A Molecular Model for Illinois No. 6 Argonne Premium Coal: Moving Toward Capturing the Continuum Structure

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Results and Discussion

The largest molecular model constructed to date for Illinois No. 6 Argonne Premium coal[1] contains 50,789 atoms within 728 cross-linked aromatic clusters. The aromatic fringe size distribution was determined from multiple high-resolution transmission electron microscope (HRTEM) lattice fringe micrographs and was duplicated with automated construction protocols (Fringe3D) in molecular modeling space. Organic oxygen, nitrogen, and sulfur functionalities were incorporated primarily into the aromatic clusters according to X-ray photoelectron spectroscopy and X-ray adsorption near-edge structure spectroscopy data. Aliphatic carbons are in the form of cross-links (bridges and loops) and pendant alkyl groups based on the combination of laser desorption ionization mass spectrometry (LDIMS), ruthenium ion catalyzed oxidation, elemental analysis, and NMR data. Bound and bulk water were also included. The coal molecules were constructed by use of Perl scripts developed in Materials Studio. The large-scale model captures a broad and continuous molecular weight distribution in accordance with LDIMS data ranging from 100 to 2,850 Da, enabling inclusion of structural diversity to capture a portion of the continuum structure. A theoretical pyridine extraction yield, determined by a group contribution approach, accords with the experimental value. The extract and residue representations were generated from the large-scale Illinois coal model and are consistent with NMR, elemental analysis, and LDIMS trends. The distribution of heteroatomic classes and double bond equivalents is also well-defined experimentally, based on electrospray ionization Fourier transform ion cyclotron resonance mass spectrometry. Those data further constrain the molecular weight and are consistent with the limited scale of the pyridine extract model heteroatom classes.

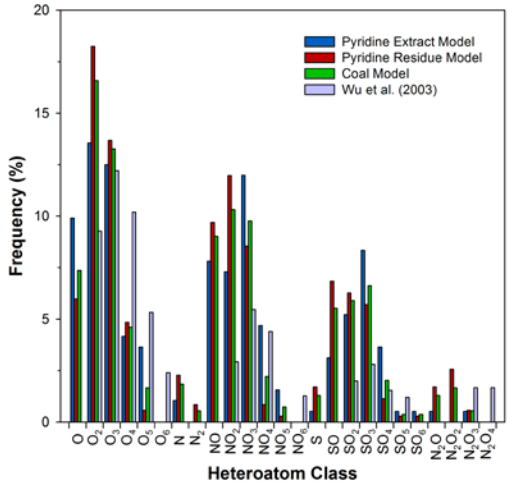

Figure 1. Distribution of the most abundant heteroatomic classes identified in the coal model and its respective pyridine extract and residue models. Experimental FT-ICR MS data[2] for the pyridine extract of Illinois No. 6 coal is also included.

Acknowledgements

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References

[1] Castro-Marcano, F., *et al.*, Fuel **95**, 35-49 (2012).
[2] Wu, Z. G., *et al.*, Energy & Fuels, **17**, 946-953 (2003).