



Analysis of Petroleum Products by Gel Permeation Chromatography Coupled Online with Inductively Coupled Plasma Mass Spectrometry and Offline with Fourier Transform Ion Cyclotron Resonance Mass Spectrometry

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Results and Discussion

We have examined the aggregation behavior of a typical atmospheric residue feedstock by gel permeation chromatography (GPC). The size profiles for compounds containing sulfur, vanadium, and nickel were determined online from elemental detection by inductively coupled plasma (ICP) mass spectrometry. Four fractions that vary in aggregation state were analyzed by NHMFL's positive atmospheric pressure photoionization (APPI) 9.4 T Fourier transform ion cyclotron resonance mass spectrometer (APPI FT-ICR MS—see Figure 1). Results showed an inverse relationship between fraction aggregate size and monomer ion yield and revealed that aggregation tendency did not correlate with higher polar or aromatic species abundance. Aggregation in the atmospheric residue more closely correlated with increased relative abundance of larger and more aliphatic compounds. The molecular composition of the GPC aggregate fractions suggests that nonpolar intermolecular forces between saturated, longchain alkyl substituents contribute more to aggregation than pi-pi interactions.

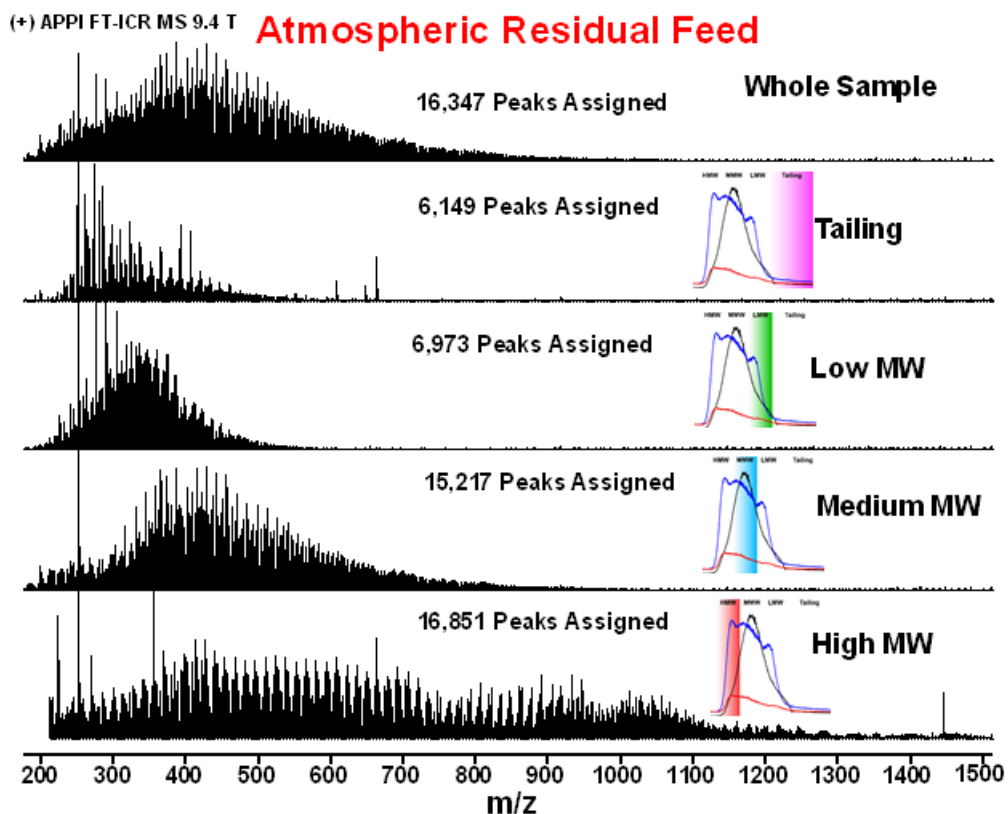


Fig. 1. Positive ion atmospheric pressure photoionization (APPI) broadband 9.4 T FT-ICR mass spectra for the feedstock atmospheric residue and its aggregate fractions.

Acknowledgments

Work supported by National Science Foundation Cooperative Agreements No. DMR-11-57490 and DMR-1644779, the State of Florida, Conseil Régional d'Aquitaine (20071303002PFM), and FEDER (31486/08011464). The authors thank TOTAL for supplying oil samples and Steven M. Rowland for helpful discussions and feedback.

References

[1] Putman, J. C., *et al.*, *Energy & Fuels*, **32**(12), 121198-12204 (2018).