

CH₄/CO₂/H₂ Storage and Transport in Nanoporous Media: Microscopic Mechanisms and Scale Effects

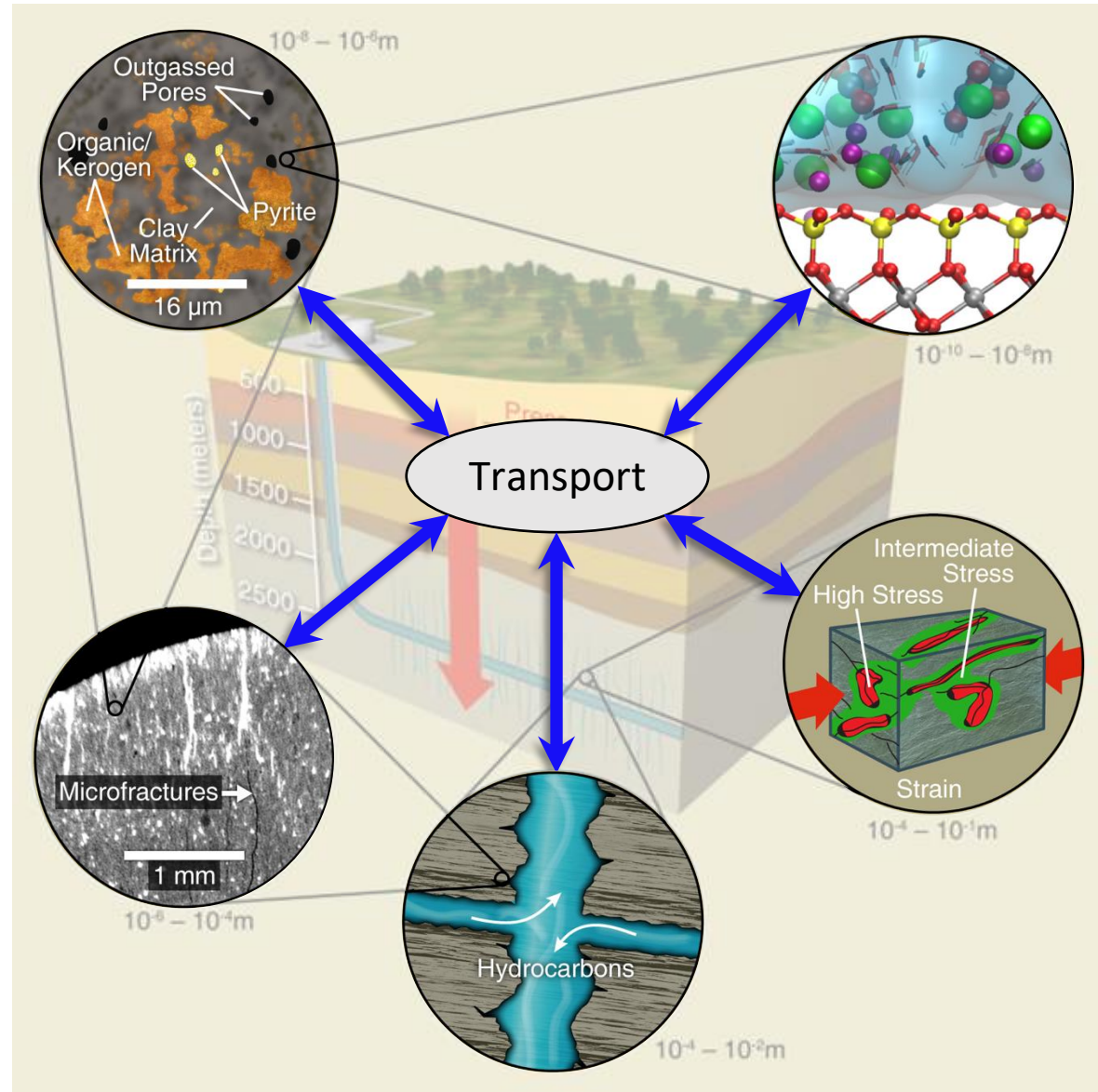
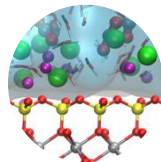
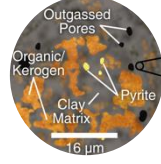
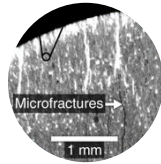
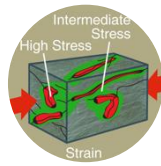
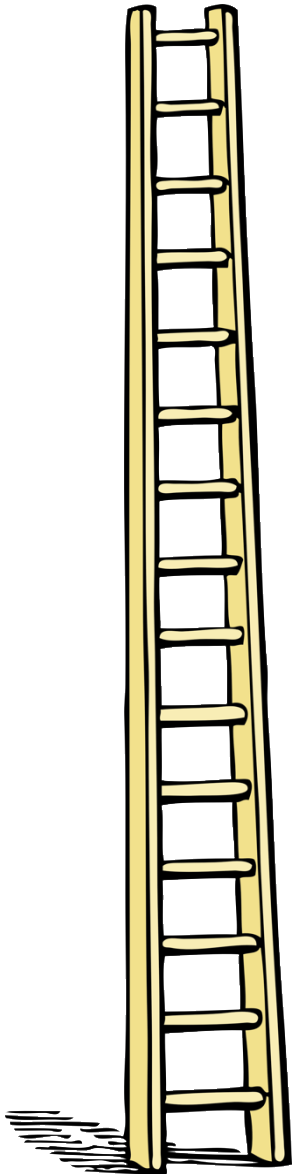
Lingfu Liu, Saman Aryana

