Molecular Simulation of Fluid Phase Behavior in Shale Systems

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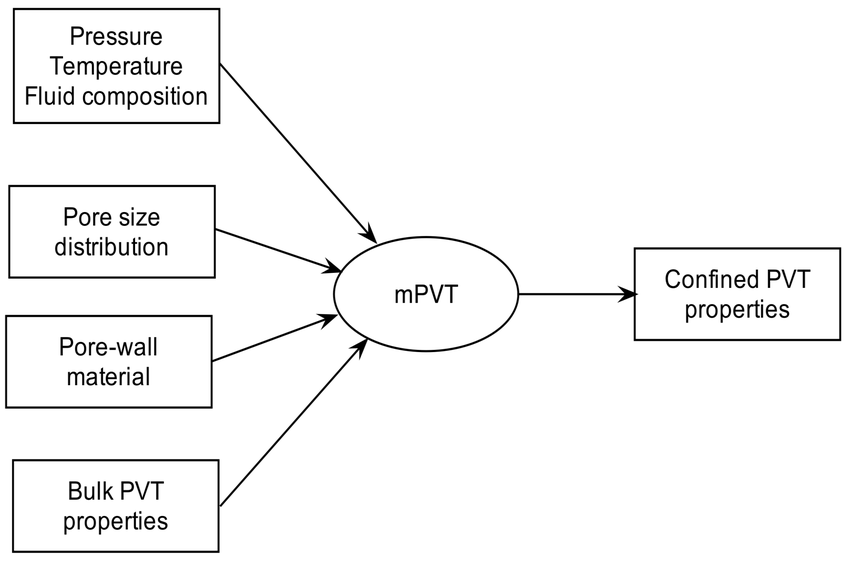
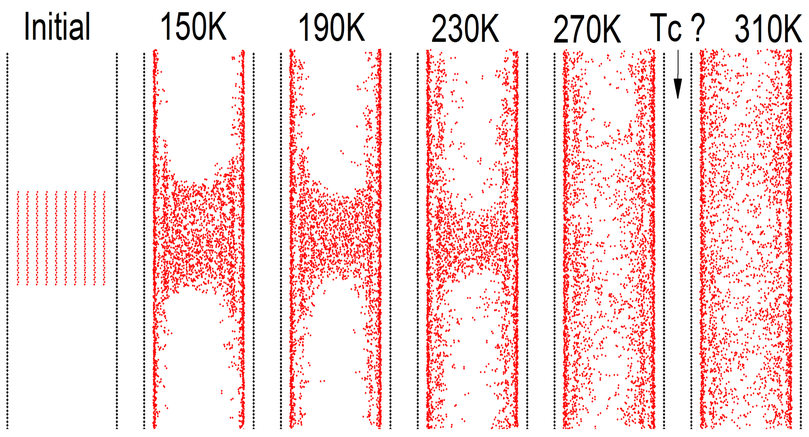
OBJECTIVE

In this project, we will use molecular simulation to accurately model the effect of solid-fluid and fluid-fluid interactions in shale, and calculate the confined phase behavior.

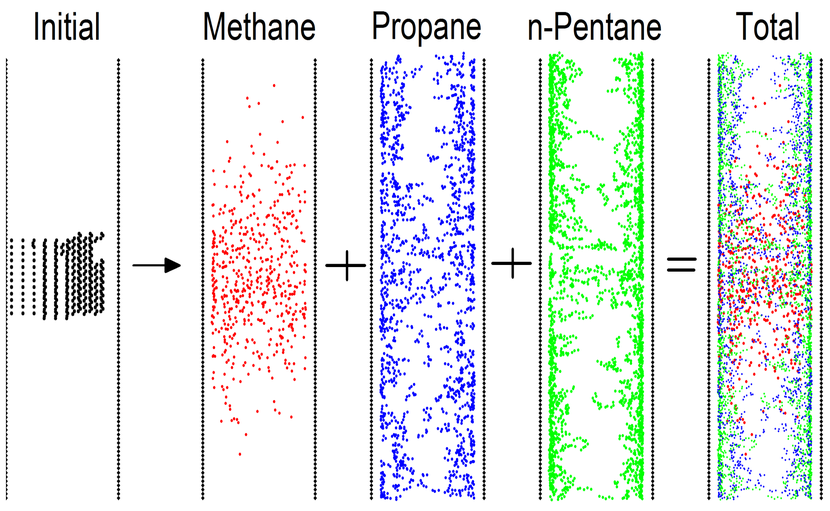


APPROACH

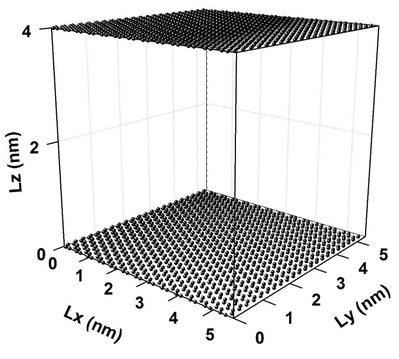
1: Liquid-vapor phase coexistence of pure substance;

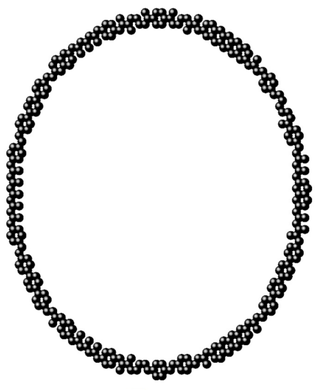


2: Liquid-vapor phase coexistence of multi-component fluid;



3: Simulation of PVT properties for hydrocarbons in model I (slit pore model) with unique diameters;





4: Repeating above processes in model II (cylindrical pore model) by considering different pore size distributions.

