

## Modeling of Transport Processes in Aqueous Li-O Cathodes

Timo Danner<sup>a,b</sup>, Birger Horstmann<sup>a,b</sup>, Norbert Wagner<sup>a</sup> and Wolfgang G. Bessler<sup>a,b,c</sup>

a) *German Aerospace Center (DLR), Institute of Technical Thermodynamics, Pfaffenwaldring 38-40, 70569 Stuttgart, Germany*

b) *University of Stuttgart, Institute for Thermodynamics and Thermal Engineering, Pfaffenwaldring 6, 70550 Stuttgart, Germany*

c) *Helmholtz-Institute Ulm for Electrochemical Energy Storage (HIU), Albert-Einstein-Allee 11, 89069 Ulm, Germany*  
*Email: Timo.Danner@DLR.de*

Metallic Lithium-Oxygen (Li-O) batteries with a very high theoretical energy density (11.680 Wh/kg) are a very promising alternative to conventional combustion technologies in the mobility sector [1].

In this talk we will present results from our multi-phase modeling framework for lithium batteries and fuel cells. The framework is capable of describing the formation and transport of multiple gaseous, liquid and solid phases in aqueous and aprotic Li-O batteries.

Major problems in Li-O systems arise from the formation of solid products within the porous structure of the oxygen electrode [2]. In our model of an aqueous Li-O battery we take into account the formation of solid  $\text{LiOH}\cdot\text{H}_2\text{O}$  in the porous electrode and separator.  $\text{LiOH}\cdot\text{H}_2\text{O}$  clogs the pore space and limits the transport of reactants, to the active surface sites.

The performance of the system can be greatly improved by Gas Diffusion Electrodes (GDE). As previous research on Alkaline Fuel Cells (AFC) provides a good basis for modelling of GDE in alkaline media [3], it is somehow surprising that only non-aqueous systems are tackled in the modeling literature so far [2, 4].

Simulation results for our detailed modeling approach of the GDE-Cathode in aqueous lithium hydroxide solution are presented. We model capillary-pressure driven transport of the liquid electrolyte in the GDE and discuss the dynamic equilibrium between the liquid electrolyte and gaseous oxygen. Capacity limitations due to the formation of a  $\text{LiOH}\cdot\text{H}_2\text{O}$  film at the anode surface are predicted by the simulations. Model parameters are calibrated and validated against experimental data of half-cell experiments at model GDEs in an aqueous one molal LiOH solution, which were also conducted at our institute.

[1] J. Christensen, P. Albertus, R.S. Sanchez-Carrera, T. Lohmann, B. Kozinsky, R. Liedtke, J. Ahmed, A. Kojic, J. Electrochem. Soc., 159 R1-R30.

[2] P. Albertus, G. Girishkumar, B. McCloskey, R.S. Sanchez-Carrera, B. Kozinsky, J. Christensen, A.C. Luntz, J. Electrochem. Soc., 158 A343-A351.

[3] F. Bidault, D.J.L. Brett, P.H. Middleton, N.P. Brandon, Journal of Power Sources, 187 (2009) 39-48.

[4] S.S. Sandhu, J.P. Fellner, G.W. Brutchon, Journal of Power Sources, 164 (2007) 365-371.