# Multiphysics Model For Performance Analysis Of Rechargeable Zn-Air Flow Batteries

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## Abstract

The increasing demand for electrochemical energy storage (EES) in stationary applications underscores the urgent need for advanced battery technologies. Among these, zinc-based systems, particularly rechargeable zinc-air flow batteries (RZAFBs), are gaining attention due to their favourable combination of technological, economic, and environmental advantages.[1-3] Despite their relative maturity, challenges in materials science persist, requiring the development of engineered prototypes beyond the laboratory scale and robust modelling frameworks to analyse the performance.
This study [4] presents a comprehensive Multiphysics model of RZAFBs, specifically focusing on a zinc plate anode configuration, which remains sensitive to issues such as corrosion, dendrite formation, and zinc oxide precipitation. The flowing electrolyte system in RZAFBs provides key advantages, including enhanced mass transport of zincate ions and improved dendrite suppression during charge-discharge cycles.[5,6]
The developed model integrates fluid dynamics in the electrolyte, concentration fields in both gas and liquid phases, electrochemical reactions at the anode and gas diffusion electrode (GDE), and a detailed physics-based formulation for gas-liquid phase exchange.[7,8] To do that, the model is developed involving the use of five coupled Physics: Secondary Current Distribution (cd), Transport of Diluted Species (tds), Laminar Flow (spf), Transport of Concentrated Species (tcs) and Darcy's Law (dl). These modules are coupled in such a way that: (i) the electrochemistry of the Butler-Volmer equations in cd depends on the concentrations of tds, (ii) the Butler-Volmer equations are incorporated into the source reactions of tds, (iii) the potential resulting from cd acts as the driving force for migration in tds, (iv) the fields resulting from spf and dl represent the convection of tds and tcs, respectively, and (v) the variable PO2, derived from tcs, acts as a source term for cO2 in tds. In Figure 1 a scheme is reported.
This approach enables an in-depth examination of:
- The influence of flow rate and current density on hydroxide ($OH^-$), zincate ion ($Zn(OH)_4^{2-}$) and dissolved O2 distributions (see Figure 2).
- Polarization curves with particular attention to the effects of gas feed pressure and electrolyte flow rate during both discharge and charge processes (see Figure 3).
- Limiting current density distribution, mapped over the Zn anode during charging to estimate shape change effects (see Figure 4).
With a view toward potential industrial scale-up, we developed a model to perform the tasks described above to characterize various cell prototypes and identify the one offering the best performance in terms of electrical output and material degradation.
Our findings indicate that optimizing the electrolyte flow rate, in conjunction with a well-designed cell geometry, ensures uniform $OH^-$ and $Zn(OH)_4^{2-}$ distribution, preventing stagnant zones and minimizing dendrite formation at the anode. Additionally, simulations reveal that variations in O2 partial pressure significantly affect both the equilibrium potential and the discharge limiting current. Flow rate changes were also found to impact polarization behaviour by altering ionic transport, ultimately influencing limiting current densities during charging.
In summary, this research provides a solid foundation for the design and optimization of RZAFBs, offering a complete characterization that advances their potential as scalable energy storage solutions.

## Reference

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## Figures used in the abstract