Chemical & Biomedical Engineering
University of Wyoming

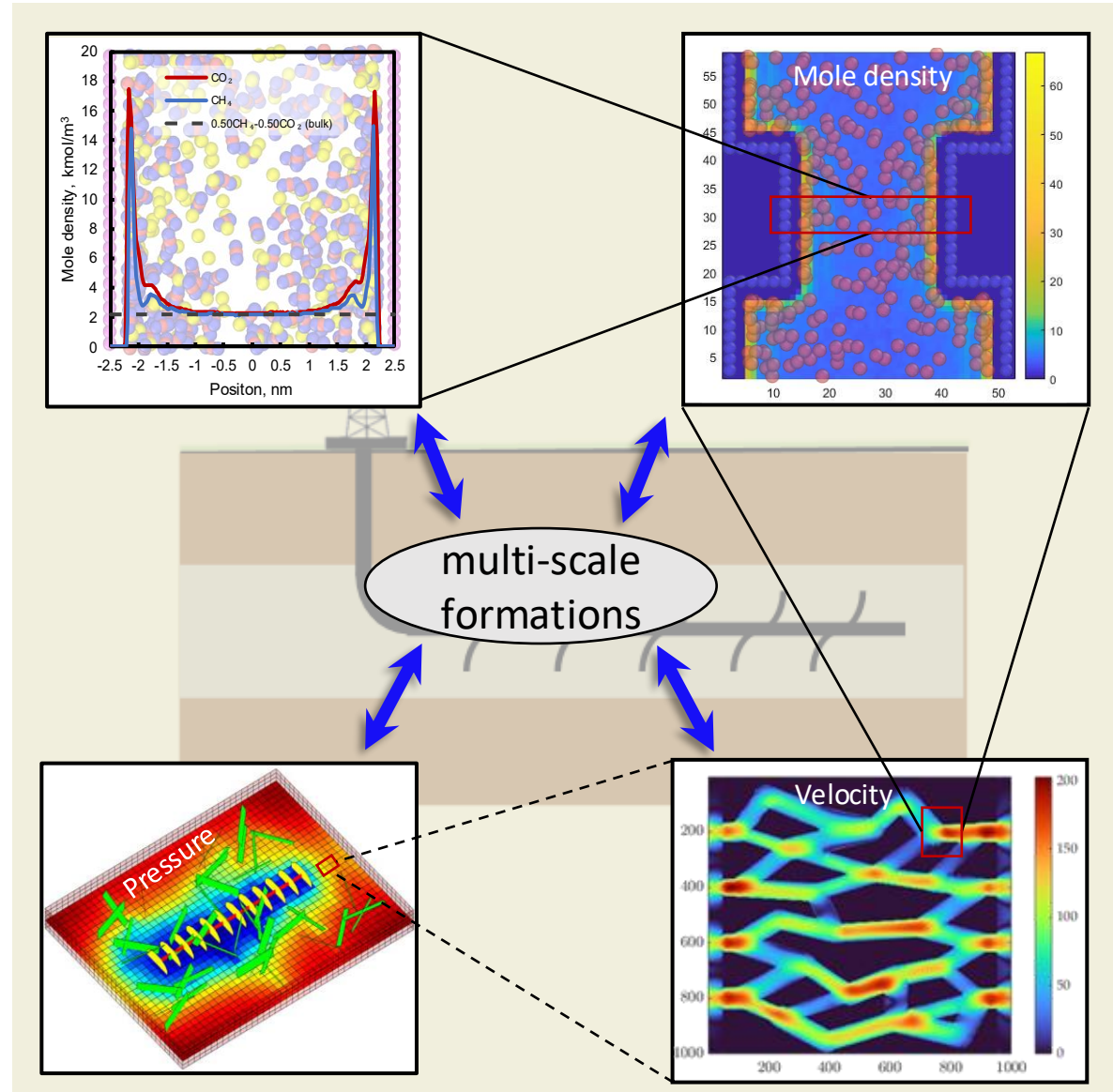


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Context



Overall Aim



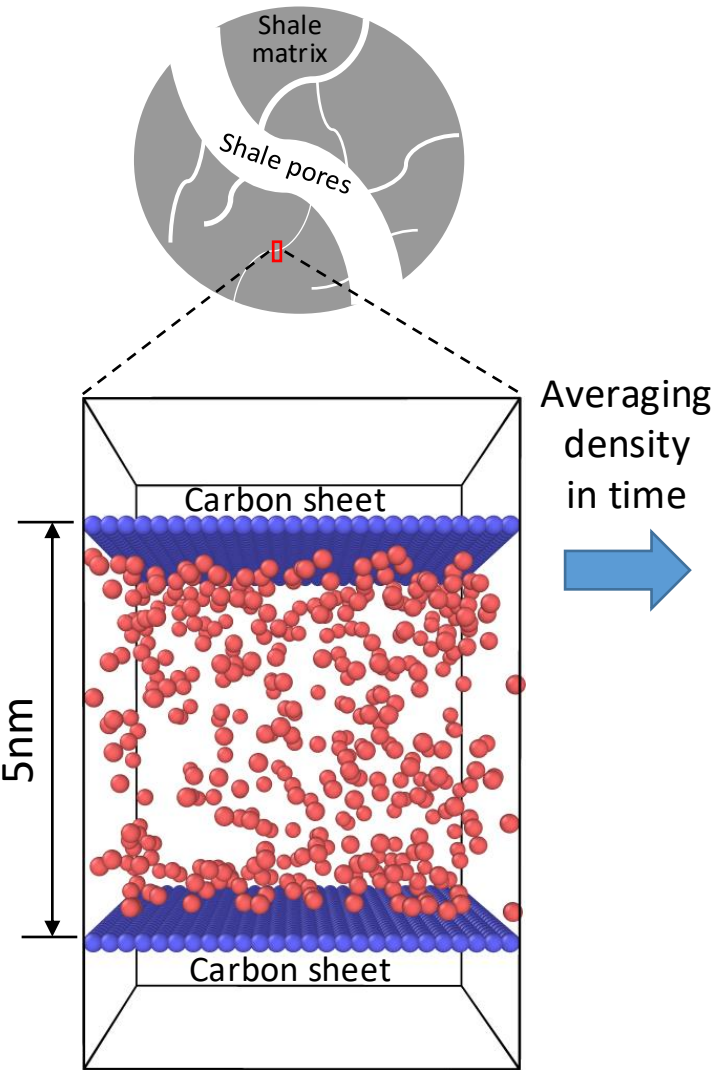
Q1. How does heterogeneity affect CH₄ adsorption in nano-sized pores?

Q2: How does nanoconfinement affect binary mixtures transport?

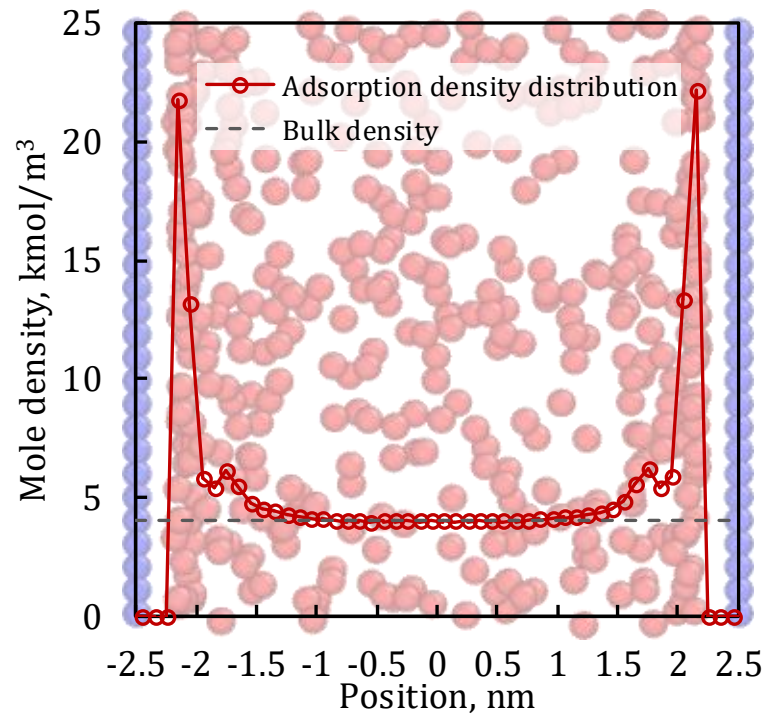
Keyword: Mont Carlo simulations; Gas adsorption; Lattice Boltzmann method; slippage flow; diffusion;



Adsorption of CH₄ Molecules in Nanoslits

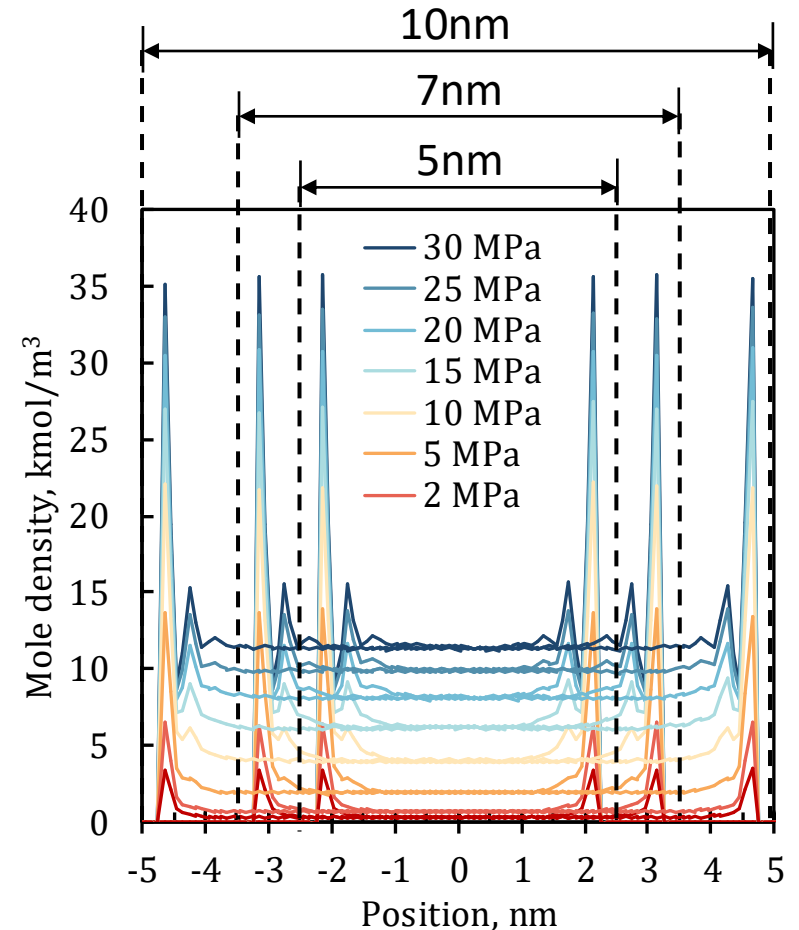


Molecule distributions of CH₄ in a 5nm pore connected to a non-confined pore at 10MPa and 333K



Density profiles of CH₄ in a 5nm pore connected to a non-confined pore at 10MPa and 333K

