



Contribution ID: 696

Type: Oral 20 Minutes

## Phase Equilibria in CO<sub>2</sub>-Multicomponent Hydrocarbon Systems in Shale Organic Nanopores: A Coarse Grained Molecular Simulation Study

Thursday, 17 May 2018 08:32 (15 minutes)

Studying the phase behavior of complex hydrocarbon and hydrocarbon/CO<sub>2</sub> mixtures in kerogen structures is extremely important for understanding the mechanisms involved in enhanced gas recovery, storage, and production of hydrocarbons from shale. The objective of this work is to determine the phase behavior of a number of binary, ternary, and multicomponent CO<sub>2</sub>/hydrocarbon systems using molecular dynamics simulation in three dimensional kerogen structure of type IIA. These systems include CO<sub>2</sub>/n-Hexadecane, CO<sub>2</sub>/n-Eicosane, CO<sub>2</sub>/n-Butane/n-Decane, and CO<sub>2</sub>/synthetic oil.

The kerogen molecule is prepared based on detailed structural analysis of NMR experiments. In order to build a representative solid state model of kerogen, eight kerogen molecules are placed in a periodic cubic cell. Once the initial configuration of kerogen molecules is prepared, constant-temperature constant-volume (NVT) simulations and then constant-temperature constant-pressure (NPT) simulations are performed to obtain the final structure. The SAFT- $\gamma$  coarse graining methodology is used to develop force fields for the fluid-phase behavior of hydrocarbon/CO<sub>2</sub> mixtures comprising CO<sub>2</sub> and n-alkanes. The densities, phase compositions, and volume of each phase in kerogen are determined at different overall compositions and pressures and compared with unconfined case.

For the final kerogen structure, density values are calculated and compared with the reported density range for kerogen density. A good agreement is found between the experimental densities and our kerogen molecular structure density. Calculated phase equilibria for the unconfined system (where experimental measurements are available) are in fair agreement with experimental data. The liquid phase density did not change significantly in confined case (in kerogen) compared with that of unconfined (or bulk). However, the heavier components tend to vaporize in kerogen structure compared with the unconfined case. For example, n-decane have much higher composition in vapor phase in kerogen compared to bulk condition. Furthermore, as the pore diameter increases, the phase envelopes approach the bulk conditions.

Experimental measurements of the phase behavior of hydrocarbon mixtures in confined systems are extremely difficult, if not impossible, with current technologies. This work is one of the few in-depth investigations of the phase behavior in organic matters of shale. The results of this study can potentially modify the equation of state for shale reservoirs and help in understanding the transport mechanism in nanoscale pores.

### References

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**Session Classification:** Parallel 9-A

**Track Classification:** MS 4.19: Rock/fluid Interactions and Their Impact on Flow and Transport in Geologic Media