

Thermal Modelling of a Lithium-Ion Aqueous Battery

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Introduction

Thermal modelling is presented here for a novel lithium-ion aqueous battery [1] using the commercial multi-physics package COMSOL with extensions consisting of an energy balance and temperature dependence of properties of the battery. The model is based on the pseudo two-dimensional Doyle-Fuller-Newman (DFN) [2, 3] battery model and a thermal, electrochemistry coupled model, which can capture high-rate transient effects and makes the task of relating model parameters back to physical quantities, such as diffusivity and porosity relatively easy.

Model development

The thermal behavior of a lithium-ion aqueous battery is studied during the galvanostatic cycling, and it was found that the diffusion coefficient of the lithium ions in the solid phase and in the electrolyte, the reaction rate constants of the electrochemical reactions, the open circuit potentials and the thermal conductivity of the binary electrolyte depend on the temperature assigned to the model used here. A schematic of the battery model is shown on Fig. 1.

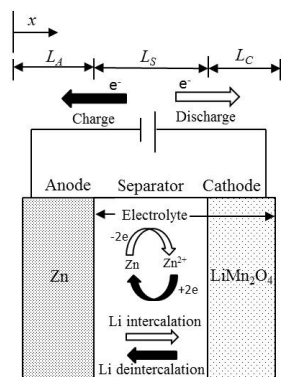
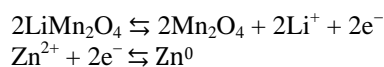


Fig. 1 Schematic of the battery model and its dimensions.

A lithium-ion cell model consisting of the anode and cathode made of non-porous and porous materials, respectively, and a porous separator, immersed in an aqueous solution of zinc and lithium salts as an electrolyte, sandwiched between them was used. The following reactions were considered upon the cell charge/discharge



i.e. when the cell is fully charged, the anode consists of non-porous zinc and a porous Mn_2O_4 cathode; on discharging, zinc of the anode dissolves and Li-ions intercalate into the cathode structure.

The model used here calculates local lithium-ion concentrations and potentials using coupled partial differential equations and these equations account for the linear diffusion of lithium-ions in the electrolyte, spherical diffusion of lithium-ions in the solid and the spatially distributed electrochemical reactions driving them to transfer between the solution and the solid. The

concentration of lithium-ions within the electrolyte is governed by Fick's law of linear diffusion combined with an intercalation current density term, transferring lithium-ions between the solution and solid. The intercalation reaction current density, acts as an input to the dynamics of the lithium-ion diffusion within the solid, and this diffusion occurs at every point in the cathode. This can be modelled using a spherical, radially symmetric diffusion law. The effective diffusion coefficient of the aqueous electrolyte solution is corrected by porosity of the cell components, and the charge balance in the liquid and solid phases is governed by Ohm's law.

Fig. 2 presents the experimental data of the electrolyte conductivity, κ_i used in the aqueous battery modelling.

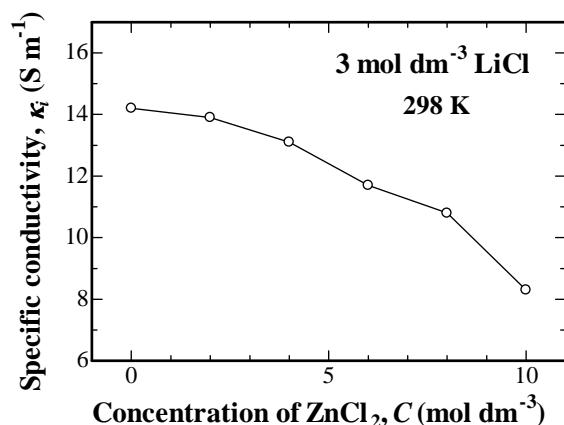


Fig. 2 Conductivity data for an aqueous electrolyte consisting of $3 \text{ mol dm}^{-3} \text{ LiCl}$ and various concentration of ZnCl_2 used in the model development.

The potential in the solution phase and its flux are continuous at the interfaces of the electrodes and the separator. The intercalation reaction current density is driven by potential differences between the solid and electrolyte solution, and governed by the Butler-Volmer equation.

Quantities calculated include the potential profile including that for different current densities, temperature on the cell surface and the cell voltage during cycling under different cooling conditions, comparison of concentration profiles of the ternary electrolyte for several operation rates, and the temperature on the cell surface during the discharge process under different operating conditions. The results will be verified by experimental results.

References

1. J. Yan, J. Wang, H. Liu, Z. Bakenov, D. Gosselink, P. Chen, *J. Power Sources*, 216 (2012) 222.
2. M. Doyle, T. F. Fuller, J. Newman, *J. Electrochem. Soc.* 140 (1993) 1526.
3. T. Fuller, M. Doyle, J. Newman, *J. Electrochem. Soc.* 141 (1994) 1.

Acknowledgments

This research was supported by the "Nazarbayev University Corporate Fund of Social Development" grant.