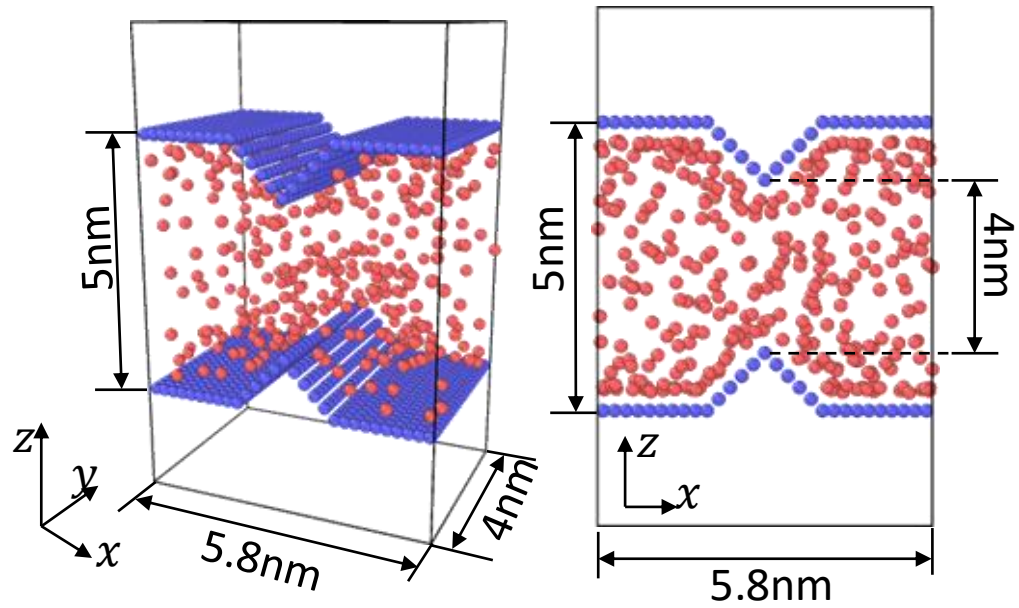
Change pressure
→
Change pore size



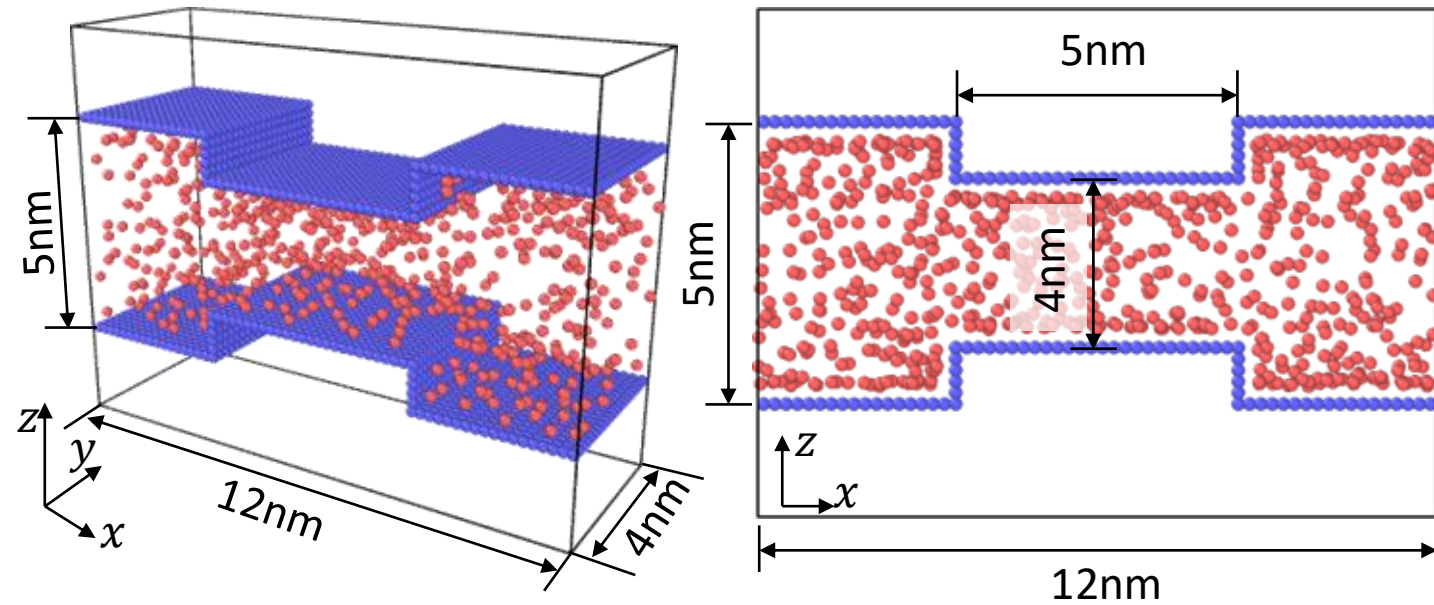
Density profiles vary with pressure and pore size is fixed at 333K

Adsorption of CH₄ in Irregular Nanopores

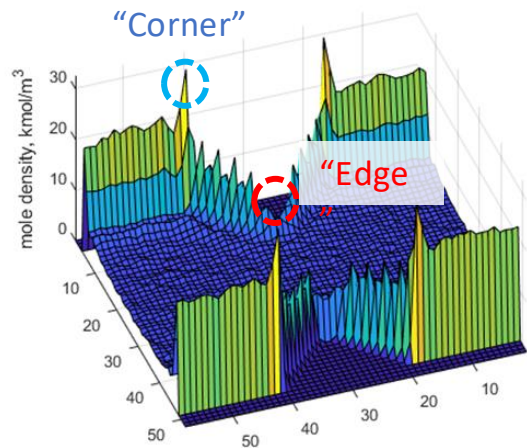
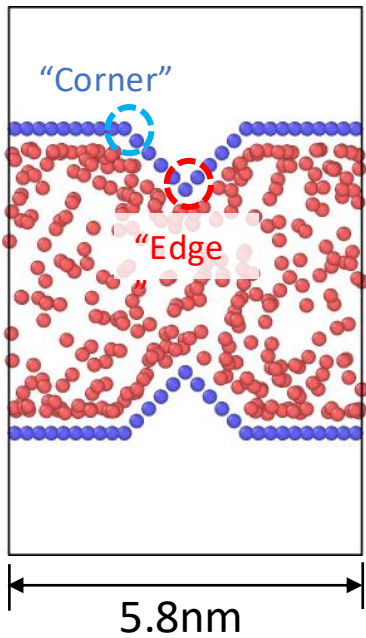
□ Nanopores with triangle structure on surface



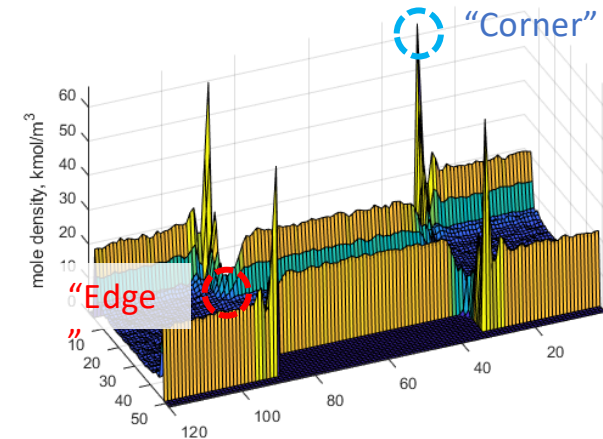
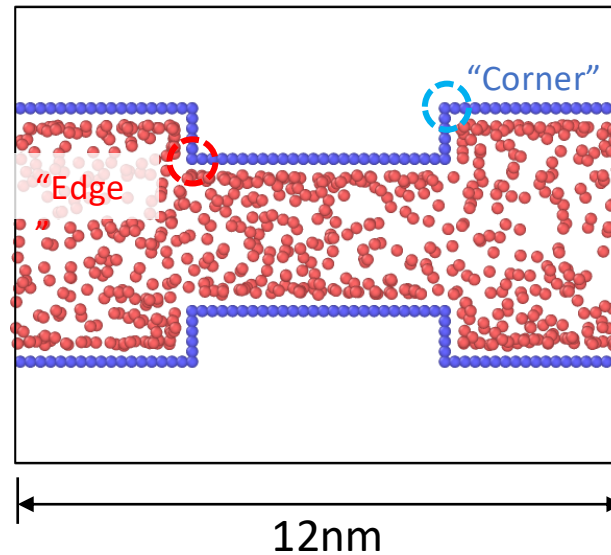
□ Nanopores with rectangle structure on surface



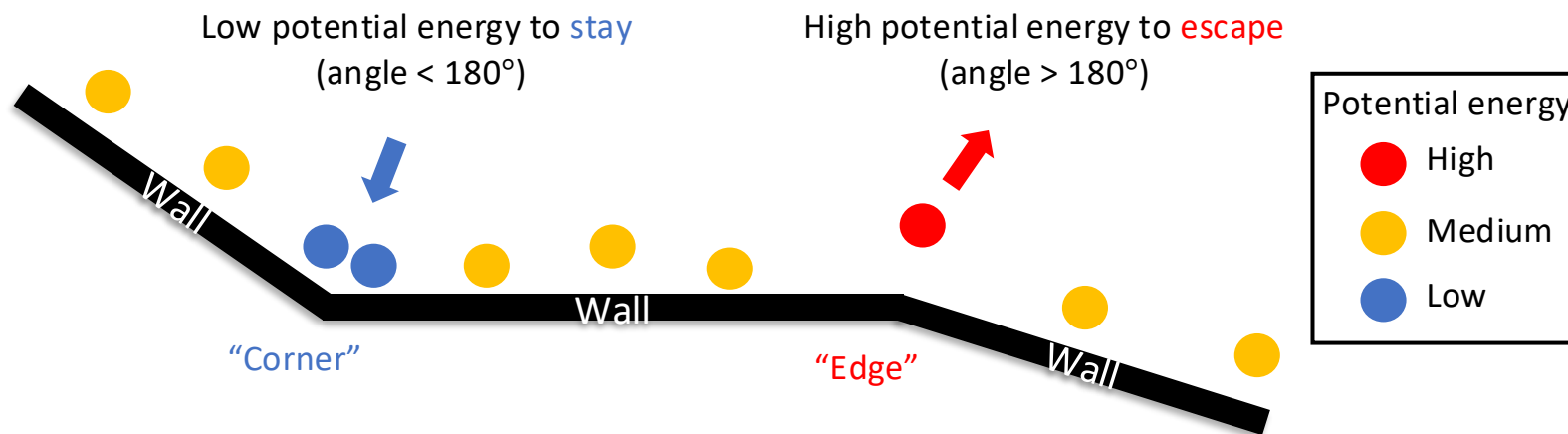
Adsorption of CH₄ in Irregular Nanopores



Density profiles from GCMC-MD simulations
(T=333K, P=10MPa)

