Characterization of Asphaltene Nano-aggregation using Molecular Dynamics

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Asphaltenes are aromatic compounds that are problematic to the oil industry due to their ability to form large nano-aggregates that clog oil pipes, decreasing oil production and increasing costs. Their ability to aggregate stems from the conjugated ring systems, which are capable of pi stacking. The formation of nano-aggregates decreases the solubility of the asphaltene constituents, which leads to pipeline obstructions. It is thought that the alkyl constituents on the conjugated ring system are an important component of aggregation. Using the molecular dynamics software suite AMBER, *in vacuo* simulations of representative asphaltenes allowed for the characterization of aggregation, calculation of energetics and the description of nano-aggregates with the primary goal being to develop an aggregation inhibitor and to understand the process of nano-aggregate formation.