Molecular Modeling of Carbon Dioxide Sequestration Utilizing A Molecular Representation of Pocahontas No. 3 A Low-Volatile Bituminous Coal

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OBJECTIVE

Utilize a molecular modeling approach to investigate CO_2 sequestration issues in coal.

ACCOMPLISHMENTS TO DATE

A large-scale molecular representation of Pocahontas No.3 coal was generated. This model was constructed based on a the review data of Stock and Muntean[1], and the combination of Laser Desorption Mass Spectroscopy, and HRTEM[2], enabling an appropriate molecular weight distribution and structural diversity to be implicitly represented. The molecular representation contains over 20,000 atoms and was utilized to test our understanding of coal behavior during carbon dioxide sequestration. Carbon sequestration requires that carbon dioxide be bound within the pores of the coal. The sorption rate and carbon dioxide sequestration capacity depends on the nature and connectivity of the pore structure. The transport, of carbon dioxide and other molecules of interest, is dependent on the size, distribution, connectivity, and shape of the pores, and the sorption or diffusion processes that occur. The micropore size distribution was determined for the model. Representation of the coal model containing appropriate quantities of: methane, carbon dioxide, and equilibrium moisture have been generated with low-level molecular modeling approaches. Force field parameterization has been performed for future higher-level molecular simulations.

FUTURE WORK

Investigate coal swelling/contraction with the appropriate gases. Investigate pore interconnectivity and diffusion of gases and their mixtures through the pore structure.

LIST OF PAPER PUBLISHED, U.S. PATENT/PATENT APPLICATION(S), CONFERENCE PRESENTATIONS, AWARDS RECEIVED AS A RESULT OF SUPPORTED RESEARCH, STUDENTS SUPPORTED UNDER THIS GRANT

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