Molecular modeling of interaction between kerogen and pore fluid

TUAN A. HO,* YIFENG WANG, LOUISE J. CRISCENTI

Sandia National Laboratories, Albuquerque, New Mexico 87185, USA (*taho@sandia.gov)

Kerogen is defined as insoluble organic matter found in sedimentary rocks. During the kerogen maturation process, kerogen breaks down into petroleum products, including methane. Once methane is produced, it resides in and is transported through the kerogen pore network. Understanding the interaction of gas with the kerogen, and transport of gas through the kerogen matrix are therefore important for shale gas production. We employ molecular modeling to investigate methane (CH_4) and carbon dioxide (CO_2) adsorption and release from nanoporous kerogen structures, the effect of water on CH_4 and CO_2 transport, the volumetric strain of the kerogen bulk structure associated with gas adsorption, and the wettability of kerogen under subsurface conditions. Our results show that kerogen retains more CO_2 than CH_4, and that the kerogen structure expands up to 5% and 11% at ~200 atm CH_4 and CO_2 pressure, respectively. Our simulations also indicate that gas release from the kerogen matrix is characterized by two steps; first the fast release of pressurized free gas followed by slow release of adsorbed gas. Significant amounts of gas in kerogen can be trapped in isolated pores and thus are not recoverable. Furthermore, kerogen wettability varies from wetting to non-wetting depending on the subsurface conditions. Our results provide insight into kerogen properties and its interaction with multiple chemical components under subsurface environments.

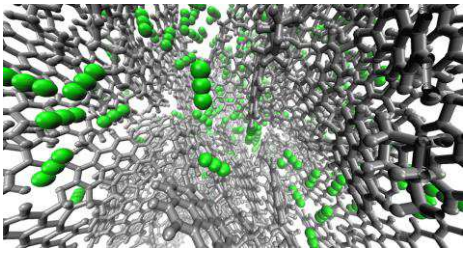

Fig. 1 CO_2 molecules (green) reside within kerogen (silver) pore network

Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. This research was funded by a DOE National Energy Technology Laboratory project (to Y. Wang).