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

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Introduction: This research looks at evaluating the sequestration potential of carbon dioxide (CO₂) gas in kerogen nanopores at varying pressures and temperatures.

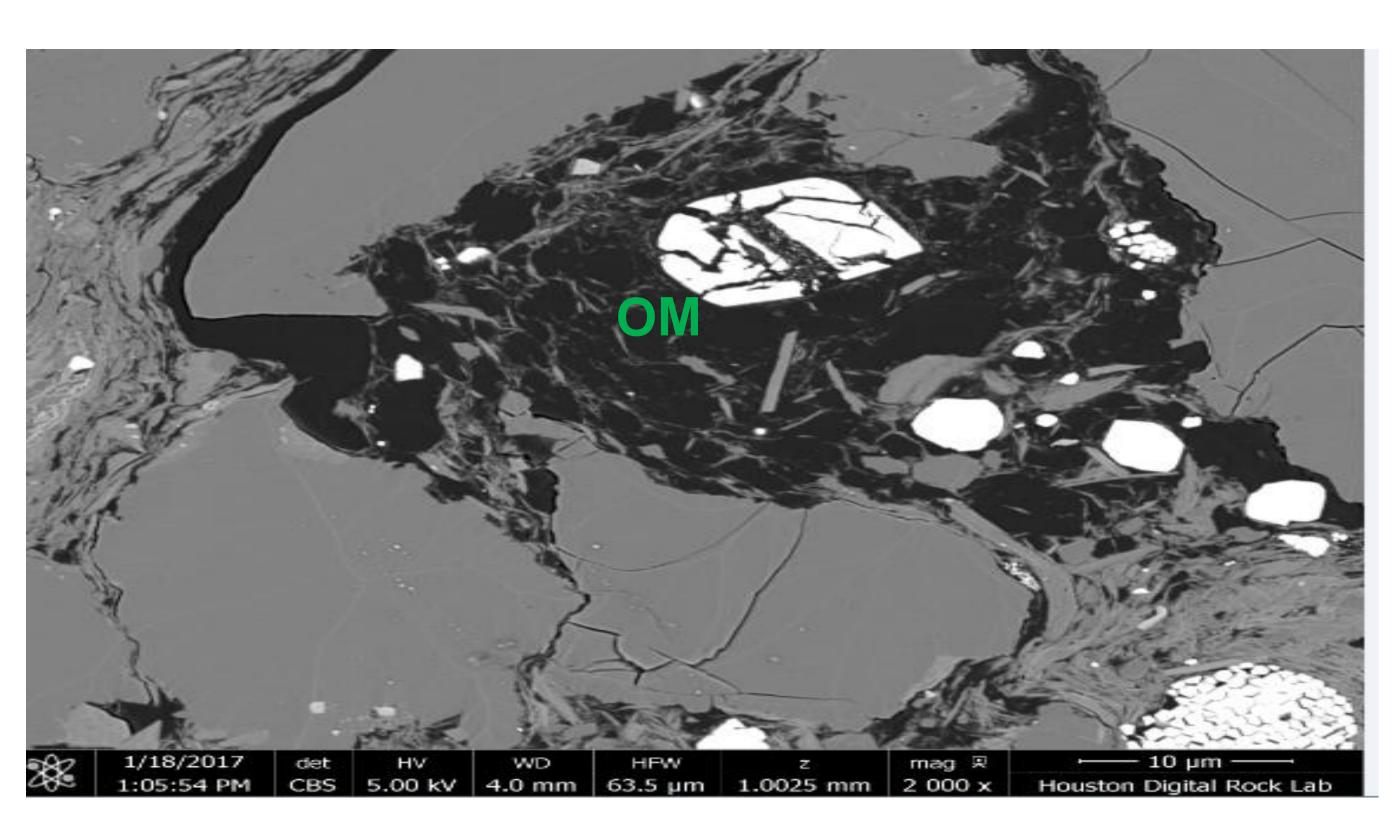


Figure 1. FE-SEM image of an organic-rich shale sample

Computational Methods: Gas flow in micro-/nano-pores deviate from continuum methods due to the dominant pore wall effects. Thus, implementing a slip boundary condition accurately captures the slip effect given as¹

$$U_{slip} = \frac{2 - \sigma_v}{\sigma_v} \lambda \frac{\partial U}{\partial y_{wall}}$$

A 6um long by 0.6 um wide pore-slit is built to reflect a kerogen pore size. Fluid domains (CO₂ and CH₄) are driven by a pressure gradient.