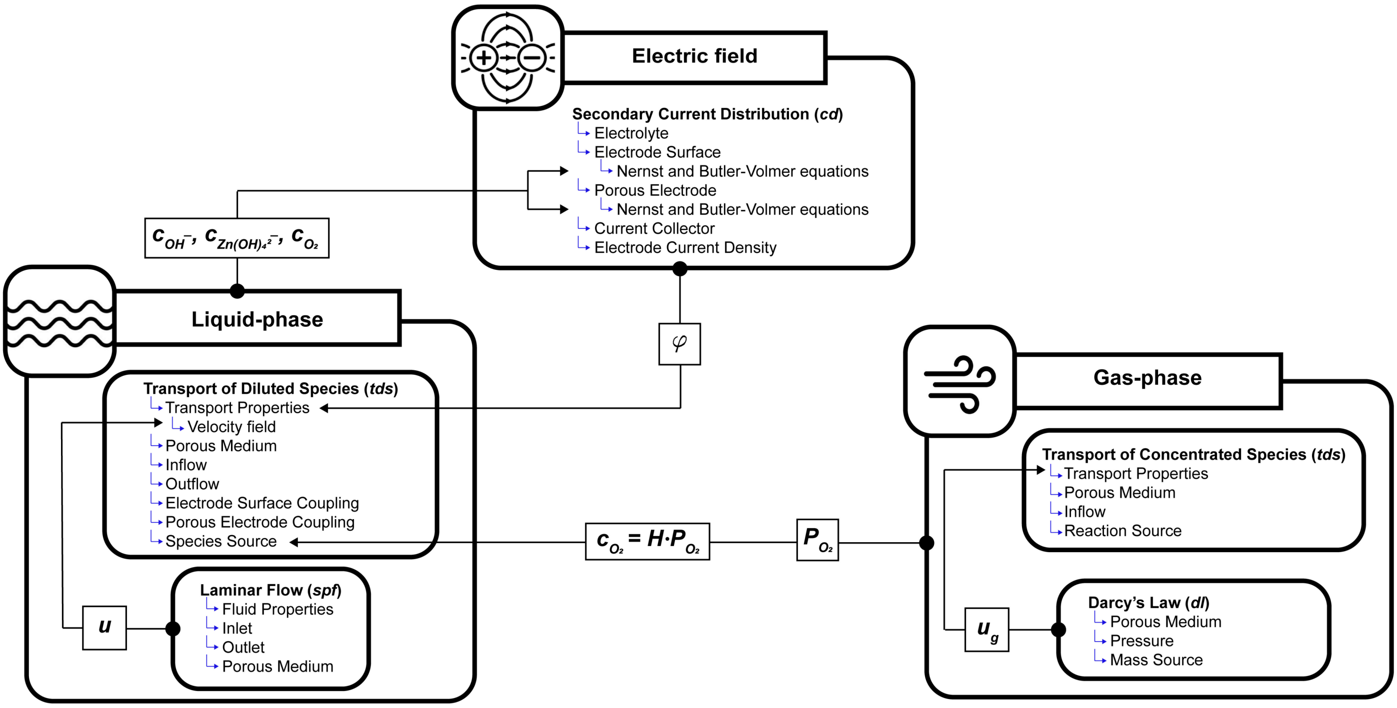


**Figure 1** : Schematic flowchart of physics and modules for the implementation in COMSOL.

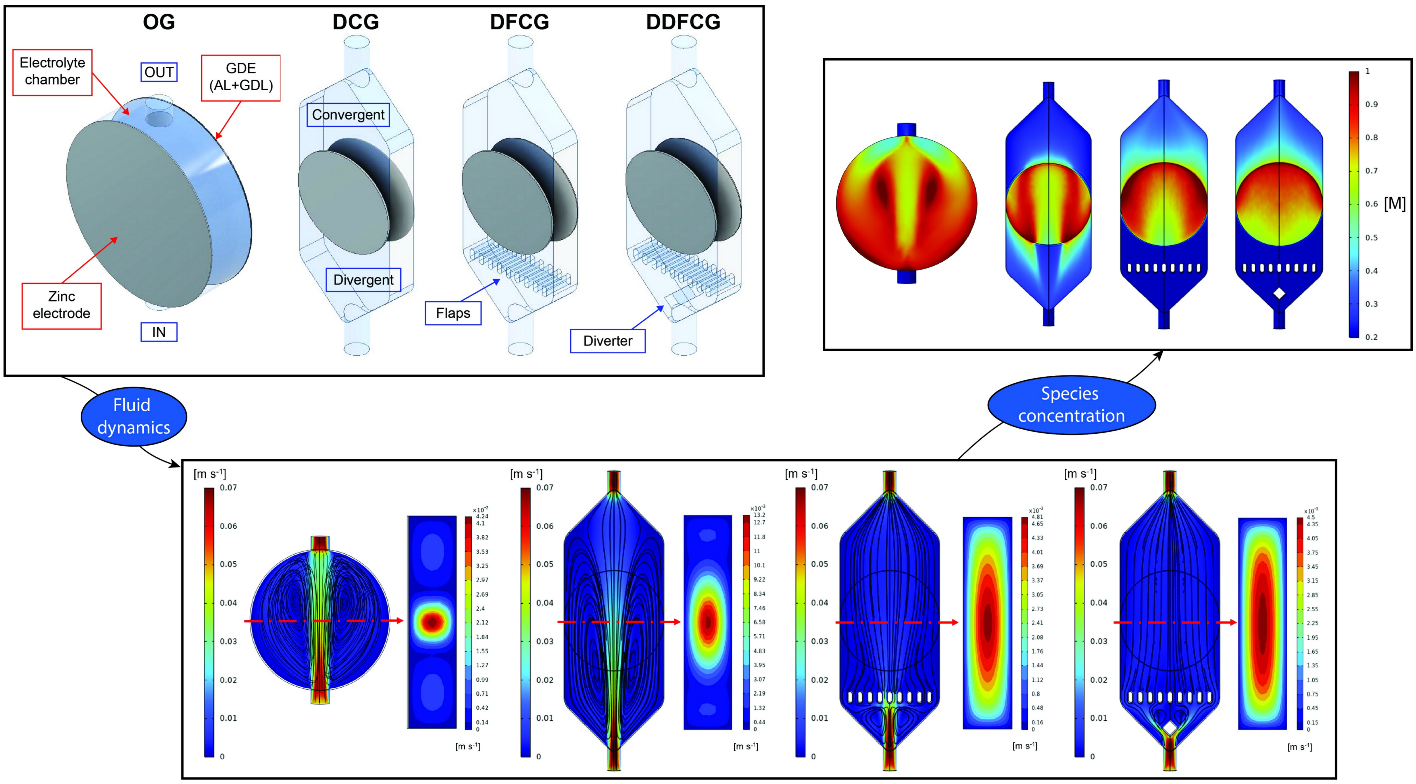


**Figure 2** : Representation of the electrolyte flow field