ACKNOWLEDGEMENTS

All computations are supported by Texas A&M High Performance Research Computing

SIGNIFICANCE

1. Ada cluster in HPRC is used;
2. Open source code *Towhee* and *GOMC* are used in this project;
3. Typical job size:

   20 jobs / 20 cores, 22 MB memory

   3 hour per million Monte Carlo steps
4. Liquid-vapor phases coexistence in nano pore;
5. Under confinement:

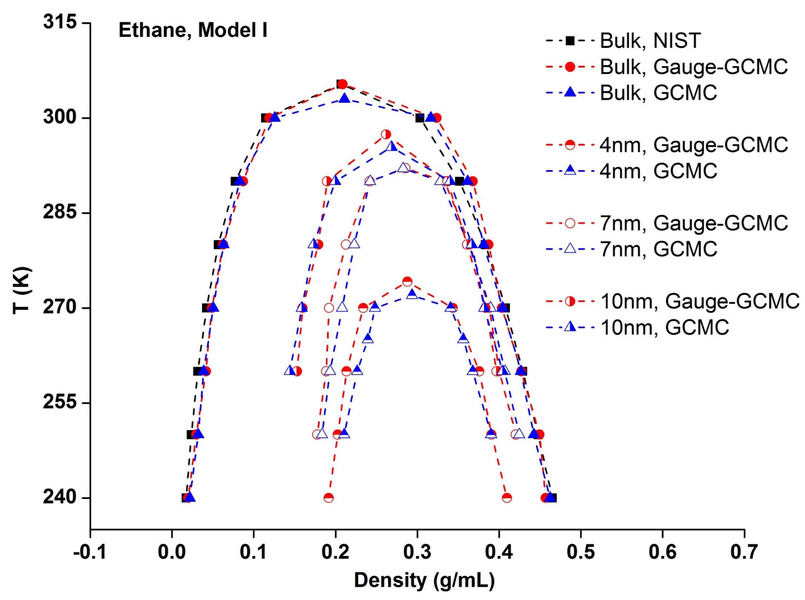
   1) Critical density is increased while critical temperature is reduced for pure fluid;

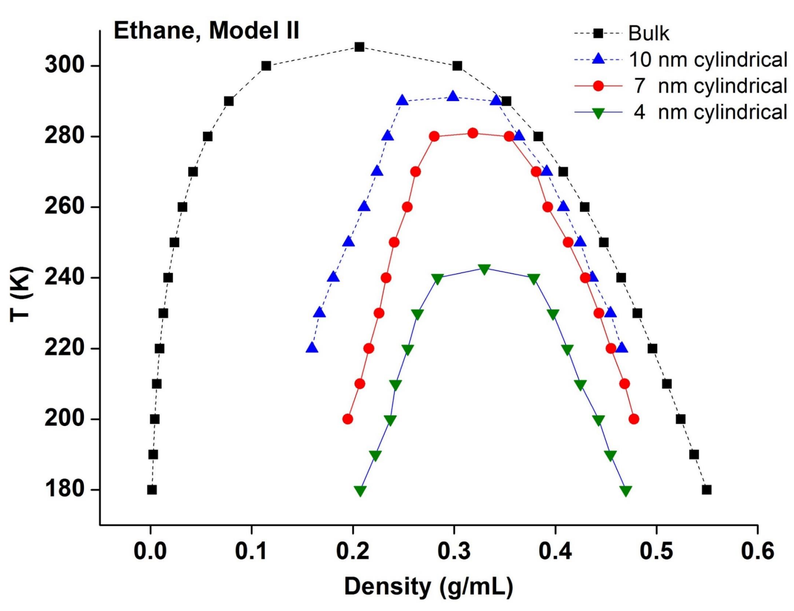
   2) Critical density is increased while C_1 composition is reduced for C_1/C_2 system;

   3) Critical density is increased while C_3 composition is reduced for $C_1/C_3/nC_5$ mixture;
6. A new method is developed for multi-component fluid simulation.

