Application of Nuclear Magnetic Resonance Spectroscopy for the *in-situ* Measurement of Vapor-Liquid Equilibria of Fluid Mixtures

Mark McLinden^{C, S}, Jason Widegren and Christopher Suiter Applied Chemicals and Materials Division, NIST, Boulder, CO, U.S.A. markm@boulder.nist.gov

Fluid mixtures are important in the chemical process industry and in numerous applications involving fuels and working fluids, among others. Vapor-liquid equilibrium (VLE) data (*T*, *p*, *x*, *y*) are the most important data needed to fit the parameters of mixture thermodynamic models, yet the literature VLE data are generally characterized by large scatter within data sets and systematic differences between data sets. This data situation hinders the further improvement of mixture models, and better experimental methods are clearly needed. In this talk we introduce nuclear magnetic resonance (NMR) spectroscopy for the measurement of VLE data. A quantity of a binary mixture, sufficient to establish separate liquid and vapor phases, is filled into a standard high-pressure sample tube and loaded into the NMR instrument. The measurement of the equilibrium liquid and vapor-phase compositions is then carried out inside the NMR; the composition is provided by integrating the NMR signal. The pressure is either measured directly with a connected pressure transducer or indirectly by combining the NMR signal with a virial representation of the vapor phase density. Beyond being simply a different VLE method, NMR offers a possible resolution to some of the systematic errors encountered in traditional VLE methods due to the *in-situ* nature of the composition determination. Finally, we discuss the types of mixtures where this method would be feasible (and where it would be impossible).