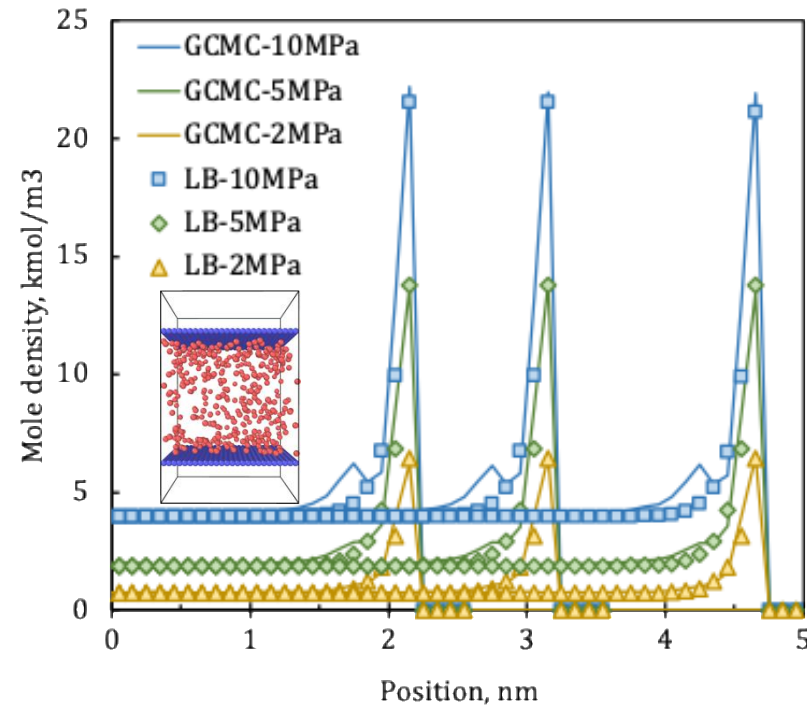


Density profiles from GCMC-MD simulations
(T=333K, P=10MPa)



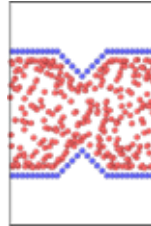
Comparison between LBM and MS

Nano slits

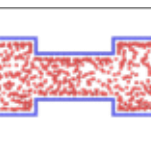


T = 333 K

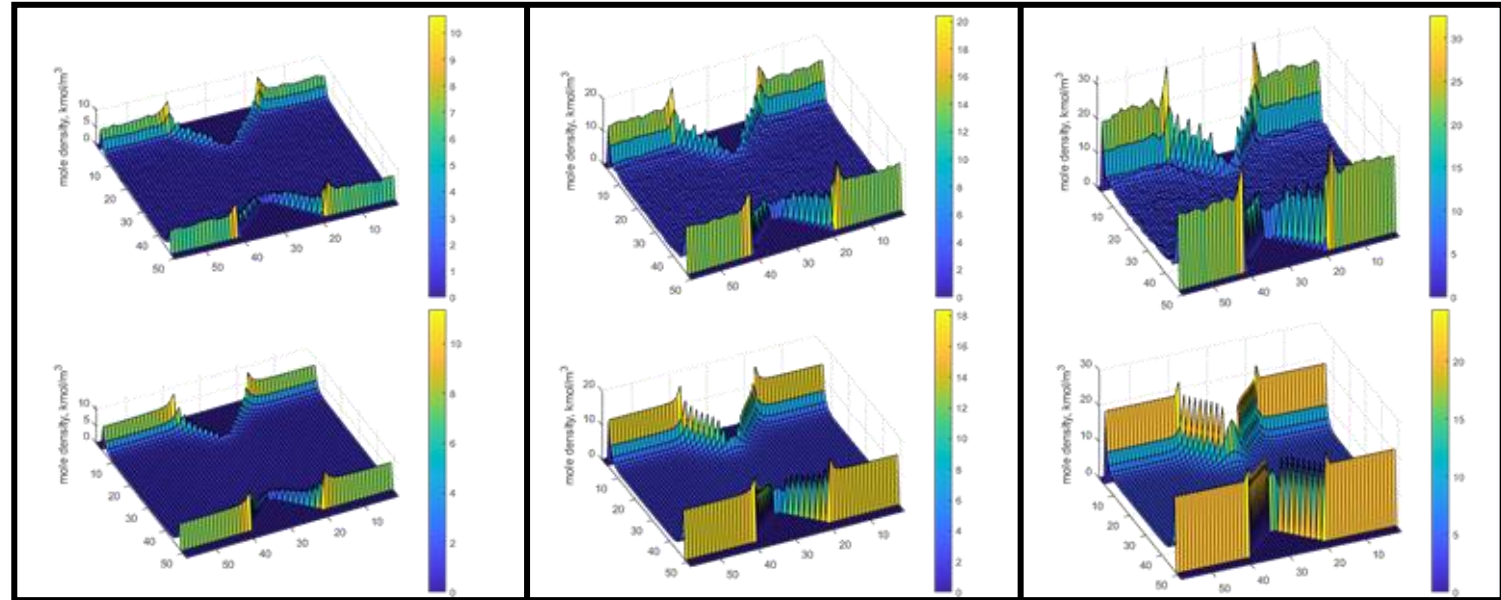
GCMC



LBM



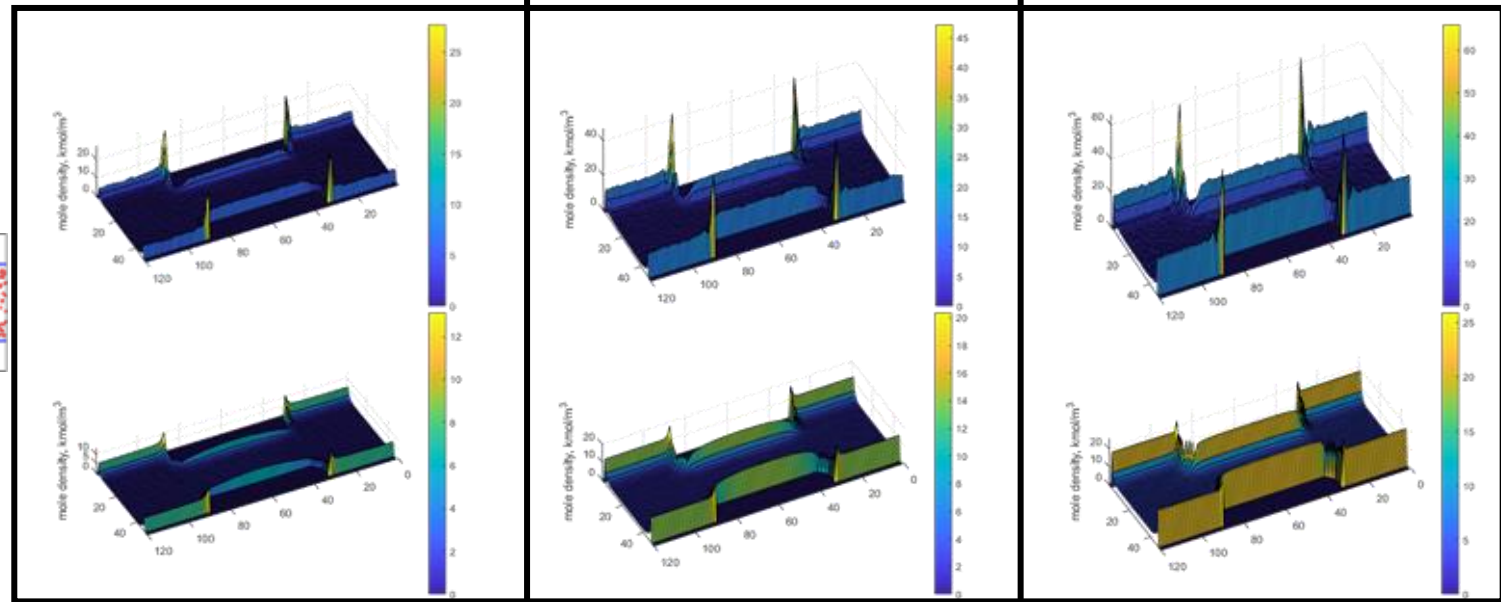
LBM



2 MPa

5 MPa

10 MPa



mole density, kmol/m³

mole density, kmol/m³

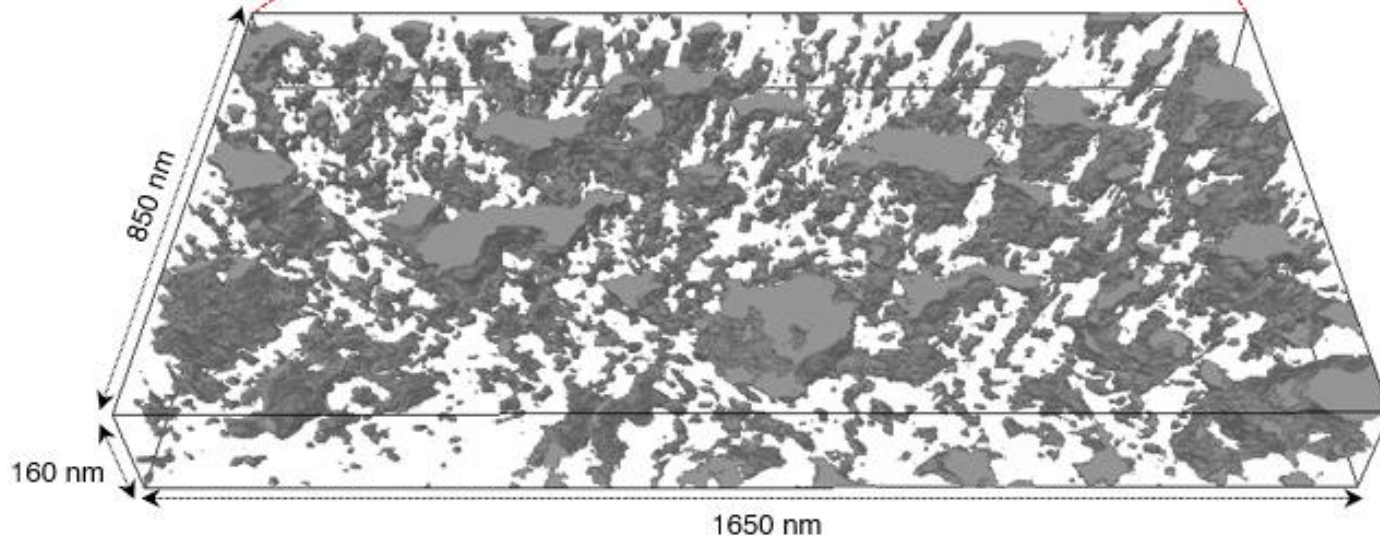
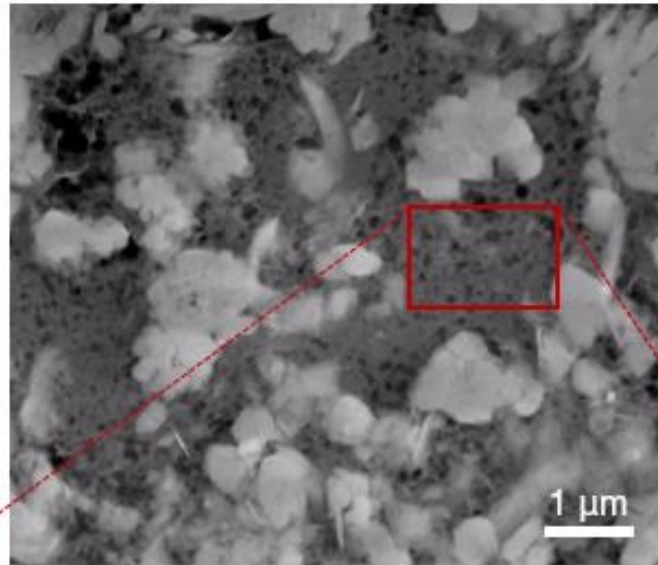
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STEM Characterization of Shale Nanopores



