Carbon Dioxide Sequestration in a Bituminous Coal Representation

Marielle R. Narkiewicz & Jonathan P. Mathews
Department of Energy & Geo-Environmental Engineering & The Energy Institute
The Pennsylvania State University

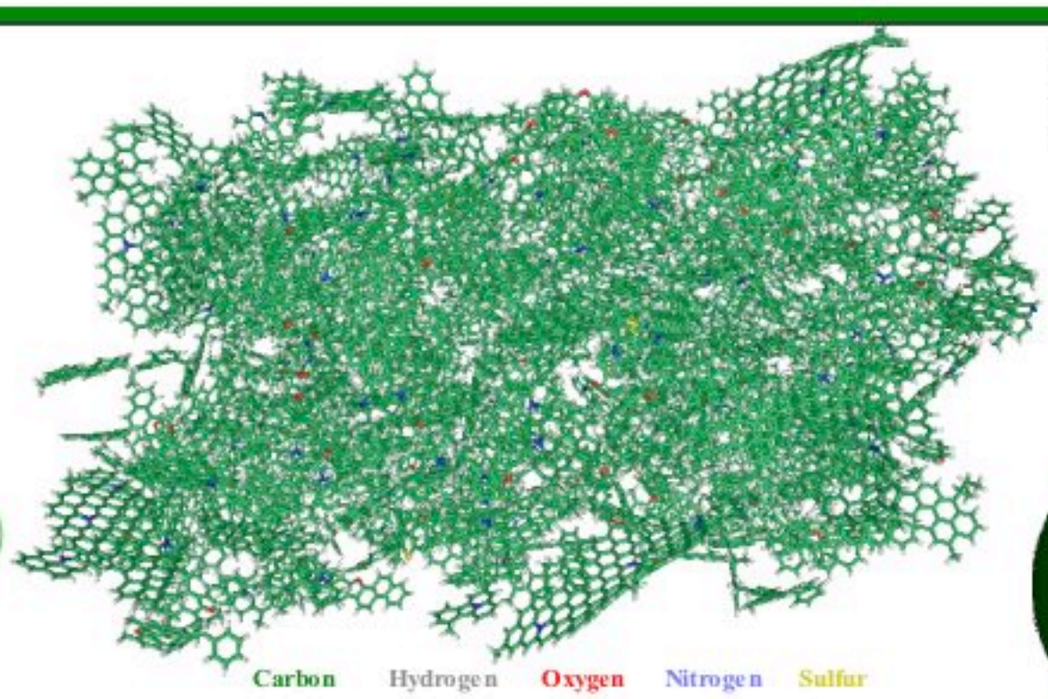
Objective

A molecular representation of a bituminous coal was constructed and used for visualization of sequestration. Specifically, small sorbates (carbon dioxide, methane, and water) were evaluated on their behavior inside the structure.

Model Creation

A model of bituminous coal was generated based on experimental data, such as HRTEM, as seen below.

a) HRTEM image b) colored by length c) colored by angle[1]

