but becomes more pronounced when pore pressure is high. For example, the relative reduction of mass flux under 50 MPa of gas pressure is 23%, 29%, 40%, 49%, and 64% for slit pores of size 40 Å, 30 Å, 20 Å, 15 Å, and 10 Å, respectively. Similar trends are also observed for the apparent gas permeability calculated from the total mass flux using Darcy's law. Moreover, the permeability ratio between the rigid and flexible slit pores declines hyperbolically with the increasing pore size and gradually approaches unity.

Acceptance of the Terms & Conditions

Click here to agree

MDPI Energies Student Poster Award

Yes, I would like to submit this presentation into the student poster award.

Country

Australia

References

Time Block Preference

Time Block A (09:00-12:00 CET)

Participation

Unsure

Primary author: Mr WU, Jian (The University of Sydney)

Co-authors: Dr HUANG, Pengyu (The University of Sydney); Prof. SHEN, Luming (The University of Sydney)

Presenter: Mr WU, Jian (The University of Sydney)

Session Classification: Poster

Track Classification: (MS13) Fluids in Nanoporous Media