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# Asymptotic Homogenization - Modeling the charging behavior of Li-ion batteries

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The modeling of lithium-ion cells plays an important role in the electrification of many industries, such as the automotive industry. Models with high accuracy and low computational complexity are essential for the optimization of such applications.

To achieve this, a fully homogenized macroscale (FHM) model has been proposed [1]. This reduced model is based on effective mass and charge transport equations in isothermal active particles and electrolyte.
In current-limited battery operation, and thus at low C-rates, the FHM model works very well. At high C-rates, the predictions of the FHM model deviate significantly from those of the Direct Numerical Simulations (DNS). A high C-rate leads to high current densities between the active particles and the electrolyte and thus to steep concentration gradients near the interface. The resulting deviation between the inner concentration and surface concentration can no longer be covered by the homogenized value. Consequently, the FHM model is not applicable to diffusion-limited battery operation.

Therefore, we propose an extension of the FHM model based on Wang's diffusion length concept for spheres [2]. Here, the diffusion length is an additional variable that characterizes the correlation between the homogenized concentration and the surface concentration as a function of the C-rate.
This extension allows to consider the diffusion limitation within the active particles, thus allowing a reliable application at higher C-rates.
The extended FHM model is validated using a direct numerical simulation (DNS) for the charge of a graphite half-cell. Despite the non-spherical properties of the graphite electrode, the diffusion length concept can be successfully applied. The concentrations and potential distributions of the FHM model are in good agreement with the DNS results.

## Participation

In-Person

## References

[1] Arunachalam, H., & Onori, S. (2019). Full homogenized macroscale model and pseudo-2-dimensional model for lithium-ion battery dynamics: comparative analysis, experimental verification and sensitivity analysis. Journal of The Electrochemical Society, 166(8), A1380
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https://doi.org/10.1149/1.1838820

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