Calculation of Solubility Parameters of Crude Oil Systems as a Function of Pressure, Temperature and Composition using Experiments, Thermodynamic Modeling and Molecular Simulations

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Asphaltenes are the heaviest and most complex fraction of the crude oil. They are polydisperse and are defined as a solubility class which is soluble in aromatic solvents and insoluble in n-alkanes. Asphaltenes can precipitate and deposit in wellbores due to changes in temperature, pressure and composition. Such asphaltene deposition problems reduce the oil production and cost millions of dollars in mitigation and remediation efforts. Our group focuses on the development and implementation of advanced thermodynamic models and experiments to address the thermo-physical characterization and the phase behavior of crude oils in general and asphaltene precipitation in particular. Solubility parameter significantly influences the asphaltene precipitation behavior and is therefore a critical parameter in the context of understanding flow assurance issues related to Asphaltenes. This work focuses on the exploration of the solubility behavior of asphaltenes in various model crude oil samples at a molecular level by calculating solubility parameters of the mixtures over a wide range of temperatures and pressures. Based on previous work, the solubility parameter can be correlated with the density and the refractive index at ambient conditions. By measuring the density and the refractive index data, experiments can be executed to evaluate the solubility parameter at ambient conditions. Using this information and advanced equation-of-state modeling, solubility parameters over wide range of temperatures and pressures (covering reservoir/wellbore conditions) are calculated and will be presented. Molecular dynamics simulations in predicting solubility parameter values of solvent mixtures and asphaltene molecular models under reservoir conditions will also be presented.