A Molecular Model for Upstream Engineering Applications: Phase Behavior, Interfacial Properties, and Microstructure

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Abstract: Simulation of flow assurance issues, compositional grading, and enhanced oil recovery requires accurate modeling of phase behavior, transport properties, interfacial properties, and molecular level self-assembly of surfactant formulations. Past approaches in the industry have required specialized thermodynamic models for varying conditions and for each separate phase with sometimes unsatisfactory results. Advances in statistical mechanics at Rice University are enabling engineers to predict fluid properties in the hydrocarbon, aqueous, and gaseous phases as well as the interfacial properties between these phases with a single unified model.

The approach taken at Rice University is based on our SAFT equation of state. This model is widely applied in industry to describe the phase behavior of complex fluids from high performance polymer solutions to asphaltene phase behavior. The model is also used to predict partitioning of inhibitors between aqueous and hydrocarbon phases. In this presentation, the molecular basis of the SAFT approach will be described. Applications of the SAFT model to asphaltene phase behavior and deposition as well as compositional grading of asphaltenes will be presented. Successes in predicting water content in hydrocarbons using SAFT will also be discussed. Further extension of the model in the form of a classical density functional theory to predict interfacial properties such as surfactant behavior will be presented.

Biography: Professor Walter Chapman is the Associate Dean of Engineering for Energy Research and the William W. Akers Chair Professor of Chemical Engineering at Rice University. He is widely recognized in industry and academia for his molecular models to predict phase behavior and interfacial properties of complex fluids in the energy, petrochemical, and polymer industries. Among Walter's publications are some of the highest cited papers in Industrial & Engineering Chemistry Research (I&ECR) and in Fluid Phase Equilibria. Walter has been recognized with the Donald L. Katz award from the Gas Processors Association, multiple university wide teaching awards, and an Outstanding Young Alumni Award from Clemson University where he received his B.S. degree in Chemical Engineering. He received his Ph.D. in Chemical Engineering from Cornell University. After a brief career with Shell Development Company, Walter joined the Rice University faculty in 1990. His wife and two sons are also engineers.

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