



Correlations between Molecular Composition and Adsorption, Aggregation, and Emulsifying Behaviors of PetroPhase 2017 Asphaltenes and Their Thin-Layer Chromatography Fractions

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Introduction

The optimization of refinery processes in the petroleum industry requires comprehensive knowledge of the effects of heavy oil fractions, such as asphaltenes, on the crude oil deposit behavior. The immense compositional complexity of asphaltenes changes between crude oils from different reservoirs as a result of variations in the source rock temperature, reservoir depth and pressure, and geologic conditions. Asphaltenes are operationally defined as the fraction of crude oil insoluble in paraffinic solvents (e.g., *n*-heptane and *n*-pentane) but soluble in aromatic solvents (e.g., benzene and toluene); they are also, and arguably, the most polydisperse and compositionally complex organic mixture known. In this work, we access the molecular composition of the thin-layer chromatography fractions from PetroPhase 2017 asphaltenes by FT-ICR MS and correlate composition to near-infrared (NIR) scattering measurements of heptane/toluene (HepTol) dispersions.

Experimental

Positive atmospheric pressure photoionization (+APPI) coupled to 9.4 T FT-ICR mass spectrometry was used to analyze thin layer chromatography fractions derived from the interlaboratory sample *PetroPhase 2017*.

Results and Discussion

PetroPhase 2017 asphaltenes were fractionated by thin-layer chromatography (TLC) and characterized by FT-ICR MS to correlate asphaltene adsorption and aggregation to aromaticity, heteroatom content, and alkylation. TLC fractionation of asphaltenes produces three TLC fractions determined by retention on silica gel. Subsequent characterization by positive-ion atmospheric pressure photoionization (APPI) FT-ICR MS reveals that the most retained species on silica plates consist of highly saturated, polar asphaltenes enriched with heteroatom-containing groups and low DBE values, in contrast to medium- and low-retained species. Near infrared (NIR) radiation scattering measurements of heptane/toluene (HepTol) dispersions, by Turbiscan Lab, of each fraction and the whole asphaltene sample identify a direct correlation between asphaltene adsorption on TLC silica plates and aggregation: The more the fraction is retained on the silica, the faster it precipitates. In addition, emulsion stability tests suggest that the most polar asphaltene fraction produces the most stable emulsions. These findings suggest a clear and distinct relationship between asphaltene polarity, aggregation, and emulsion stability.

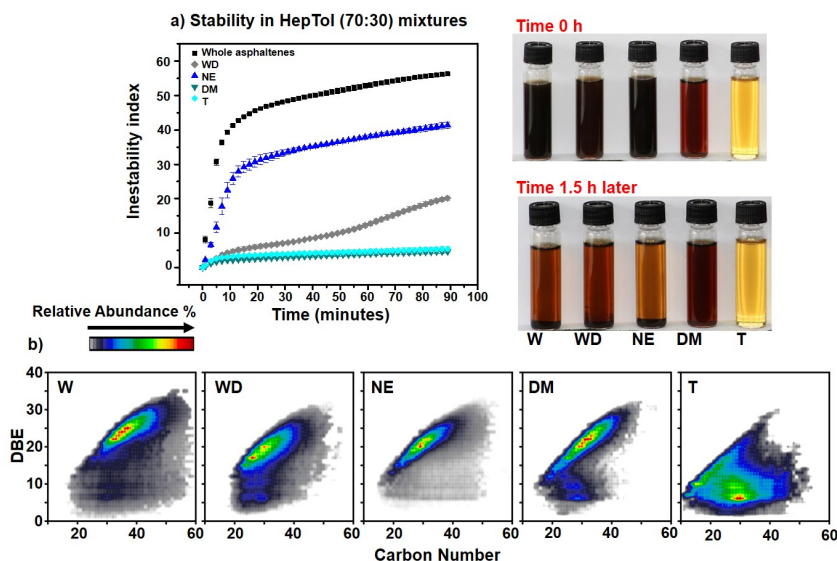


Figure 1. a) Stability of whole asphaltenes W and TLC fractions WD, NE, DM, and T fractions determined by Turbiscan Lab; b) DBE versus carbon number plots for the class S_1 for whole asphaltenes and TLC fractions.

Conclusions

Collectively, the results suggest that not all asphaltene species exhibit a similar adsorption/aggregation/molecular composition, and indicate a direct relationship between asphaltene polarizability, aggregation tendency, and emulsion stability.

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References

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