

Simulating Transport Behavior of Room Temperature Ionic Liquids for Li-Ion Applications

Vyran L. George, Thomas F. Fuller

School of Chemical & Biomolecular Engineering,
Georgia Institute of Technology, Atlanta GA 30332, USA

Using room temperature ionic liquids (RTILs) as electrolytes in Li-based batteries provides important safety and performance benefits over the more volatile, combustible organic solvents currently used¹⁻². However, in order to gain a better understanding of transport in these electrolytes, properties such as conductivity, transference numbers, diffusion coefficient and salt activity must be measured as a function of salt concentration.

Experimental methods are explained for measuring these transport properties for a room temperature ionic liquid system³⁻⁴. For example, electrical conductivity, Figure 1, was calculated using impedance measurements across a conductance cell for ionic liquids with varying N-lithiotrifluoromethanesulfonimide (LiTFSI) salt concentrations (0M – 1.5M).

Furthermore, a model is proposed to predict the competing effects of each transport property on the discharge behavior of a dual insertion cell. The model is based on concentration solution theory and derived from the work of Newman⁵. It is generalized to simulate any cell composed of two insertion electrodes, electrolyte, and an inert conducting material. Our focus is characterizing the transport of the species in the electrolyte, by incorporating the concentration dependence of the electrical conductivity, the transference number, and the diffusion coefficient of the lithium salt.

The validity of the model and simulation results were tested by experimental results. Full lithium-ion coin cells in 2032 configuration with commercial $\text{LiNi}_{0.8}\text{Co}_{0.15}\text{Al}_{0.05}\text{O}_2$ cathodes and graphite anodes were built. The RTIL used as electrolyte was 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide (EMITFSI). Electrochemical tests were performed on these cells by varying current densities. Cell performances that were measured included capacity and power fade over the total cycling period.

ACKNOWLEDGMENTS

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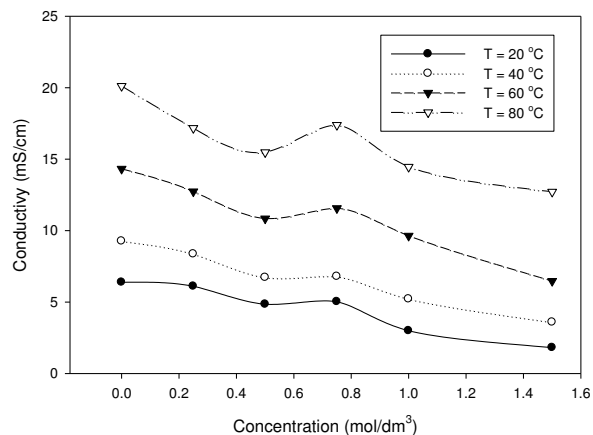


Figure 1. Electrical conductivity of 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide (EMITFSI) as a function of LiTFSI salt concentration and temperature.

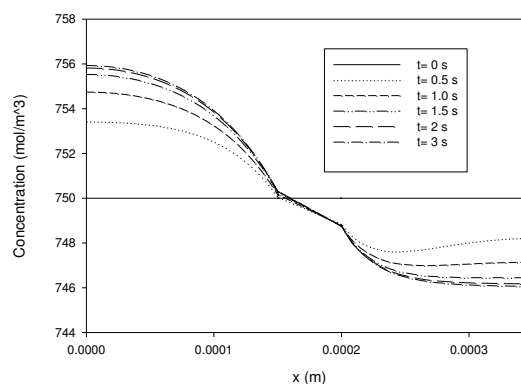


Figure 2. Simulation of concentration profiles across cell during galvanostatic discharge at $I = 0.5\text{mA/cm}^2$.