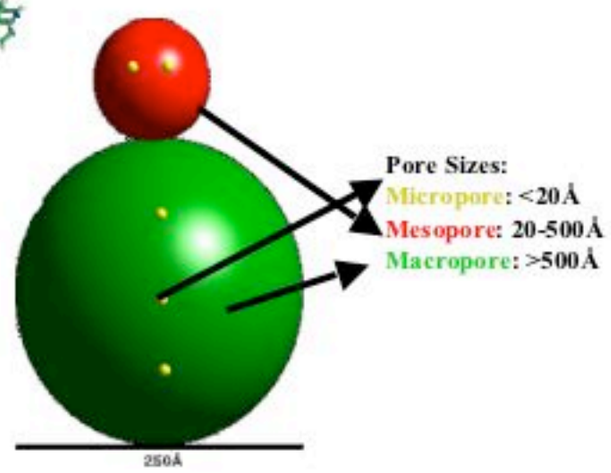


Carbon Hydrogen Oxygen Nitrogen Sulfur

$C_{13,471}H_{8,143}O_{113}N_{181}S_{23}$

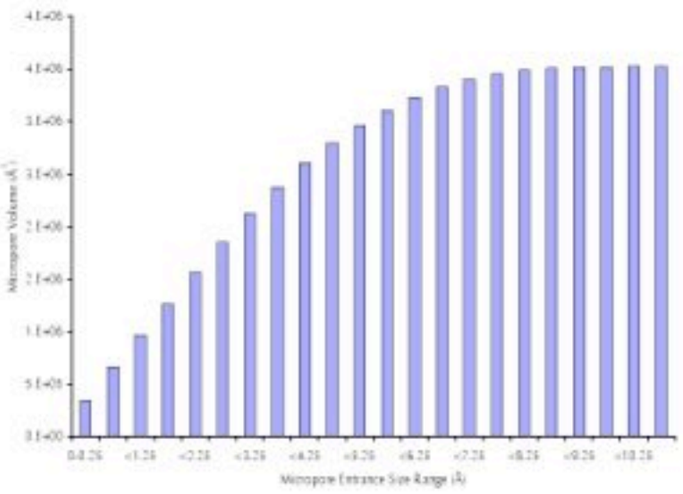
Density: 1.27g/cm^3

Due to the scale of the model, only micropores are present in the structure. Micropores are the important location for the carbon dioxide storage within coal.

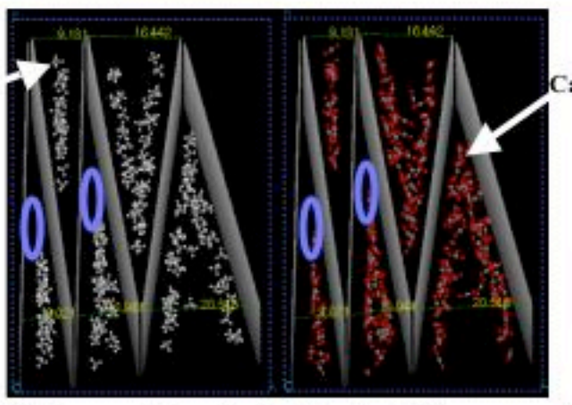


Data Collection

This plot shows that all of the micropore volume is occupied by molecules with an entrance size of at least 10.75Å.



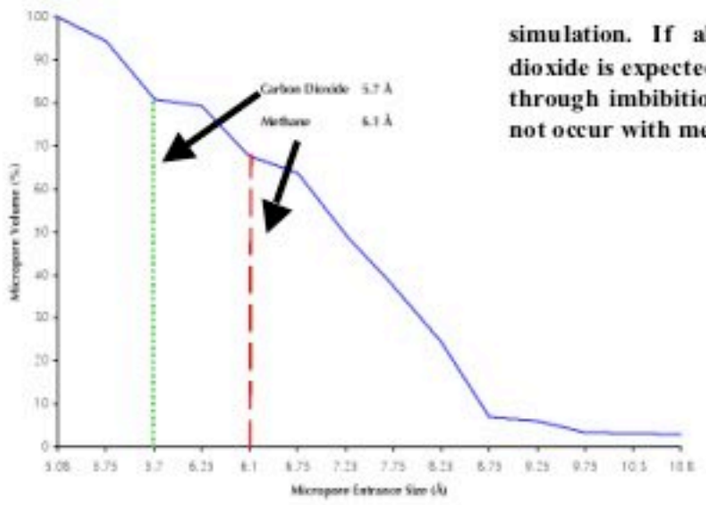
Methane



Carbon Dioxide

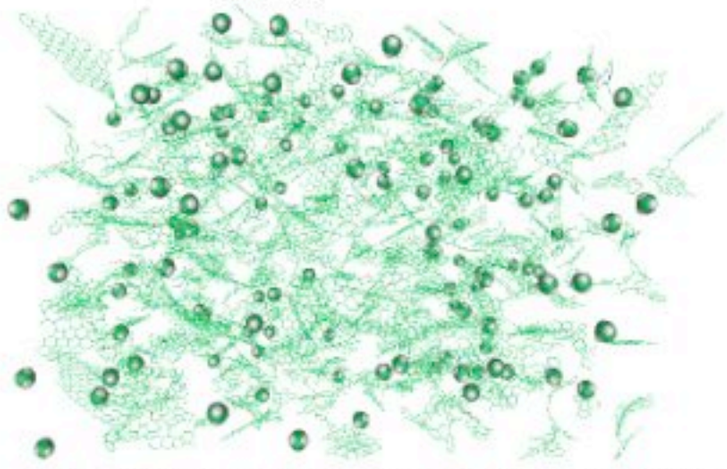
This figure confirms that molecular sieving occurs in these idealized rigid, v-shaped pores. Sieving occurs around 5Å, in which carbon dioxide can access these smaller pore entrances that methane cannot.

