## An Evaluation of CO2 Sequestration in Organic-Rich Shales Using COMSOL Multiphysics®

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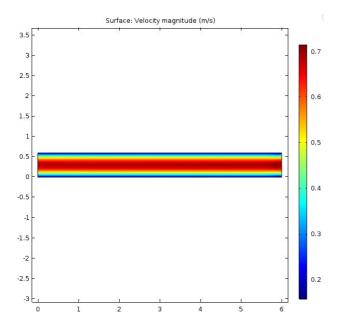
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## **Abstract**

Organic-rich shale resources remain an important source of hydrocarbons considering their substantial contribution to crude oil and natural gas production around the world. Moreover, as part of mitigating the greenhouse gas effects due to the emissions of carbon dioxide (CO2) gas, organic-rich shales are considered a possible alternate geologic storage. This is due to the adsorptive properties of organic kerogen and clay minerals within the shale matrix. Therefore, this research looks at evaluating the sequestration potential of carbon dioxide (CO2) gas in kerogen nanopores with the use of COMSOL multiphysics software under varying pressures and different pore sizes. Gas flow in micro/nano pores differ in hydrodynamics due to the dominant pore wall effects, as the mean free path ( $\lambda$ ) of the gas molecules become comparable to the characteristic length (H) of the pores. In so doing, the traditional computational methods break down beyond the continuum region, as a result of the rarefaction effect at low pressures, as characterized by the Knudsen number (Kn). The molecular flow module in COMSOL is utilized to predict low-pressure CO2 and naturally occurring methane (CH4) gas in a 0.6-µm pore-slit. The effects of gas-wall collisions (Knudsen layer effects) is incorporated into the molecular flow module, while the discontinuous velocity at the pore walls is resolved with a slip boundary condition.

Implementing the Maxwell slip model at the pore walls for both CO2 and methane (CH4) gases under similar conditions, revealed the amount of CO2 adsorbed is more than that of CH4 gas. Moreover, the underlying flow mechanism for CO2 for a typical kerogen nanopore is dominated by the slip flow regime. Increasing the equilibrium pressure, increases the mass flux due to adsorption. On the other hand, an increase in the nano pore size caused further increase in the mass flux due to free gas and that due to adsorbed gas. Thus, in the kerogen nano pores, CO2 gas molecules are more adsorptive than naturally occurring CH4. This is an indication of a multi-layer adsorption. Therefore, this study not only provides a clear understanding of the underlying flow mechanism of CO2 in kerogen nano pores, but also provides a potential alternative means to mitigate the greenhouse gas effect (GHG) by sequestering CO2 in organic-rich shales.

## Figures used in the abstract



**Figure 1**: Velocity profile of CO2 gas in a 6- $\mu$ m long pore slit with height of 0.6- $\mu$ m to reflect a kerogen pore size at a pressure of 1000 Pa and a temperature of 293.15 K. The resulting slip velocity is recorded as 0.296 m/s at the walls.