Petroleomics: Elucidation of Chemical Composition and Functionality of Compounds Resistant to Asphaltene Inhibitors

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Asphaltenes are the most aromatic and polar constituents found in crude oil and have been defined as those species that are insoluble in *n*-heptane. They are an important class of crude oil components simply because of the problems associated with flocculation during routine refining procedures. Asphaltene inhibitors have been employed to reduce the rate and extent of flocculation during reservoir extraction and refining procedures. We have employed the use of both low-resolution mass spectrometric techniques for the determination of unique fragmentation patterns for asphaltene-like molecules and high resolution mass spectrometry for the determination of chemical composition of both bulk oil and asphaltene samples. To date, we have determined the need for better extraction of pure asphaltenes and fragmentation of a number of asphaltene-like molecules. Future work will include a novel titration experiment to fractionate asphaltenes and the determination of specific inhibitor compounds to prevent flocculation.

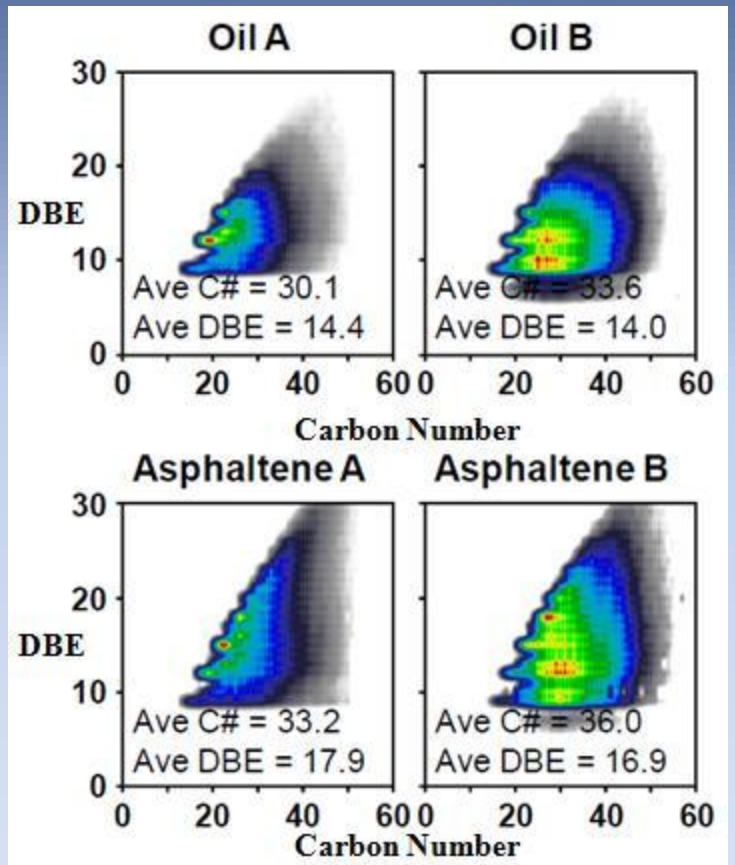

Figure 1. (-) ESI FT-ICR N-Class (Pyrrole-type compounds) composition of two representative oils and extracted asphaltenes.