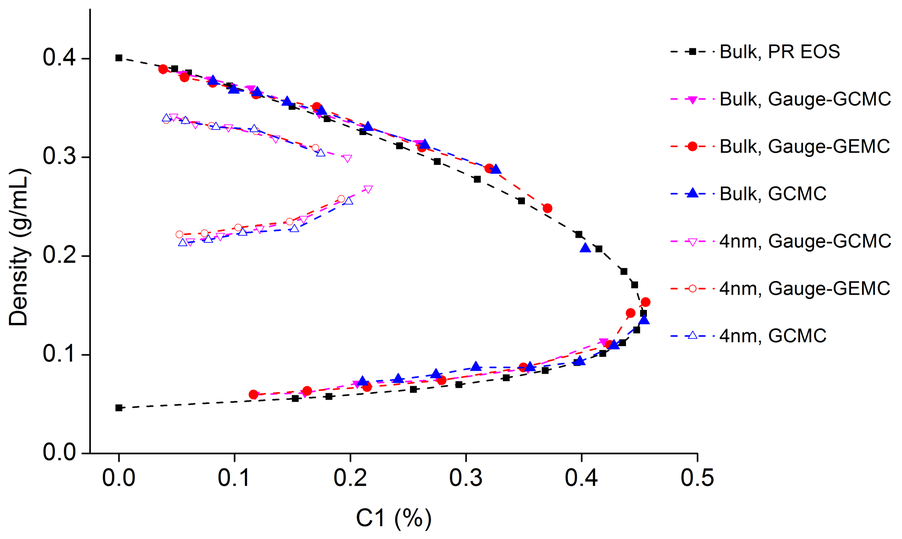
ACHIEVEMENTS

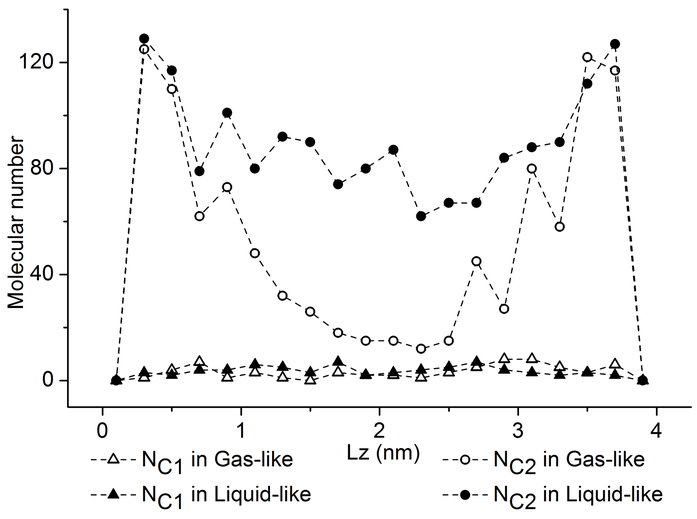
1. Single-component fluid:



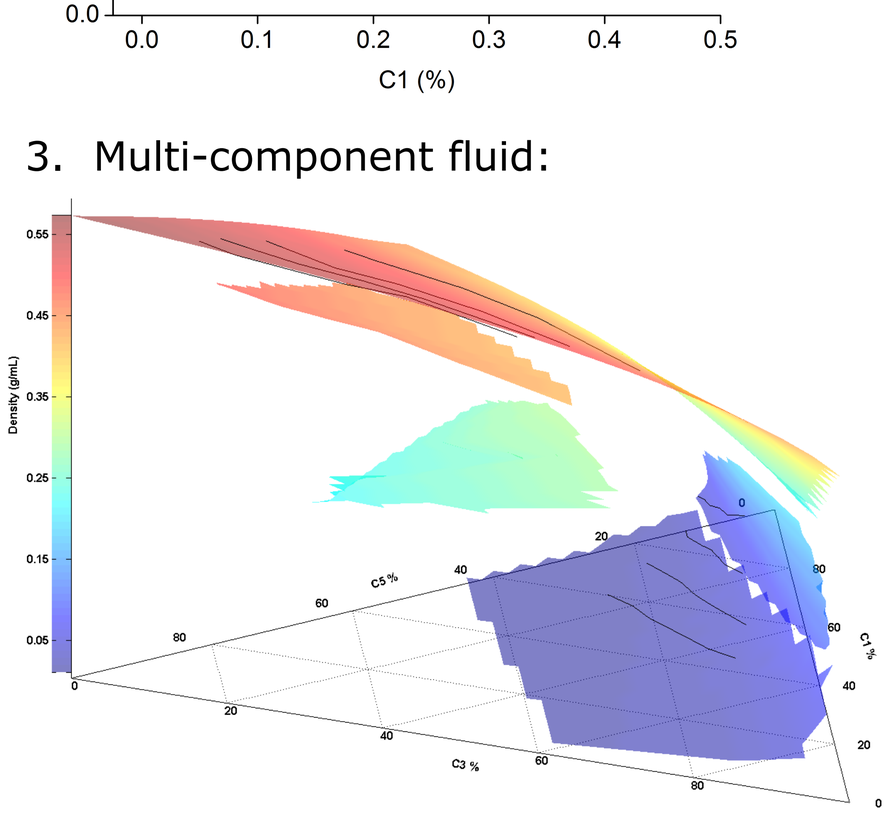


2. Two-component fluid:





3. Multi-component fluid:



4. Publication

Bikai J., Hadi N. (2016). Phase behavior of multi-component hydrocarbon systems in nano-pores using gauge-GCMC molecular simulation, *Fluid Phase Equilibria*, 425: 324-334.