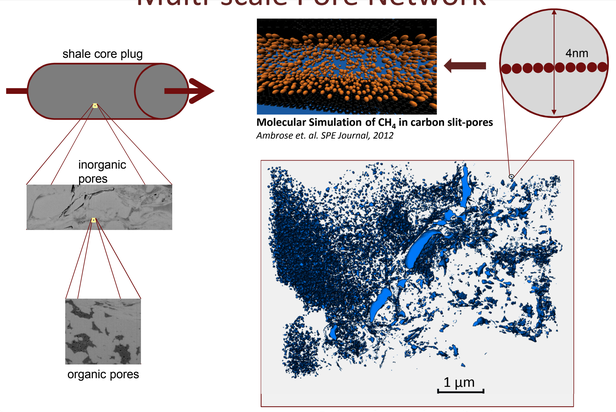
SAND2015-4704C

Fundamental Study of Disposition and Release of Methane in Shale Gas Reservoirs: Numerical Studies

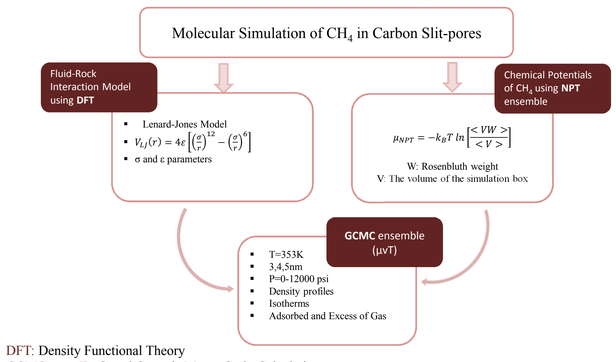
I. Y. Akkutlu[1], P.H. Weck[2], L. Criscenti[2], M.J. Rigali[2]2, D. Cristancho[1], and Y. Wang[2]

[1] Texas A&M University, College Station, Texas 77843, USA.
[2] Sandia National Laboratories, Albuquerque, New Mexico 87185-0754, USA.

Multi-scale Pore Network

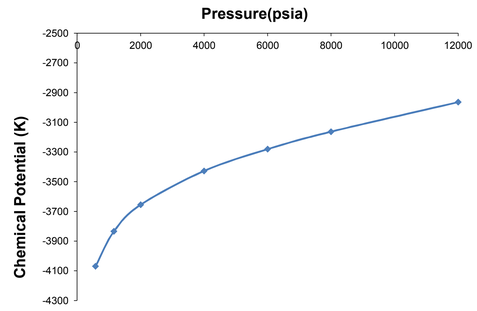


Methodology



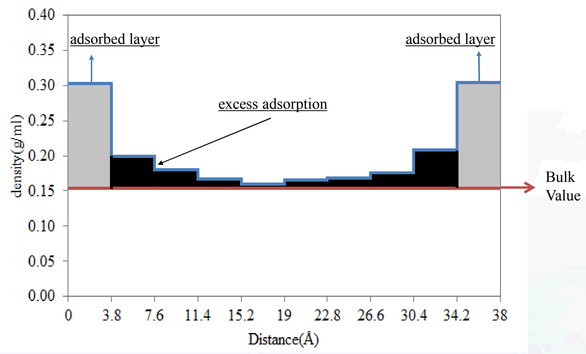
DFT: Density Functional Theory
GCMC or µVT : Grand Canonic Monte Carlo Calculations
NPT: Isothermal-isobaric ensemble

Chemical Potentials of CH_4 using **NPT** Ensemble

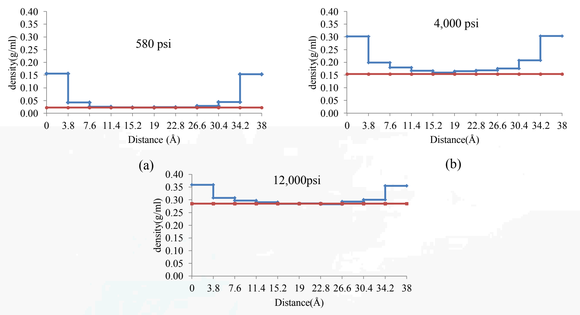


Chemical potential of CH_4 versus pressure using NPT calculations. The chemical potential increases with pressure. This information is needed as input for µVT calculations.

