FT-ICR MS Analysis of Blended Pine-microalgae Feedstock HTL Biocrudes

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Results and Discussion

Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS) is utilized for direct comparison of the chemical composition of hydrothermal liquefaction biocrudes from of 100% pine, 100% algae, 75:25 pine:algae, and 50:50 pine:algae feedstocks. This analysis reveals that of the 72:25 and 50:50 pine:algal HTL biocrudes is essentially a composite of the two parent feeds (i.e., pine and algae) with a lower relative abundance of Ox species and a higher relative abundance of nitrogen-containing species than the pine HTL biocrude. Alternatively, the biocrude blends have a lower relative abundance of nitrogen-containing species where N>2 than the algal HTL biocrude. The 75:25 pine:algal HTL biocrude has more elemental formulae in common with the pine HTL biocrude than the 50:50 blend; however, both blends have more elemental formulae in common with the algal HTL biocrude. Interestingly, >20% of the elemental formulae assigned to monoisotopic peaks within the 75:25 and 50:50 biocrude blends are species not present in either the pine or algal HTL biocrudes. The highest relative abundance of these new species belong to the N2O4-6 classes, which correspond to heteroatom classes with a moderate number of nitrogen atoms and higher number of oxygen atoms per molecules than the species within the pure algal HTL biocrude. Compositionally, the novel species have the same structural motif but are of higher DBE and carbon numbers than the species within the algal HTL biocrude. These original species are most likely generated from reactions between molecules from both feeds, which results in compounds with higher oxygen content than typically seen in the algal HTL biocrude but also higher nitrogen contents than observed in the pine HTL biocrude.

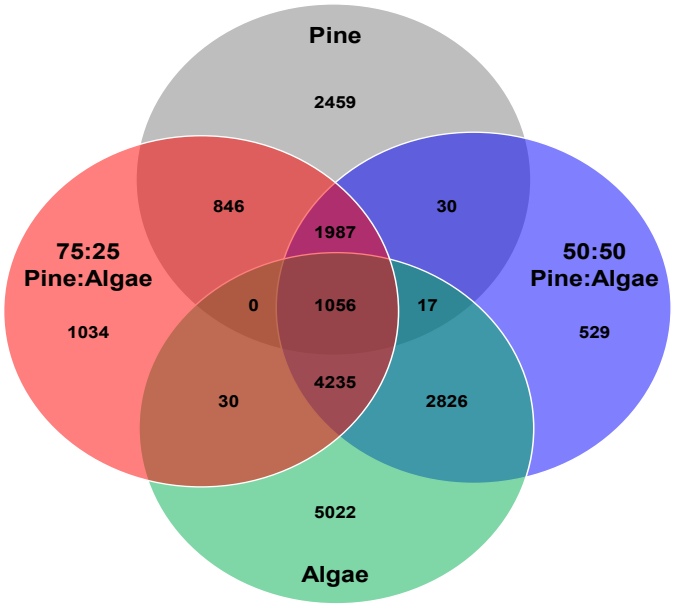

Fig.1 Venn diagram depicting the number of monoisotopic (+) APPI molecular formulae in common between the 100% pine (top circle), 75:25 pine:algal (left circle), 50:50 pine:algal (right circle), and 100% algal (bottom circle) HTL biocrudes. There are 5 molecular formulae that are only common to the pine and algal biocrudes and 2010 molecular formulae that are only in common to the 75:25 and 50:50 pine:algal blends that cannot be visualized by the Venn diagram. Proportions not to scale.

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Reference

[1] Jarvis, J., *et al*., Fuel **216**, 341-348 (2018)