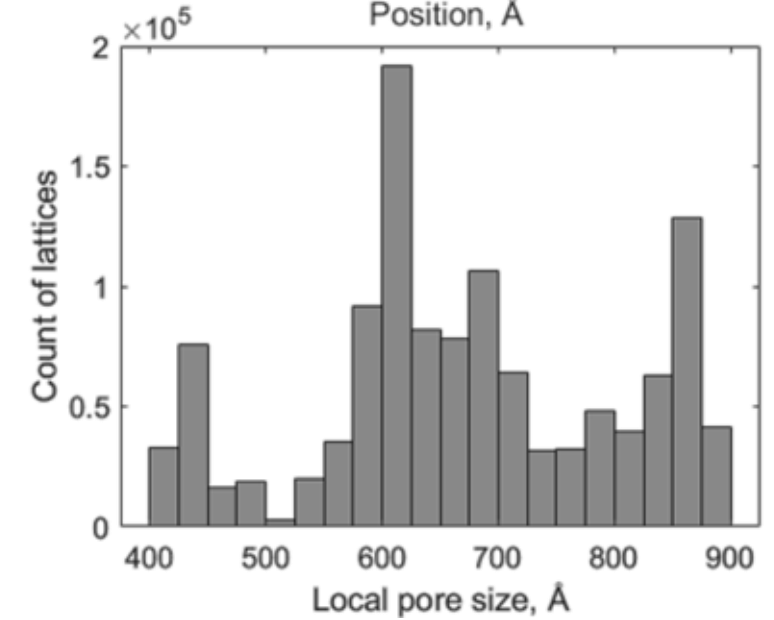
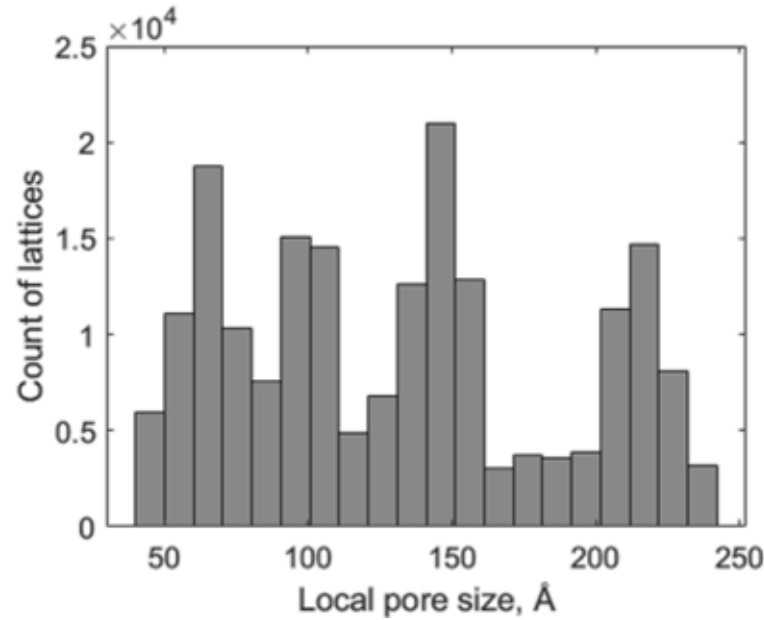
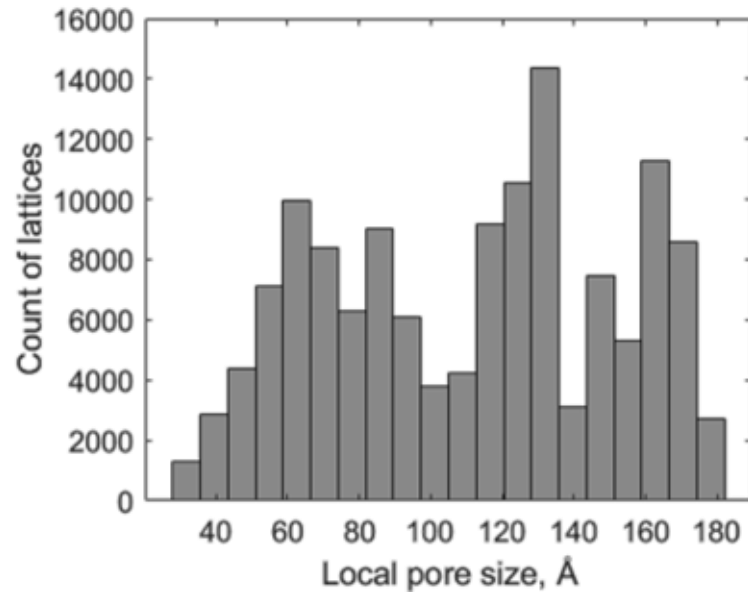
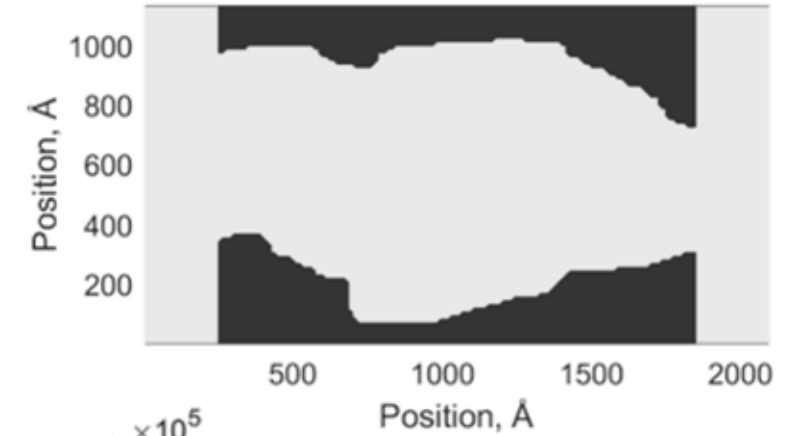
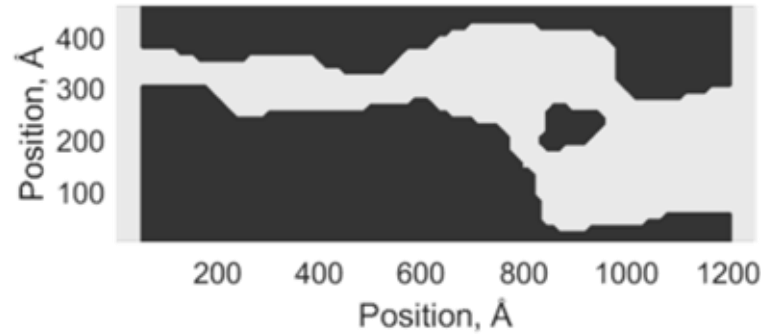
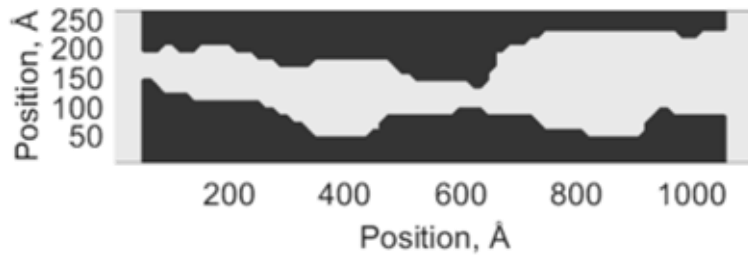
A sample from the Vaca Muerta formation
(well SR1001, 2654.2 m depth)

Organic pore network reconstructed by STEM
tomography*. (voxel size: 1.24 nm).

(Gray shading indicates the pore network identified after image segmentation.)

