Designing Aqueous Neutral Electrolytes for Zinc-Air Batteries

Birger Horstmann*[1,2,3], Simon Clark[1,2,3,4], A.R. Mainar[5], E. Iruin[5], L.C. Colmenares[5], J.A. [5]Blazquez, J.R. Tolchard[4], Arnulf Latz[1,2,3]

[1] *German Aerospace Center, Pfaffenwaldring 38-40, 70569 Stuttgart, Germany.*

[2] *Helmholtz Institute Ulm, Helmholtzstraße 11, 89081 Ulm, Germany.*

[3] *Ulm University, Institute of Electrochemistry, Albert-Einstein-Allee 47, 89069 Ulm, Germany.*

[4] *SINTEF Industry, Richard Brikelands vei 2b, 7034 Trondheim, Norway.*

[5] *CIDETEC Energy Storage, P◦ Miramón, 196, Donostia-San Sebastián 20014, Spain.*

**birger.horstmann@dlr.de*

In the on-going pursuit of high-performance and sustainable energy storage, zinc-air batteries (ZAB) are among the most promising systems under development with a theoretical energy density over $6000\,\mathrm{Wh}\cdot\mathrm{L}^{-1}$ [1]. Industry-standard primary ZABs currently contain aqueous alkaline KOH electrolytes. Their lifetime is limited to just a few months due to CO_2 absorption from air [2]. ZABs with near-neutral NH_4Cl-$ZnCl_2$ electrolytes have shown good cycleability and are not subject to carbonation [3,4]. Despite the strongly oxidizing nature of chlorine and the precipitation of unwanted solids [6], aqueous near-neutral ZABs are beginning to be commercialized [7].

We have derived and implemented thermodynamic models and dynamic cell models to evaluate the performance of ZABs with a range of electrolyte compositions. Our models determine the equilibrium composition of aqueous electrolytes and the solubility of various precipitates. We then simulate the dynamic and spatially resolved 1D concentration and multi-phase volume fraction profiles that develop in a ZAB cell during operation.

In this contribution we present a validated method for designing new aqueous electrolytes for next-generation ZABs. Beginning with fundamental thermodynamics and moving up to cell-level engineering, we identify the requirements for new electrolyte materials and highlight an example of electrolyte design. Our simulations are validated by experimental characterization techniques including full cell cycling, operando pH monitoring, and ex-situ XRD, SEM, and EDS measurements.

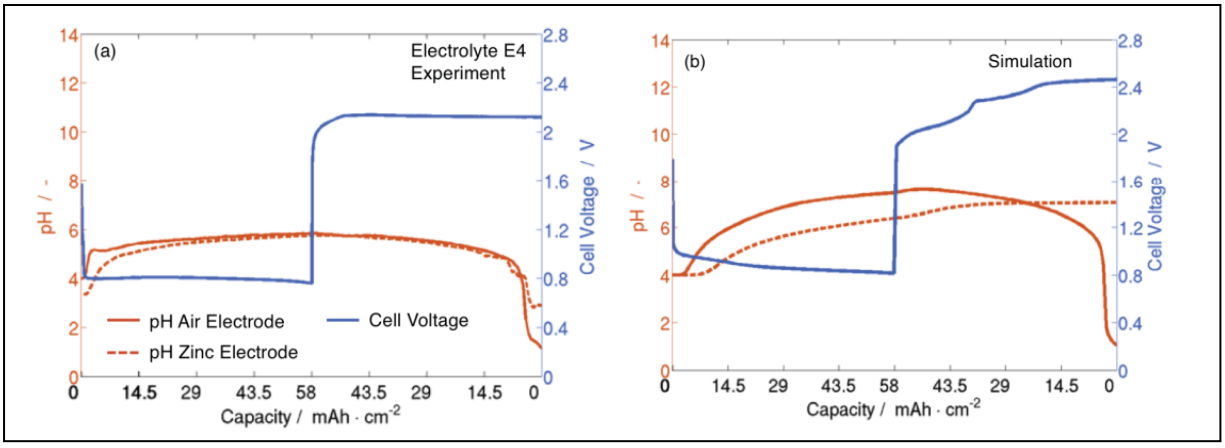

Figure 1: Comparison of measured and predicted pH profiles near the air electrode and the zinc electrode from (a) experiment and (b) simulation.

References:

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