

Master topic From February 2017

Title of the research topic	Determination of electrolytes transport properties for Li-ion batteries
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Scientific Project :

The development of the electric vehicle is tied to that of Li-ion cells from which the battery pack is made. The driving range of the vehicle directly relates to the energy stored in the battery pack. Besides, the vehicle mileage depends upon the aging of the battery pack, which itself depends upon the conditions (under storage, acceleration, cruise, and regen) the pack experiences. In order to forecast how a cell design will translate to the vehicle performance, as well as how a vehicle usage will affect the battery life, it is important to set forth reliable battery models. Physics-based models, which are based on mathematical equations that describe the various underlying phenomena (reaction kinetics, transport, etc.), are probably the most predictive in this regard. However, they rely on a number of input parameters which must be determined as accurately and independently as possible. Among these, the electrolyte properties are crucial, because electrolyte transport is known to have a strong impact on limitations across the porous electrodes. The full set of properties includes ionic conductivity, lithium transference number, salt diffusion coefficient, and a thermodynamic factor that relates to nonideality. Looking at the literature, there are only a few reports on battery electrolytes [1-8]. As example, for some commonly used mixtures of carbonates with LiPF_6 as the lithium salt (e.g., dimethyl carbonate and ethylene carbonate – as LP30), there is no report of above mentioned properties, to the best of our knowledge. In a recent work, we reported on a novel four-electrode electrochemical cell from which the three transport properties of a binary electrolyte can be determined in one shot [9]. A current pulse is applied between the two terminal lithium electrodes, and the voltage response between the two lithium reference electrodes is measured. From a model analysis of the voltage response, the three transport properties are fitted reliably.

In the master thesis work, experiments will be carried out with this novel cell in order to study how the transport properties depend upon salt concentrations and temperatures, for some selected electrolytes. The concentration dependence will be included in the model analysis, which should help decreasing the number of initial salt concentrations to be studied without compromising on accuracy. This work will pave the way toward the development of a methodology to establish a database for electrolyte properties, which is extremely relevant to the physics-based modelling community; both academic and from industry.

Techniques used :

Cell assembly, electrochemical techniques.
Model analysis of data, concentrated solution theory

Recent publications related to the topic :

- [1] Stewart, S. G. and Newman, J. J. *Electrochem. Soc.* 155(1), F13–F16 (2008).
- [2] Klett, M., Giesecke, M., Nyman, A., Hallberg, F., Lindstrom, R. W., Lindberg, G., and Furo, I. J. *Am. Chem. Soc.* 134, 14654–14657 (2012).
- [3] Valøen, L. O. and Reimers, J. N. J. *Electrochem. Soc.* 152(5), A882 (2005).
- [4] Ma, Y., Doyle, M., Fuller, T. F., Doeff, M. M., Jonghe, L. C. D., and Newman, J. J. *Electrochem. Soc.* 142(6), 1859–1868 (1995).
- [5] Zugmann, S., Fleischmann, M., Amereller, M., Gschwind, R., Wiemhöfer, H., and Gores, H. *Faraday Discuss. Chem. Soc.* 88, 43 (1987).
- [6] Nyman, A., Behm, M., and Lindbergh, G. *Electrochim. Acta* 53(22), 6356–6365 (2008).
- [7] Lundgren, H., Behm, M., and Lindbergh, G. J. *Electrochem. Soc.* 162(3), A413–A420 (2015).
- [8] Stewart, S. G. and Newman, J. J. *Electrochem. Soc.* 155(6), A458–A463 (2008).
- [9] M. Farkhondeh, M. Pritzker, M. Fowler, and C. Delacourt, *Electrochem. Comm.*, 67, 11-15 (2016)