* Froute, Stanford University, 2023

Three Representative Shale Nanopores

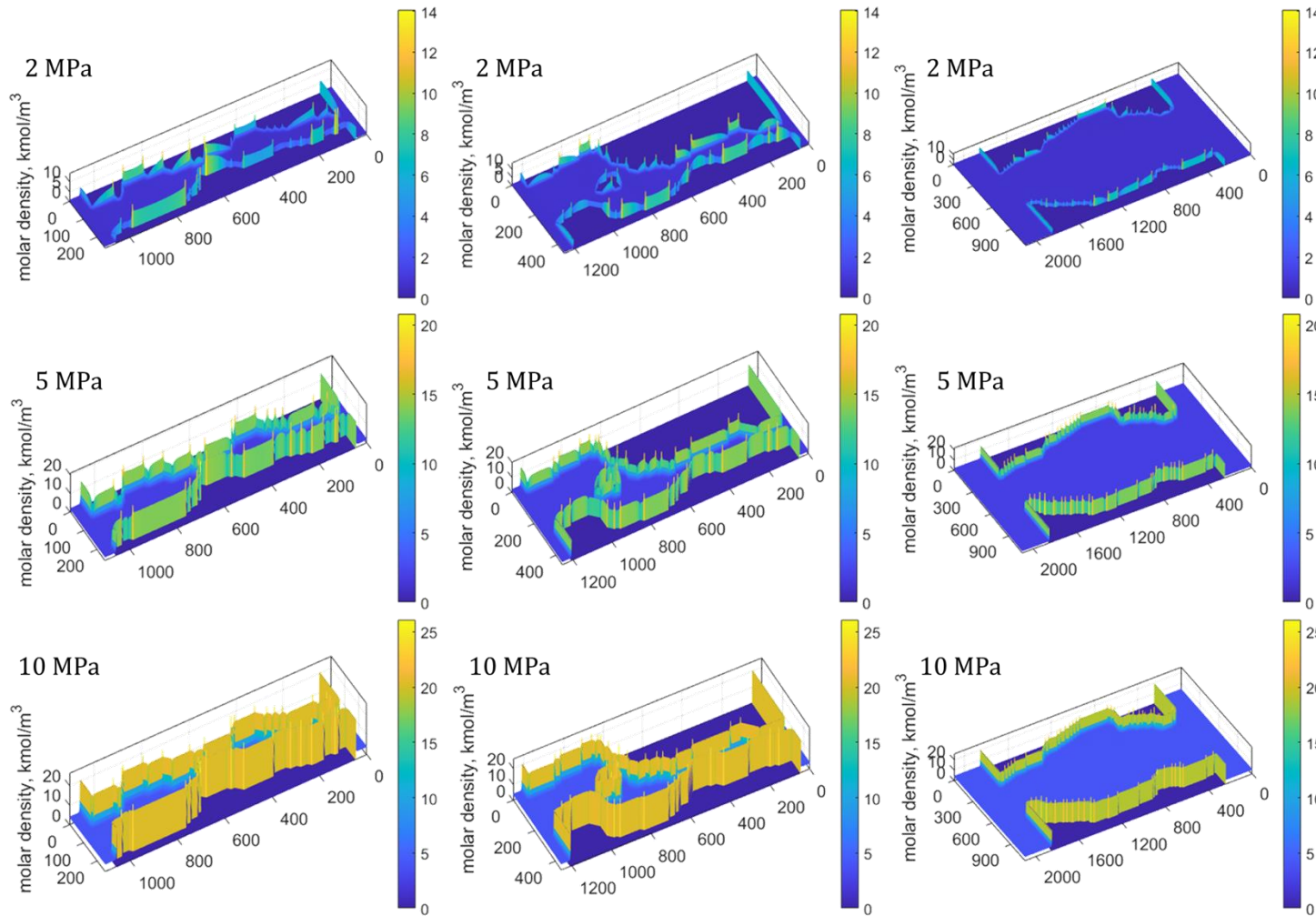


(a) Small
4-18 nm

(b) Medium
5-25 nm

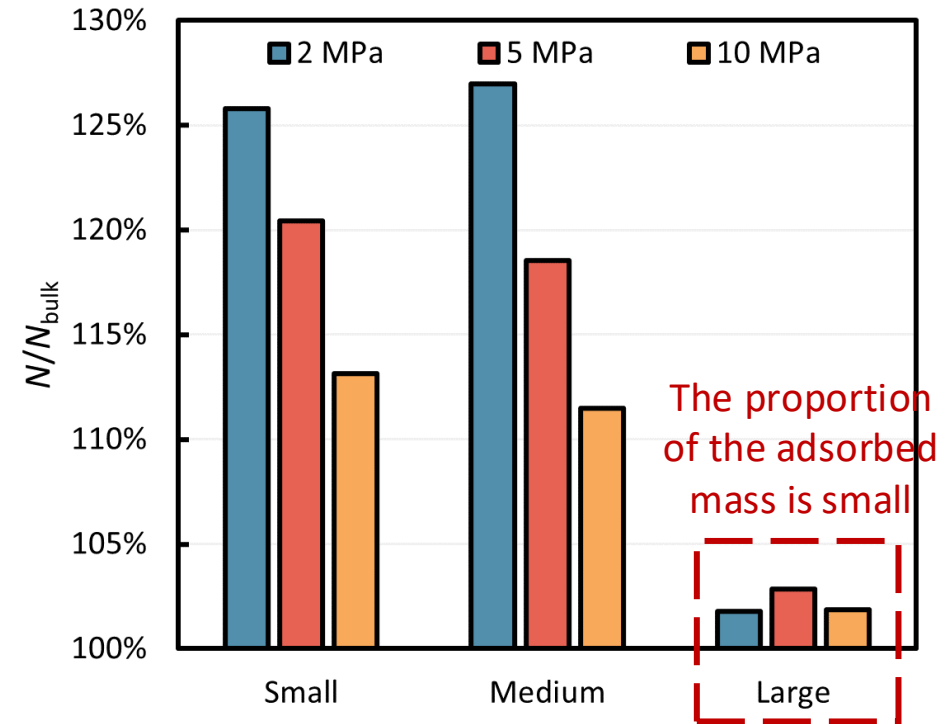
(c) Large
40-90 nm

The Scale-Effect Limit of Methane Adsorption



CH₄ density distributions (kmol/m³)

$$\frac{N}{N_{bulk}} = \frac{\text{Contained fluid in nanopores}}{\text{Bulk fluid}}$$



Ratio of fluids contained in nanopores from LB simulation results, N , to their corresponding cases of bulk fluids, N_{bulk}

Conclusion: It may be reasonable to ignore the contribution of the adsorbed methane when shale pore sizes are larger than 40 nm.

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Q2: How does nanoconfinement affect binary mixtures transport?

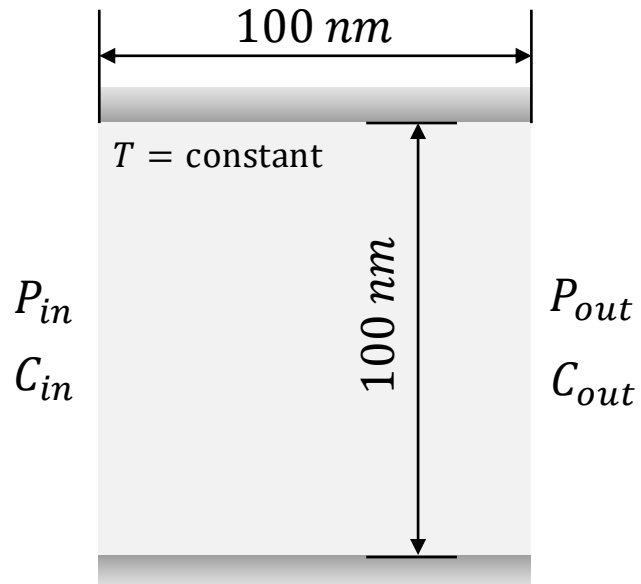
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Pressure-Gradient Driven Flow in Nano-Slits



