Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Self-assembly of Asphaltenes: Enthalpy, Entropy of Depletion and Dynamics at Crossover II - theoretical DENISE FREED, NATALIA LISITZA, PABITRA SEN, YI-QIAO SONG, Schlumberger-Doll Research — NMR spin-relaxation is directly sensitive to molecular dynamics and is therefore an excellent tool for studying the formation of nano-aggregates. When aggregates form, the molecular rotations are slowed down, and the spin-relaxation rate is enhanced, which reduces the NMR signal. This gives rises to a remarkable kink in the NMR signal intensity at the Critical Nano-Aggregate Concentration (CNAC). In this talk, we use Debye's two-state model for micelle formation to describe asphaltene aggregation. We use the temperature dependence of the CNAC to determinate the enthalpy and entropy of aggregation. The enthalpy is negative, as expected, and indicates that the aggregate formation is energetically favorable due to π-stacking interactions. On the other hand, we find that the entropy is positive, which is quite a surprise. We propose that this increase comes from the depletion entropy of the solvent. As asphaltene molecules aggregate, the free volume available for the solvent molecules increases, giving rise to a depletion effect. An estimate of the depletion entropy from the sizes of asphaltene and toluene (solvent) is very close to the measured entropy gain. We will also discuss the applicability of Debye's two-state model to aggregate formation in asphaltene solutions.

Yi-Qiao Song
Schlumberger-Doll Research

Date submitted: 30 Nov 2005 Electronic form version 1.4