and species conservation for different cell geometries.

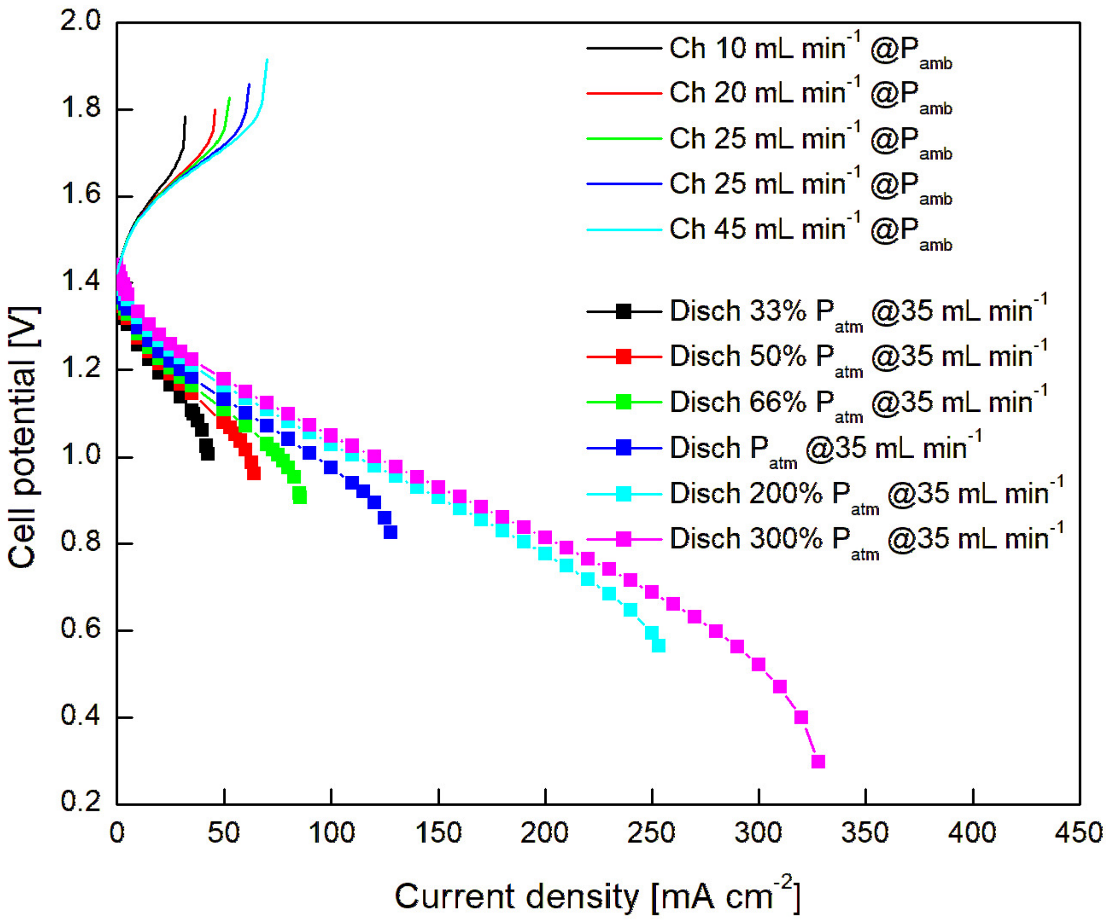


**Figure 3** : Discharge and charge polarization curves computed for different electrolyte flow rates and ambient pressure for OG cell.