□ CH₄-CO₂ mixture in nano slits



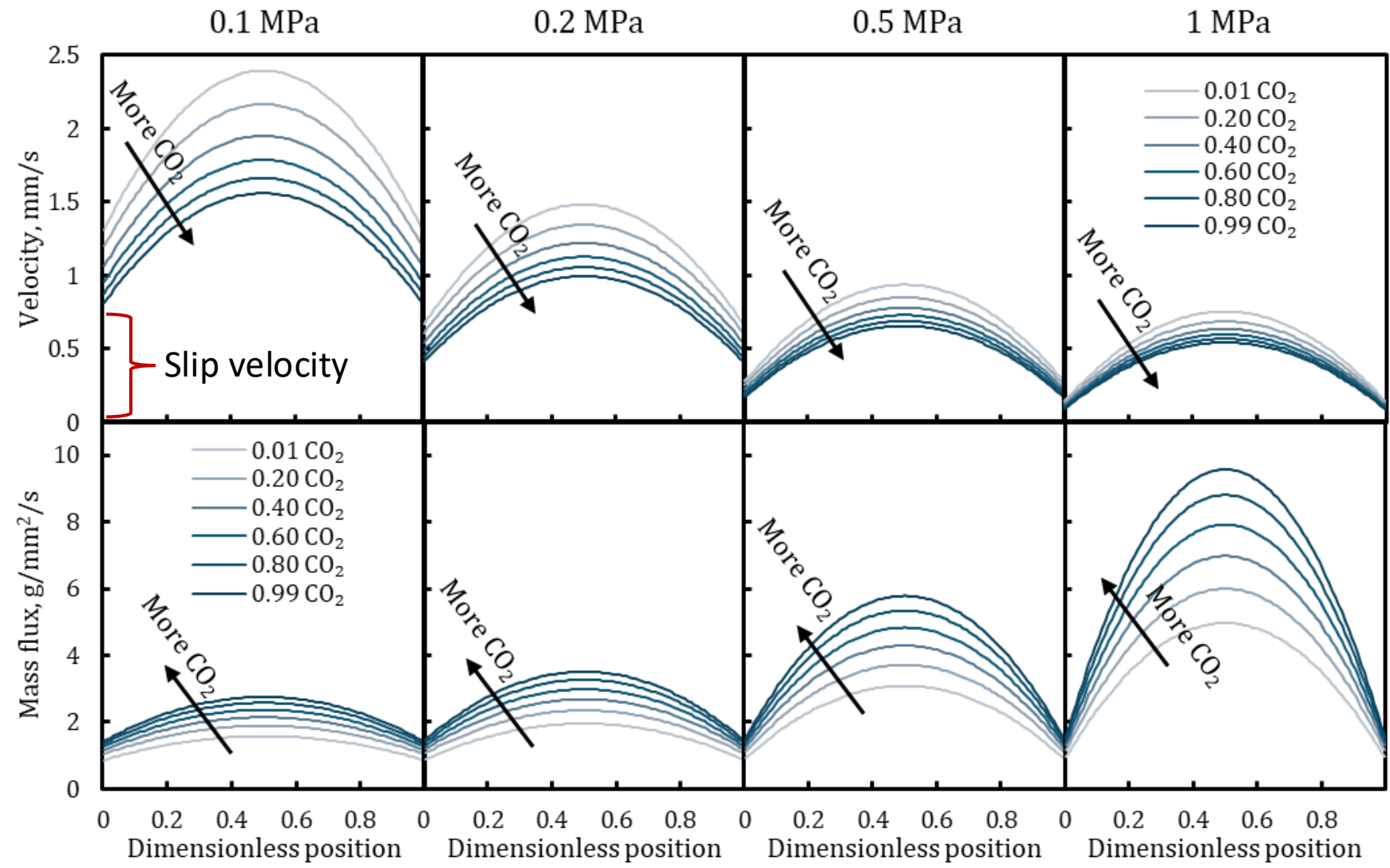
$$C_{in} = C_{out}$$

$$T = 298 \text{ K}$$

$$P_{initial} = P_{in}$$

$$P_{in} - P_{out} = 5 \text{ Pa}$$

➔ $\frac{dP}{dL} = 50 \text{ MPa/m}$

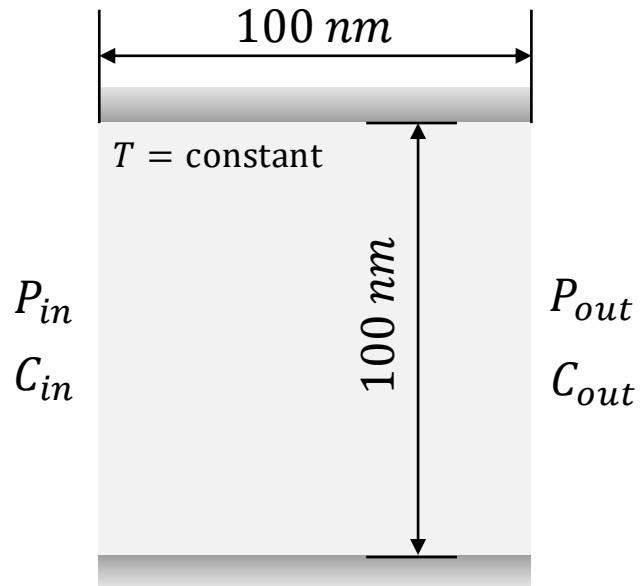


❖ Under the same pressure difference, lower pressure leads to higher slip velocity.

Pressure-Gradient Driven Flow in Nano-Slits



□ CH₄-H₂ mixture in nano slits



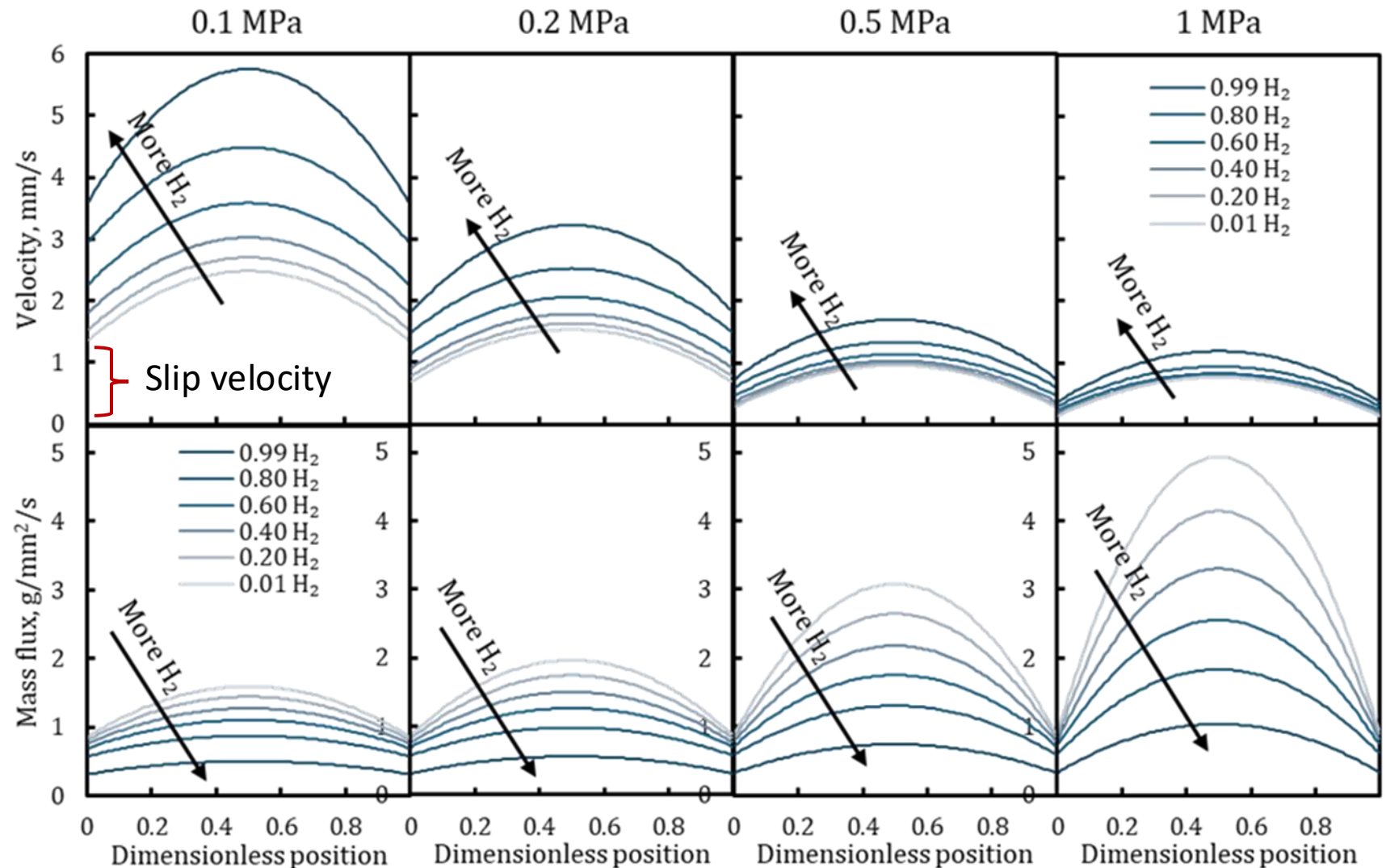
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$$\rightarrow \frac{dP}{dL} = 50 \text{ MPa/m}$$



❖ Slip effects become more pronounced with increasing light-component fraction

Apparent permeability of Binary Gas



□ Apparent permeability of mixtures

Darcy's Law $Q = k_g \frac{A dP}{\mu dL}$

Ideal Gas Law $\frac{P}{\rho} = \text{constant}$



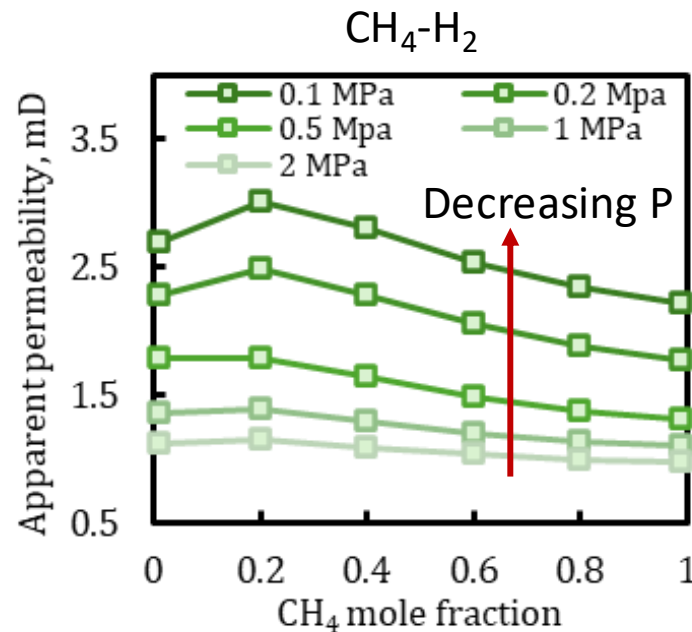
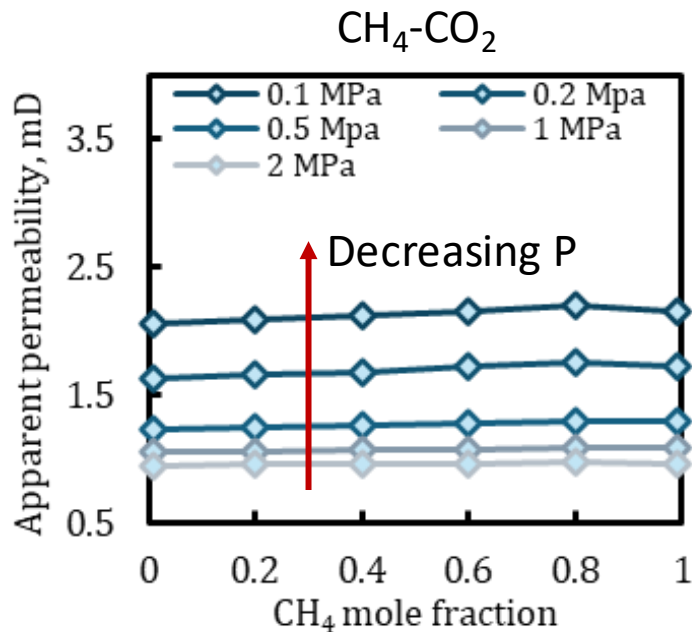
$$k_g = \frac{2\bar{q}_{out}\mu P_{out}L}{P_{out}^2 - P_{in}^2}$$

