Characterization of Pine Pellet and Peanut Hull Pyrolysis Bio-Oils by Negative-Ion Electrospray Ionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry

J. M. Jarvis (FSU, Chemistry), A. M. McKenna (NHMFL, Chemistry) R. N. Hilten (U. Georgia, Engineering), K. C. Das (U. Georgia, Engineering), R. P. Rodgers (FSU, NHMFL, Chemistry), and A. G. Marshall (FSU, NHMFL, Chemistry)

Results and Discussion

Pyrolysis of solid biomass, in this case pine pellets and peanut hulls, generates a hydrocarbon-rich liquid product (bio-oil) consisting of oily and aqueous phases. Here, each phase is characterized by negative-ion electrospray ionization Fourier transform ion cyclotron resonance mass spectrometry (ESI FT-ICR MS) to yield unique elemental compositions for thousands of compounds. Bio-oils are dominated by O_x species: few oxygens per molecule for the oily phase and many more oxygens per molecules for the aqueous phase (see **Figure 1**). Thus, the increased oxygen content per molecule accounts for its water solubility. Peanut hull bio-oil is much more compositionally complex and contains more nitrogen-containing compounds than pine pellet bio-oil. Bulk C, H, N, O, and S measurements confirm the increased levels of nitrogen-containing species identified in the peanut hull pyrolysis oil by FT-ICR mass spectrometry. The ability of FT-ICR MS to identify and assign unique elemental compositions to compositionally complex bio-oils based on ultrahigh mass resolution and mass accuracy is demonstrated.[1]

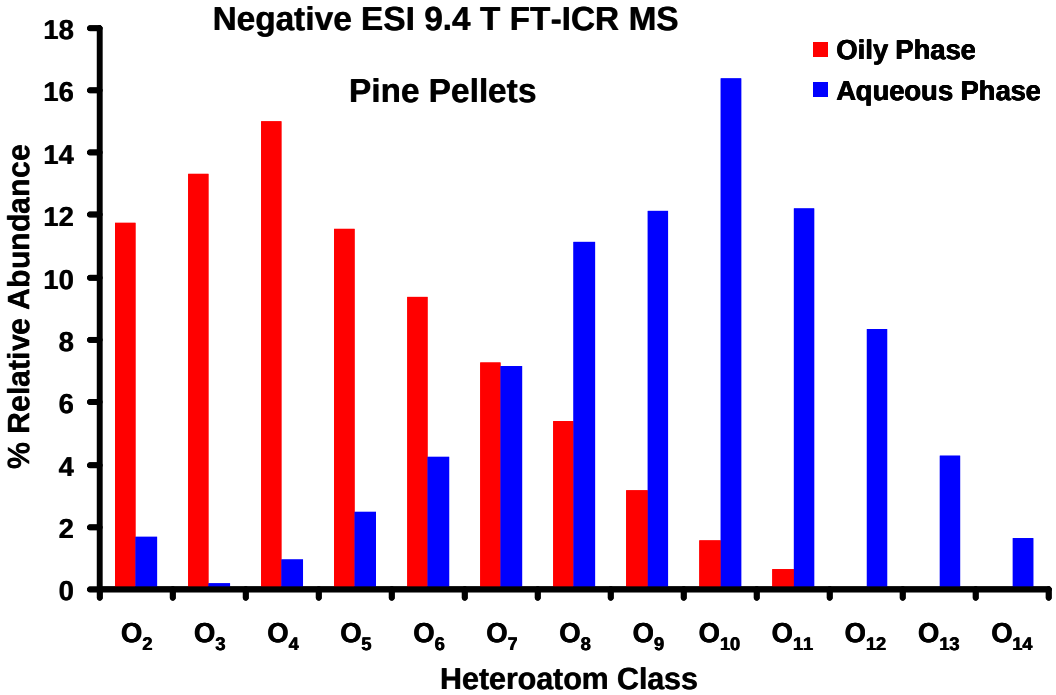

Figure 1. Heteroatom class distribution for the pine pellet oily (red) and aqueous (blue) phases derived from negative ESI 9.4 T FT-ICR mass spectra. The most abundant class in the oily phase contains 4 oxygens whereas the most abundant class in the aqueous phase contains 10 oxygens. Only classes with greater than 1% relative abundance in either phase are shown.

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References

[1] Jarvis, J. M., *et al.*, Energy & Fuels, **26**, 3810-3815 (2012).