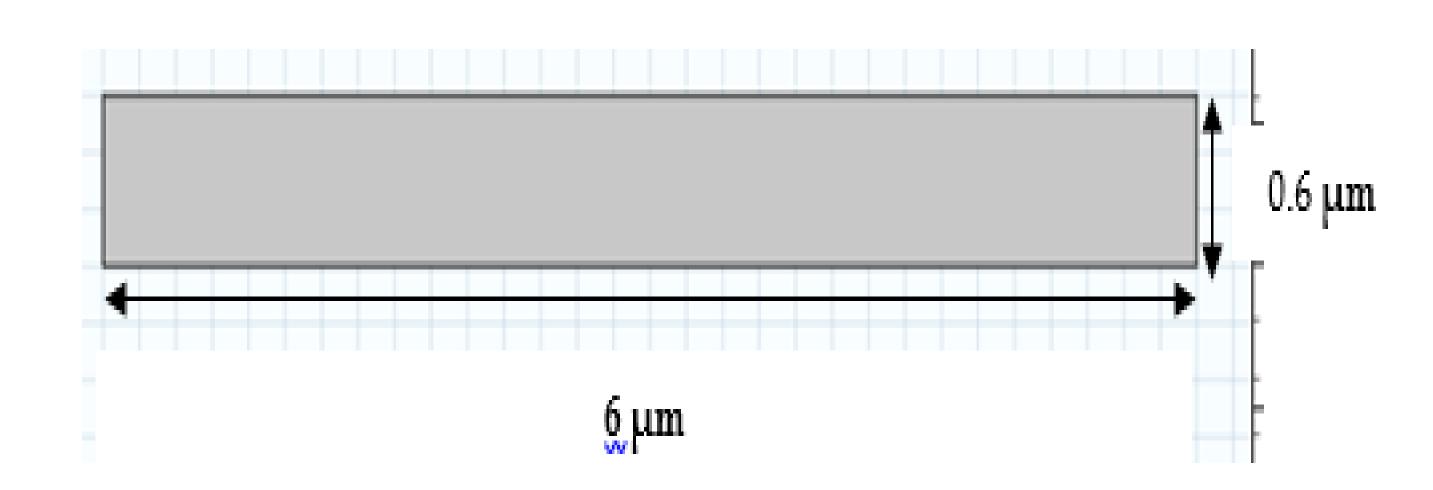


Figure 2. Geometry of pore-slit

Results: Figure 3 and Figure 4 show the velocity magnitude of CO₂ and CH₄ respectively at 1000 Pa and 273.15 K.

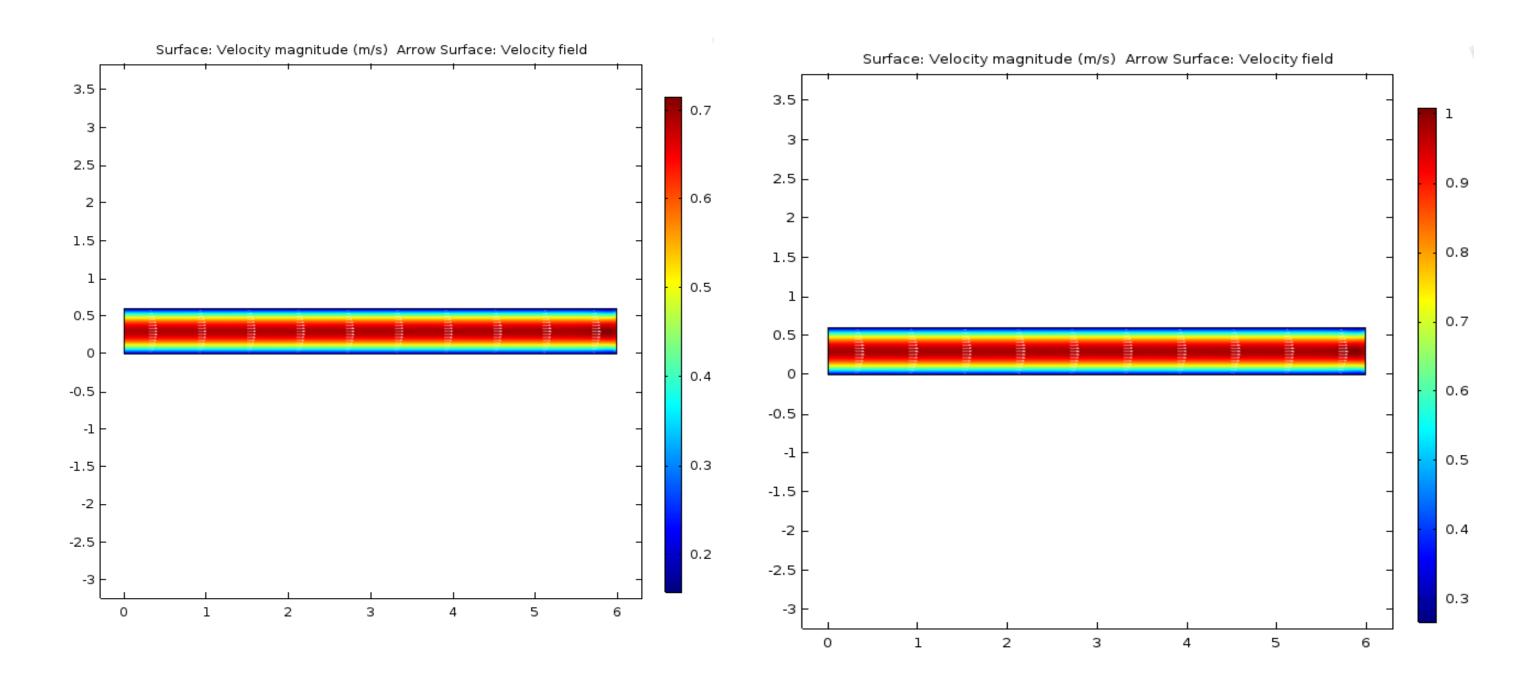


Figure 3. Velocity of CO₂

Figure 4. Velocity of CH4

Parameter	Value	Units
Slip velocity	0.177	m/s
Average velocity	0.519	m/s
Mean free path	42.4	nm
Knudsen number	0.071	

Parameter	Value	Units
Slip velocity	0.296	m/s
Average velocity	0.752	m/s
Mean free path	53.4	nm
Knudsen number	0.089	

Table 1. Simulation results of CO₂ and CH₄, respectively.

Conclusions: CO₂ gas molecules under similar conditions is twice more adsorptive than CH₄ gas molecules inferring from the slip velocity at different pressures and temperatures. Therefore, this study provides a potential alternative means to mitigate greenhouse gas effect by sequestering CO₂ in organic-rich shales.

References:

1. Zheng, L., Shi, B. C. & Chai, Z. H. Lattice Boltzmann method for simulating the temperature jump and velocity slip in microchannels. *Commun. Comput. Phys.* **2**, 1125–1138 (2007).