Molecular and Pore-scale Modeling

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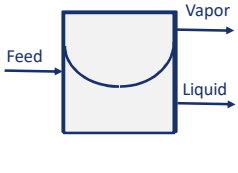
Molecular and Pore-scale Modeling

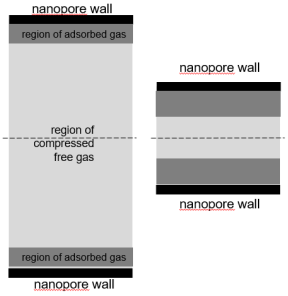
- Traditional reservoir models consider macroscopic phenomena with parameters that are averages of the pore-scale properties
- The approach works reasonably well for modeling of the conventional reservoirs
- Unconventional reservoirs have added intricacies mainly due to their much smaller pore sizes

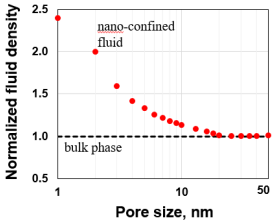
Molecular and Pore-scale Modeling: Challenges

1. Unconventional reservoir fluids far more complex
   - Inaccurate flash calculations in presence of porous medium
   - Interface curvature effect needed for liquid/gas compositions

2. Do we understand nano-confined fluids? EOS? Mass density? R_s? FVF? μ?



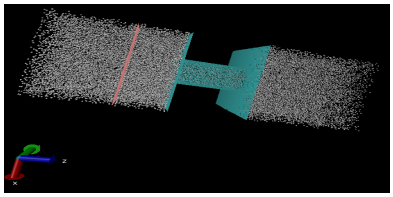


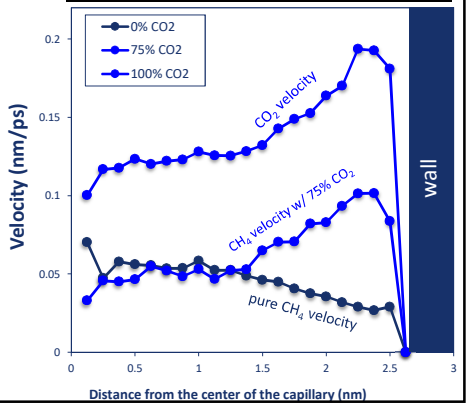


Molecular and Pore-scale Challenges

3. Uncertainties in transport calculations:
   - Are we allowed to use continuum mechanics?
   - Is Darcy law still valid?
   - How important are diffusion/slip on production?
   - Does the concept of REV exist?
   - Can we scale-up or should we go multi-scale?

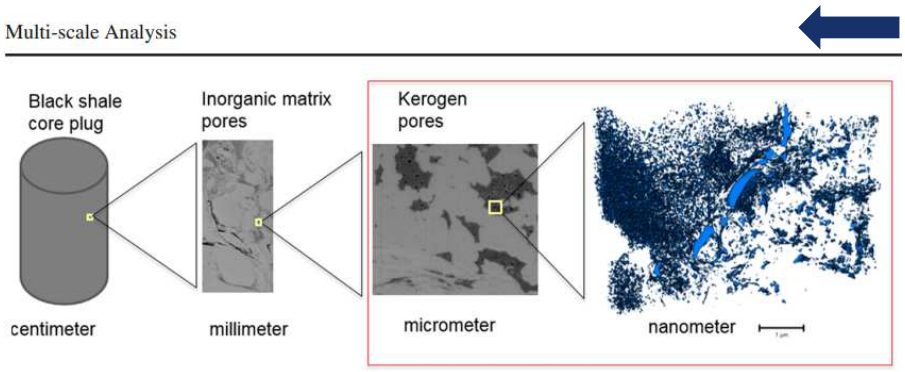
Source rock segmentation size: 4 μm high, 5 μm wide, 4 μm deep





Molecular and Pore-scale Modeling: Progress

Bottom-to-top construction & modeling: reasonable ?



Reservoir-scale, core-plug scale

Continuum models

Digital core scale — Scale of pores

Pore-scale modeling and simulation (DNS, PNM)

Scale of atoms and molecules

Molecular simulation (MD, MC)