Ionic liquids (ILs) are generally defined as salts composed of discrete cations and anions with melting points below 100°C, and many are liquid at ambient temperature. ILs are a relatively new material class with unique properties including non-volatility and excellent solvation capabilities. The extremely large number of possible ion combinations makes ILs a truly tunable material which has led to an intense worldwide academic study. Interest in commercial use of ILs in the chemical industry is also expanding rapidly, but commercialization is hampered by a lack of physical property data, particularly for mixtures of ILs with ordinary gases and liquids. Our research has focused on accurately measuring vapor-liquid equilibria (VLE) and liquid-liquid equilibria (LLE) and using thermodynamic models to understand the phase behavior of binary gas mixtures in ILs.

This presentation will focus on the importance of characterizing the global phase behavior of gases in ionic liquids and how this can provide insight into new applications. Solubility measurements of several gases in ILs will be discussed and important experimental details regarding VLE measurements using a gravimetric microbalance and VLLE measurements using a mass-volume technique will be highlighted. VLE data have been successfully correlated with a modified Redlich-Kwong equation of state (EOS), and in certain cases (e.g. hydrofluorocarbons) the EOS predicts partial immiscibilities (LLE) with lower critical solution temperatures (LCSTs) in the fluorocarbon-rich side solutions. This behavior is quite interesting and in contrast with ionic liquid solutions with various alcohols where immiscibility gaps have been well studied experimentally and show upper critical solution temperatures (UCSTs). In addition to the phase behavior, we will discuss unusually large negative excess molar volumes discovered in the present LLE experiments. We have also found that gases such as CO2 can exhibit different solubility behaviors in ILs (i.e. physical and chemical absorption) and that these behaviors can be analyzed with the EOS using a simple association model and excess thermodynamic functions. Recent ternary phase behavior (e.g. CO2/SO2/IL) experiments and model calculations will also be examined.

Knowledge of these gas and IL phase behaviors has led to several practical applications including separation of azeotropic mixtures and absorption cooling cycles. These along with a few new examples for future applications will be discussed.

Dr. Shiflett is a Senior Research Associate in DuPont and has worked for the company for 22 years. He is currently in Central Research and Development and located at the Experimental Station in Wilmington, Delaware. He has a B.S. in Chemical Engineering from North Carolina State University and a M.S. and Ph.D. in Chemical Engineering from the University of Delaware. He has worked on a variety of DuPont programs including developing refrigerant mixtures to replace chlorofluorocarbons (CFCs), plasma reactions, synthesis of nanoporous carbon membranes, hydrogen storage materials, environmentally friendly routes to producing titanium dioxide, and for the past several years has been leading a team studying new applications for ionic liquids. He has commercialized three refrigerants mixtures (R-402A, R-402B and R-404A), is a named inventor on 23 granted U.S. patents, and published over 50 papers (35 on ionic liquids). He recently received the “Heroes of Chemistry” award from the American Chemical Society for his work to replace CFCs with non-ozone depleting HFC mixtures.

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