Model-Based Development Secondary Zinc-Air Batteries with Advanced Aqueous Electrolytes

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Zinc-air batteries (ZABs) are promising candidates for next-generation electrochemical energy storage. They offer a high theoretical specific energy (1086 Wh·kg-1) and energy density (6093 Wh·l-1), are based on cheap and widely-available materials, and have superior operational safety characteristics. But after weeks of operation in air, CO2 reacts with the alkaline electrolyte to form carbonates, lowering the ionic conductivity of the electrolyte and degrading the performance of the cell. (1). Furthermore, zinc metal may undergo irreversible passivation when discharged, reducing the usable capacity of the cell. To better understand and solve these challenges, we have developed continuum models based on the principles of electrochemical thermodynamics and kinetics to simulate the performance of metal-air batteries (2, 3). Our models allow us to investigate transient and spatially resolved changes in cell potential, electrolyte concentrations, and multi-phase volume fractions.

Our simulations show that ZABs with traditional alkaline KOH electrolytes face three major design challenges: electrode shape change due to inhomogeneous Zn dissolution and ZnO precipitation, local depletion of electrolyte at the zinc interface causing passivation, and the dissolution of atmospheric CO2 in the electrolyte.

The near-neutral ZnCl2-NH4Cl electrolyte may help address some of these challenges. This electrolyte is not susceptible to the same parasitic reactions as the KOH electrolyte and could potentially extend the lifetime of the battery (4-6). However, the behavior of the electrolyte in the near-neutral pH regime is very complex. The state of the aqueous zinc ion and the final discharge product of the cell are significantly influenced by even small changes in the electrolyte environment. Our simulations show that strong pH gradients develop during operation, which may accelerate cell degradation.

In this contribution we highlight the coupled effects between electrolyte composition and ZAB performance, and discuss how modeling and simulation can be applied to accelerate the development of next-generation batteries. This work is supported by the European Commission Horizon 2020 project ZAS! (Zinc Air Secondary Batteries Based on Innovative Nanotechnology for Efficient Energy Storage).

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