Density Profile for Methane in a Slit Pore

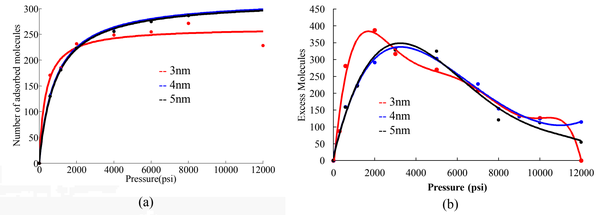


Isothermal Density Profile for CH_4 at 353K in a slit pore of 4nm



Density profile of CH_4 across the diameter of a 4nm slit pore at 353K and at (a) 580 psi, (b) 4,000psi and (c) 12,000 psi pore pressure. The density of CH_4 is not constant in the pore and higher densities are obtained near the wall (First Layer). The red lines are free gas values and the calculated density in the middle of the pore tend to match these free gas values.

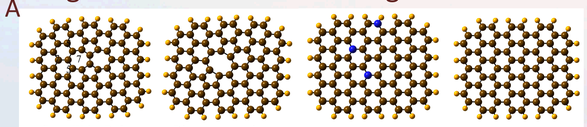
Isotherms at 353K of CH_4 in a slit pore



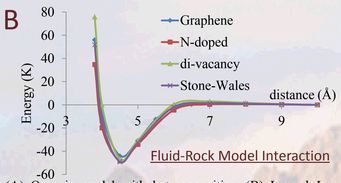
(Left) Adsorption isotherms for methane in a slit-shape pore with sizes 3, 4 and 5nm. The pore walls are pristine graphene. No significant variation is observed in the isotherms as the size of the pore increases because the surface area of the first adsorption layer does not change. (Right) Excess adsorption of CH_4 in a slit pore, excluding the first layer of adsorption by the walls. The excess amount is the largest in between 1,000-5,000 psi, which is a typical range for shale gas reservoir initial pressures

Organic Models with Heterogeneities-DFT

A



B



C

Model	ε(K)	σ(Å)
Graphene*	-44.00	3.95
di-vacancy	-46.78	4.00
N-doped	-48.32	3.90
Stone-wales	-49.18	3.92

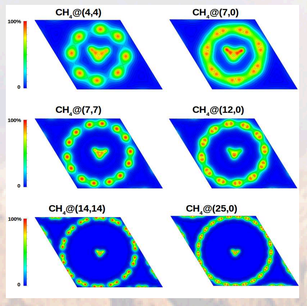
(A) Organic model with heterogeneities, (B) Lenard Jones potential profile for the interaction between methane and organic models and (C) Lenard Jones parameters obtained for the methane-organic wall interactions in the presence of the heterogeneities. The epsilon parameter slightly varies with the heterogeneities on the surface.

Carbon Nanotube Models-DFT

Density functional theory (DFT) calculations have been carried out using the VASP code within the generalized gradient approximation with the Perdew-Burke-Ernzerhof exchange-correlation functional (GGA/PBE) for the structural optimization of the following structures:

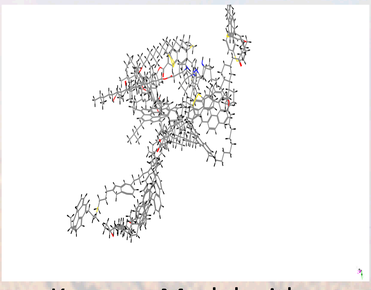
Prisitine 3-D periodic single-walled carbon nanotubes (SWCNT): calculations were carried out for both armchair- and zigzag-type SWCNTs with similar diameters, i.e. (4,4) (5.42 Å diameter), (7,0) (5.48 Å diameter), (7,7) (9.49 Å diameter), (12,0) (9.39 Å diameter), (14,14) (18.98 Å diameter) and (25,0) (19.57 Å diameter).

CH4@SWCNTs: the structure and interaction of one CH4 molecule inside (4,4), (7,0), (7,7), (12,0), (14,14) and (25,0) SWCNTs was investigated; charge distribution maps of the CH4@SWCNTs were obtained.



Molecular Modeling of Methane-Kerogen Interactions

This study is focused on kerogen interactions with methane, methane + H_2O, methane + H_2O + CO_2. The work will lead to the development of both thermodynamic and transport properties of methane in kerogen nanopores.



Kerogen Model with Molecular Formula $C_nH_mO_sS_t$

Harold Vance Department of PETROLEUM ENGINEERING TEXAS A&M UNIVERSITY

Sandia National Laboratories

This work is supported by Sandia National Laboratories under its Laboratory Directed Research and Development program.
Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

U.S. DEPARTMENT OF ENERGY — National Nuclear Security Administration