Investigation of the aggregation of asphaltenes using Molecular Dynamics

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Abstract

Asphaltenes are organic compounds composed of aromatic and saturated hydrocarbons that are commonly found in crude oil. They are problematic in that they tend to aggregate, forming a thick sludge that ultimately clogs pipelines. Previous studies have shown that pi stacking between the aromatic rings is a mechanism for the clustering of asphaltenes. The compound first forms nanoaggregates, which becomes clusters at higher concentrations. Furthermore, it is assumed that the alkyl groups on the aromatic rings play an important role in the aggregation of the compound. Our work utilizes Amber 14, a molecular dynamics software, to study the importance of the alkyl chains in the nano-aggregation of asphaltenes (Figure 1). Simulations of the compound will be run in-vacuo to generate trajectories of asphaltene aggregation. The aggregation properties of the compound will be analyzed through the determination of the binding free energy and entropy of the system.

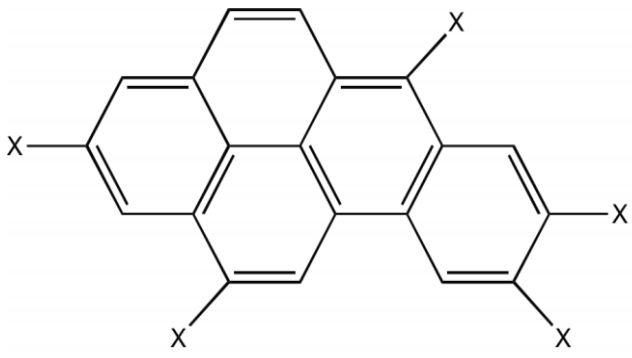

Figure 1. Model structure used to study nano-aggregation of asphaltenes. A variation of n-alkyl chains, OH, NH, and SH groups will be added to the aromatic carbons in place of the X's to investigate aggregation patterns of these compounds.