Modelling and Simulation of secondary zinc air batteries with anion-exchange-membranes

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The zinc-air battery chemistry is a promising candidate for future energy storage. However, the previously developed cells suffer from significant degradation resulting in poor cycle and shelf life. One of the main degradation mechanisms identified is the carbonation reaction with ambient CO_2 continuously lowering the alkalinity of the electrolyte.

This, amongst other performance decreasing effects such as the presence of high zincate concentrations at the gas diffusion electrode, can be addressed e.g. by incorporating a polymer membrane which is only conductive for single charged anions **[1]**, allowing for the necessary exchange of hydroxide ions OH^- . Both, $Zn(OH)_4^{2-}$ and CO_3^{2-}, are present as multivalent ions in strongly alkaline media, thus their transport is prohibited.

The usage of such membranes is a rather new approach for zinc-air battery cells and needs to be analysed and understood in further detail. One of the common approaches in modern battery research besides experiments is simulation, because it allows access to many variables at any given time and location of the simulated cell under a wide range of environmental and boundary conditions.

Within the ZABSES project, a model for secondary zinc-air batteries with anion conducting polymer membranes is developed. Due to the complexity of the considered system, the model needs to be reduced to incorporate only the main investigated effects. The used volume-averaged continuum model is a combination of reaction rate approximations using approaches such as Butler-Volmer-chemistry and kinetic reaction rates with a model for the electrochemical fluid incorporating e.g. particle and charge conservation.

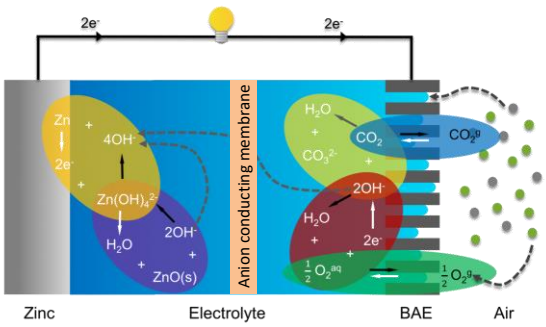

Figure 1 : Schematic representation of cell chemistry **[2]**

This modelling approach has already been used and validated for zinc air batteries by previous research **[2, 3]**. The main goal of the conducted research is the extension of the model to include the polymer membrane as well as further details such as side reactions and degradation mechanisms.

[1] Dembele, K., Chikh, L., Alfonsi, S., & Fichet, O. (2023). Effect of polyelectrolyte architecture on chemical stability in alkaline medium of anion exchange membranes. Polymer Degradation and Stability, 110462.

[2] Stamm, J., Varzi, A., Latz, A., & Horstmann, B. (2017). Modeling nucleation and growth of zinc oxide during discharge of primary zinc-air batteries. Journal of Power Sources, 360, 136-149.

[3] Schmitt, T., Arlt, T., Manke, I., Latz, A., & Horstmann, B. (2019). Zinc electrode shape-change in secondary air batteries: A 2D modeling approach. Journal of Power Sources, 432, 119-132.