A Computational Investigation of the Aggregation of Asphaltenes with Various Solvents and Aggregation Inhibitors

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Asphaltenes are chemical compounds found in crude oil that have a natural tendency to aggregate. These asphaltene aggregates tend to have lower solubility, which can result in the formation of a solid, wax-like material that clogs oil pipelines and causes a loss of time and resources during the oil refining process. It is theorized that aromatic solvents are able to subside such aggregations through π-stacking with asphaltenes, while non-aromatic solvents typically lead to increased aggregation. We hope to describe the process of aggregation at the atomic level using computational chemistry. Three solvents were used in these simulations (heptane, hexanol and toluene) along with a commercial aggregation inhibitor (limonene). These solvents were chosen to explore the effect of aggregation on solvents with varying molecular properties. The systems were run using unrestrained MD and were analyzed using MM-PBSA to determine the free energy of each system as a function of aggregation time. We also measured the average distance between asphaltene molecules to quantify aggregation. Through this investigation, we hope to gain a better understanding of how certain solvents interact with asphaltenes and the reason why inhibitors have the potential to stop aggregation so that we can use this information to develop new inhibitors to prevent asphaltene aggregation.

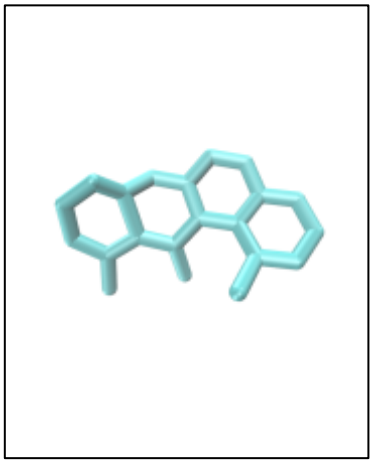

Figure 1. The asphaltene used in this experiment containing four fused aromatic, six carbon rings and three methyl “arms”.