Asphaltene self-association: Modeling and effect of fractionation with a polar solvent - DTU Orbit (18/08/2019)

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The self-association of asphaltenes in toluene is believed to occur step-wise, rather than by the formation of micelles. A number of step-wise models have been used to fit the calorimetric titration of asphaltenes in dried toluene solutions, with excellent results. All the models are based on chemical reactions equivalent to the ones found in polymerization. The study shows that the choice of the average properties of asphaltenes, such as the molecular weight, is critical in the final value of the parameter of interest, namely the average heat of self-association ΔH(a). The low values of ΔH(a) obtained suggest that a fraction of asphaltenes is not active in the calorimetric experiments. Asphaltenes from Venezuela (LM1) and Mexico (KU) have been fractionated by precipitation with a mixture of acetone and toluene. It is considered that the most polar compounds are collected in the soluble fraction. A calorimetry study was performed on the two fractions, and the results show that the soluble fraction (SOL) has a much higher heat developed than the insoluble fraction (INS). This suggests again that a fraction of asphaltenes is not active in the calorimetric experiments, either because it does not self-associate or because the dilution effect is not strong enough to break the aggregates. Fluorescence and IR spectroscopy experiments confirm there is self-association in INS fraction, leading to the conclusion that asphaltene aggregates are formed by bonds of different strengths. The stronger aggregates would be predominantly in INS fraction and would be inactive in the calorimetric experiments.

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