\bar{q}_{out} is average flow rater per length

μ is dynamic viscosity $\leftarrow \tau_s$

P_{out} and P_{in} pressure at inlet and outlet

L is length from inlet to outlet



❖ Apparent permeability with slip (k_g) is jointly controlled by pressure (P) and gas composition (z)

Apparent permeability of Binary Gas



□ Apparent permeability of mixtures

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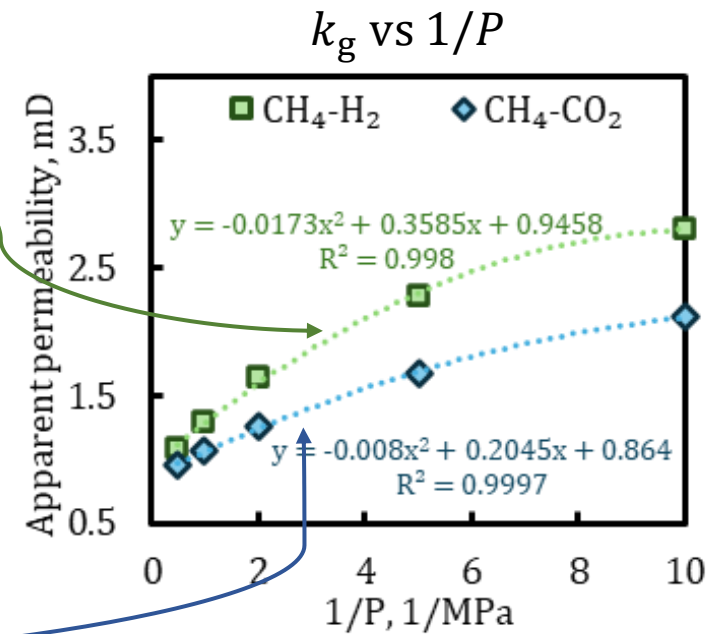
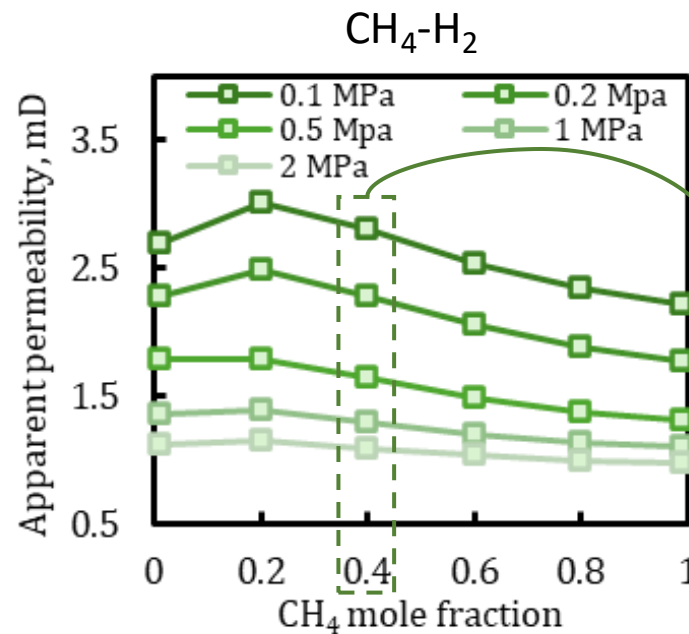
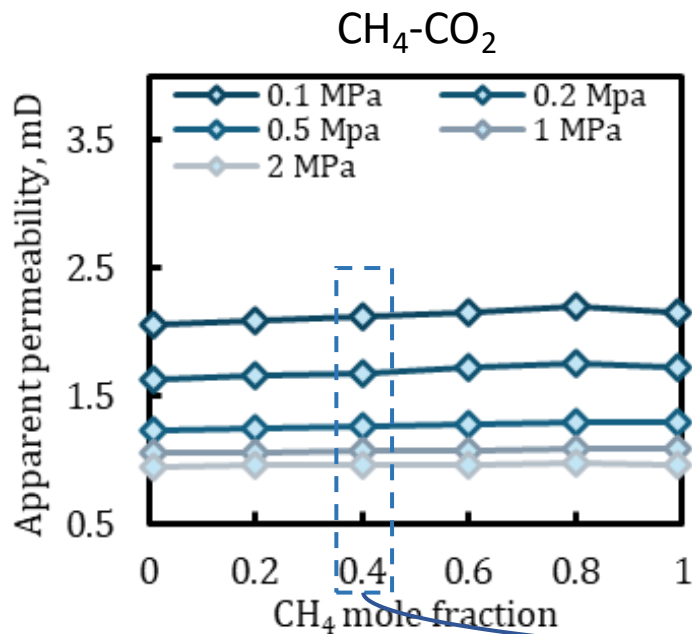
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P_{out} and P_{in} pressure at inlet and outlet

L is length from inlet to outlet



❖ Under fixed gas composition, k_g shows a quadratic dependence on $1/P$

Conclusion

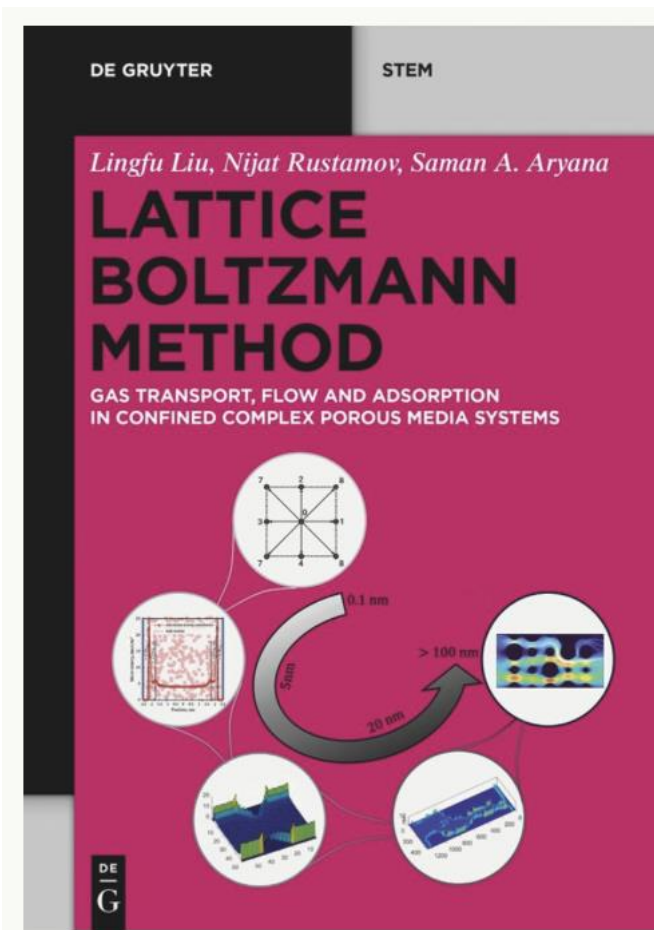
1. A cross-scale framework combining molecular simulation and LBM was established for nano-confined systems.
2. Adsorption effects become negligible in pores larger than about 40 nm.
3. Gas transport in nanoscale pores exhibits pronounced slip effects, with permeability following $k_g = a \left(\frac{1}{P}\right)^2 + b \left(\frac{1}{P}\right) + c$.
4. Molecular species strongly affect diffusion and displacement behavior.



The Center for Mechanistic Control of Unconventional Formations (CMC-UF), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science under DOE (BES) Award DE-SC0019165.



U.S. DEPARTMENT OF
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Two Postdoc Positions — PoreLab, NTNU

We are recruiting **two postdoctoral researchers** to extend a new thermodynamic framework for two-phase flow in porous media — from steady state to viscous fingering.

- **Position 1 — Numerical modeling** of Darcy-scale viscous fingers *Porous media · hydrodynamics · numerical methods · C++ / Python*
- **Position 2 — Theory** of Darcy-scale viscous fingers *Porous media · hydrodynamics · equilibrium thermodynamics · mathematical modeling*

Based at **NTNU, Trondheim**. Funded by the **European Research Council** (AGIPORE, PI: Alex Hansen). Group: A. Hansen, S. Aryana, S. Berg, S. Succi, S. Sinha, and team.

Formal announcement expected **summer 2026**. Strong candidates are welcome to send a CV and brief statement of interest in advance.

Inquiries: alex.hansen@ntnu.no