3D Continuum Modelling and Simulations of Ni/Zn Batteries

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The increasing need for electric power and the importance of renewable energy sources highlight the necessity for cost-effective, dependable and sustainable storage solutions, like innovative zinc-based batteries. These batteries are advantageous because they utilise readily available and inexpensive materials, are environmentally friendly, recyclable, and feature non-flammable components.[1,2]

Among these, the nickel-zinc (Ni/Zn) battery stands out as a particularly promising option for e.g. stationary energy storage. Nonetheless, a comprehensive understanding of the physicochemical processes occurring during battery operation remains elusive, which complicates achieving consistent and reliable performance. Issues such as the shape change of the Zn electrode, its compaction and thus reduction in pore volume, as well as gas production impacting electrolyte levels are factors influencing cell efficiency and longevity.

Leveraging models developed for lithium-ion batteries,[3] a 3D+1D continuum model incorporating thermodynamic principles and volume averaging has been developed. This model enables detailed examination of transport phenomena and electrochemical reactions of Ni/Zn cells during cycling in real-time. The 3D aspect of the simulations reveals how phases and chemical constituents redistribute within the cell over time (e.g. Zn, see Figure 1),[4] with the additional dimension focusing on solid diffusion at the particle level. By comparing these simulation outcomes with experimental data, the model can serve as a tool for enhancing cell design and composition. This includes improving cell performance and cycle life, and mitigating degradation mechanisms.

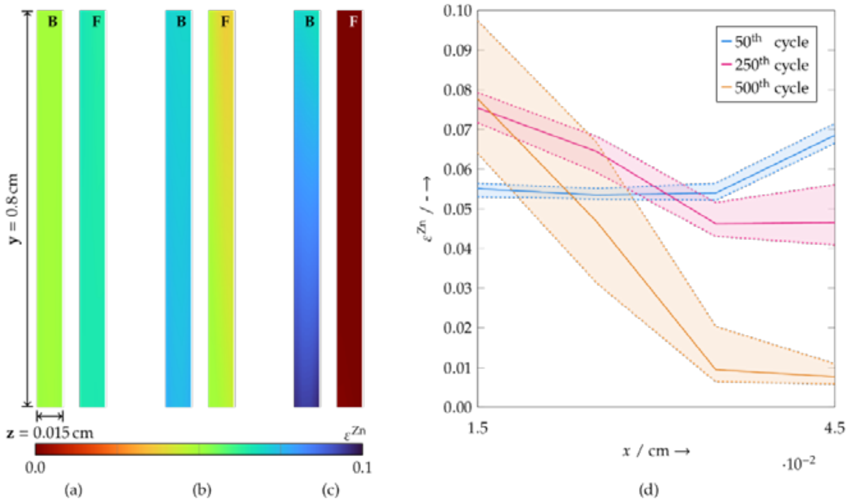

Figure 1: The observed shift in zinc distribution through the anode's thickness upon full discharge shows zinc migrating from the front (F) to the back (B) across cycles 50, 250, and 500, as depicted in panels (a) to (c). Panel (d) visually represents this internal redistribution for the same cycles, using a cross-sectional average.

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References
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