Motivation

Advanced numerical simulation tools are important for both the improvement of existing battery systems as well as the development of superior future battery systems such as Li-air batteries. To provide insight into physical and chemical aspects of such battery systems, it is necessary to develop computer models based on

- thermodynamically consistent models for ion-transport in porous media consisting of electrolyte solution, active and electrically conducting electrode material and non-conducting materials
- accurate and reliable geometrical parameters and transport parameters

Mathematical model

Ion transport in porous separator filled with electrolyte solution [1] governed by

$$\frac{\partial c}{\partial t} = - \nabla \cdot \left( \varepsilon \mathbf{J} \right) + \nabla \cdot \left( \frac{\varepsilon}{\tau} \kappa \nabla c \right) = 0$$

$$\mathbf{J} = - I + g_\phi \nabla \ln c$$

Experimental determination of transport parameter for binary electrolyte solutions

Transference number & thermodynamic factor

Concentrated solution theory:

$$g = 2 \left( 1 + \frac{d \ln f_s}{d \ln c} \right) (1 - e^-)$$

for small concentration variation:

$$g \simeq g_s (1 - e^-) \frac{1}{D_+}$$

$$g = \frac{F^2 c_0 f_s 0 \Delta \phi}{R T ^ \tau}$$

$$\Delta \phi = \frac{R T}{F} g_\phi \nabla \ln c$$

Factor $g_s$ can be determined in a concentrated cell [4]:

<table>
<thead>
<tr>
<th>c [M]</th>
<th>0.01</th>
<th>0.1</th>
<th>1.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>$g^* \cdot D_+ [-]$</td>
<td>0.306</td>
<td>0.309</td>
<td>0.052</td>
</tr>
</tbody>
</table>

Future work

- Numerical validation of determined parameters
- Determination of physically motivated transport parameters for
  - tertiary electrolyte solutions
  - ionic liquids
  - based on thermodynamically consistent transport equations

Acknowledgement

Nikolaos Tsiouvaras gratefully acknowledges the Alexander von Humboldt Foundation for his scholarship.

Financial support through the TUM EE-Bat program is greatly acknowledged.