The micropore volume of the structure was determined and plotted as a function of entrance size of both carbon dioxide and methane. It is shown that carbon dioxide can enter 81% of the micropore volume, while methane can only enter 68% of the micropore volume. The structure was kept rigid during this simulation. If allowed to relax more carbon dioxide is expected to access the micropore volume through imbibition into the structure, which does not occur with methane.



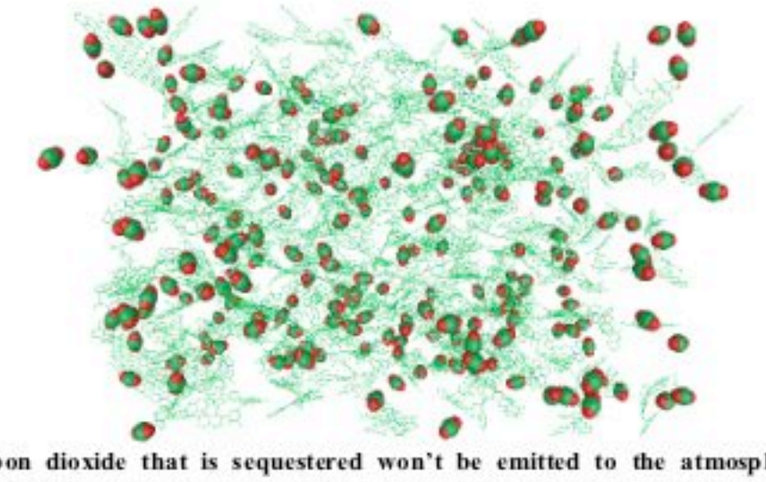
Model Utilization

Methane



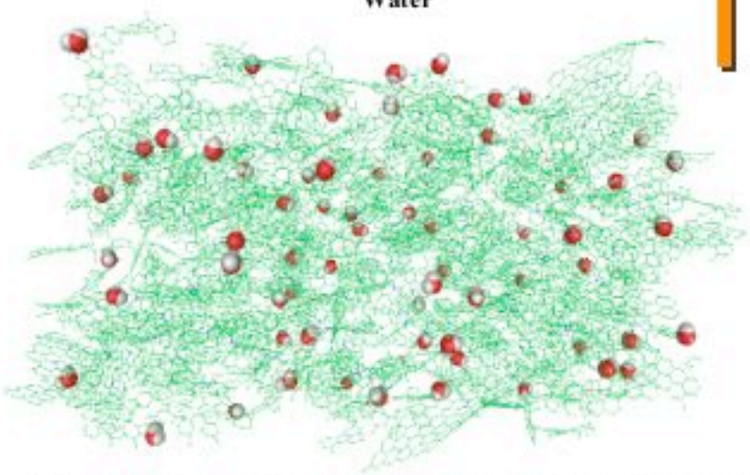
The methane from the coal bed can be used as a domestic energy source. This representation shows an average amount (470 Scf/ton) of methane found in bituminous coal based on the molecular mass that this model has.

Carbon Dioxide



Carbon dioxide that is sequestered won't be emitted to the atmosphere, and therefore won't add to the potential global climate change. Based on the 2:1 CO_2 to CH_4 ratio expected in bituminous coal, this model has twice the number of methane molecules represented as carbon dioxide molecules.

Water



Water is known to reduce the capacity of CO_2 that the coal bed can hold. This representation depicts the as-received moisture of bituminous coals, which is based on the molecular mass of this structure.

Contact Information: Address: 131A Hosler Building University Park, PA 16803 Voice: 814.865.2711 Email: mrn134@psu.edu
Address: 126 Hosler Building University Park, PA 16803 Voice: 814.863.6213 Email: jmathews@psu.edu

1. Mathews, J. P.; Jones, A. D.; Pappano, P. J.; Hurt, R.; Schobert, H. H. In *New Insights into Coal Structure from the Combination of HRTEM and Laser Desorption Ionization Mass Spectrometry*, 11th International Conference on Coal Science, San Francisco, CA, 2001.