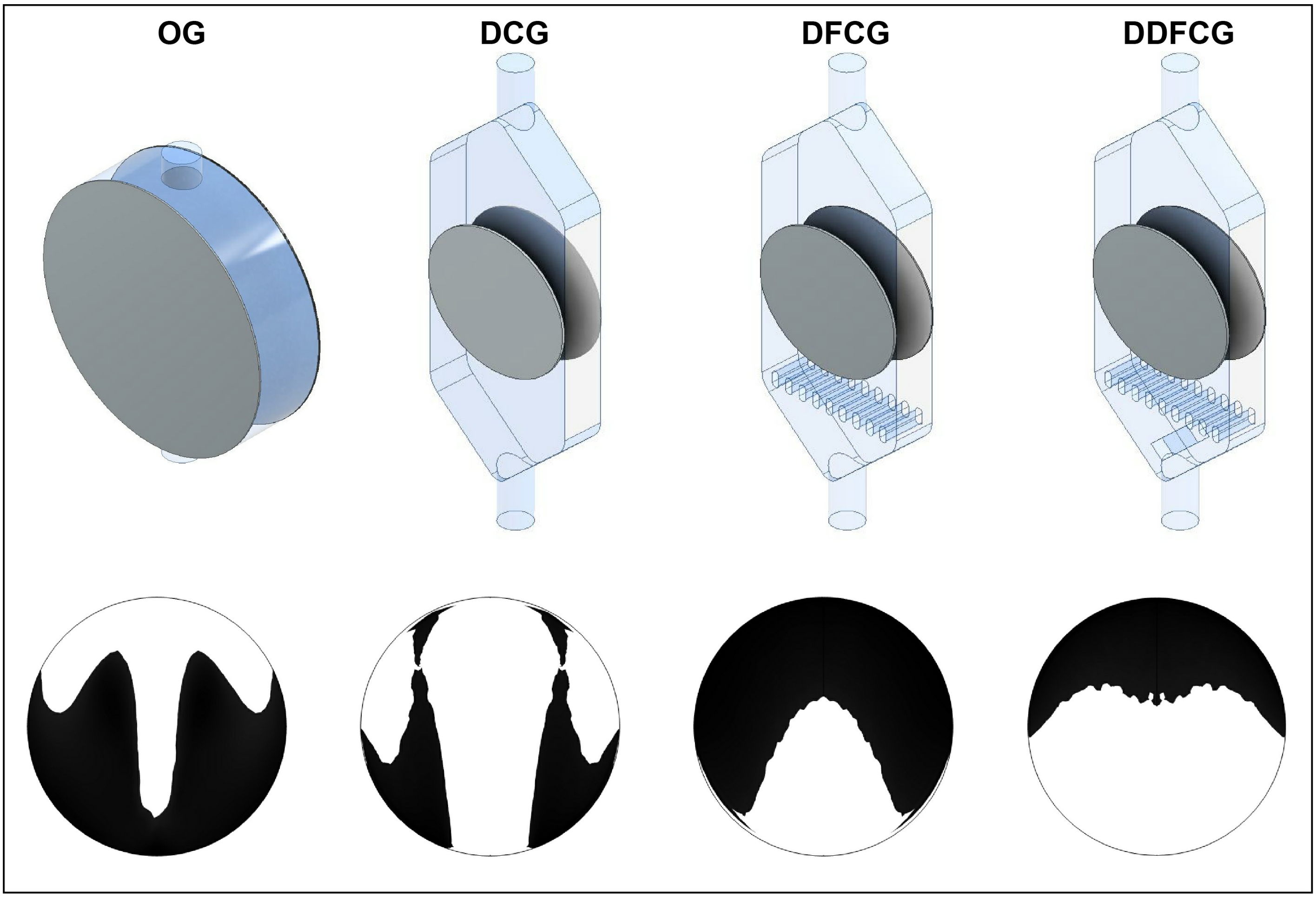


**Figure 4** : Maps of the regions in which a zincate concentration is low (< 10 mM), denoting establishment of limiting current density, between different cell geometries.