543d Predicting Gas Diffusivity in Room Temperature Ionic Liquids

Lee Ferguson and Paul Scovazzo

One of the big sales pitches for using Room Temperature Ionic Liquids (RTILs) as an alternative to traditional volatile organic solvents is the potential for there to be “trillions” of RTILs to choose from in order to fine tune the solvent system. This advantage is also a disadvantage since there are also “trillions” of RTILs to synthesis, prior to testing their thermodynamic and transport properties. We have been working on models for predicting both gas solubility and diffusivity in order to produce a tool for screening RTILs for a proposed gas separation. In this paper, we will focus on our correlations for predicting gas diffusivities in RTILs. In the past, we developed a correlation for predicting molecular diffusivity in imidazolium ionic liquids. Now we present RTIL transport data (diffusivity, solubility, and permeability) for phosphonium, ammonium, piperidium, and pyrrolium based ionic liquid membranes using a lag-time technique. We will also compare and contrast these cation classes of RTILs with the imidazolium class of RTILs. Finally, we will update our diffusivity correlations to encompass all of the tested classes of RTILs. The gases used in the study include carbon dioxide, nitrogen, oxygen, methane, ethene, propene, 1-butene, and 1-3 butadiene. The anions used in the training set for the correlations include: trifluoromethylsulfonate [CF3SO3], chloride [Cl], hexafluorophosphate [PF6], bis((trifluoromethyl)sulfonyl)amide [Tf2N], bis((perfluoroethyl)sulfonyl)amide [BETI], dicyanamide [DCA], and diethylphosphate.