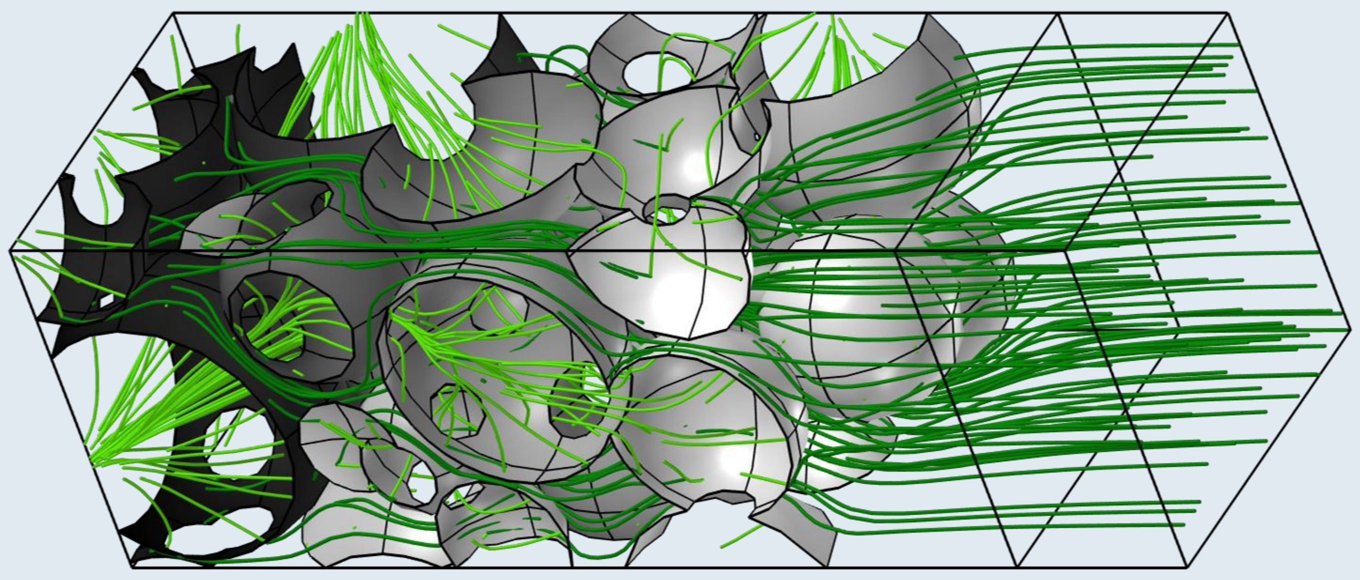

Comparative Analysis on the Impact of Electrode Morphologies on Lithium-Ion Battery Performance

Comparing three different electrode geometries to show the impact of the morphology on the battery discharge process.

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Introduction & Goals

The morphology of electrode materials strongly influences lithium-ion battery performance. Traditional models often oversimplify graphite as uniformly sized spheres, limiting predictive accuracy. This study introduces a flexible and reproducible computational workflow that incorporates more realistic morphological descriptions, enabling efficient evaluation of electrochemical behavior across diverse structures. Results show that increasing morphological complexity causes significant deviations from classical predictions but improves agreement with experimental data. The developed code, fully compatible with the COMSOL® API, ensures easy adoption and adaptation by researchers. This framework bridges modeling and experiments, supporting the optimization of material design and processing for advanced battery technologies.

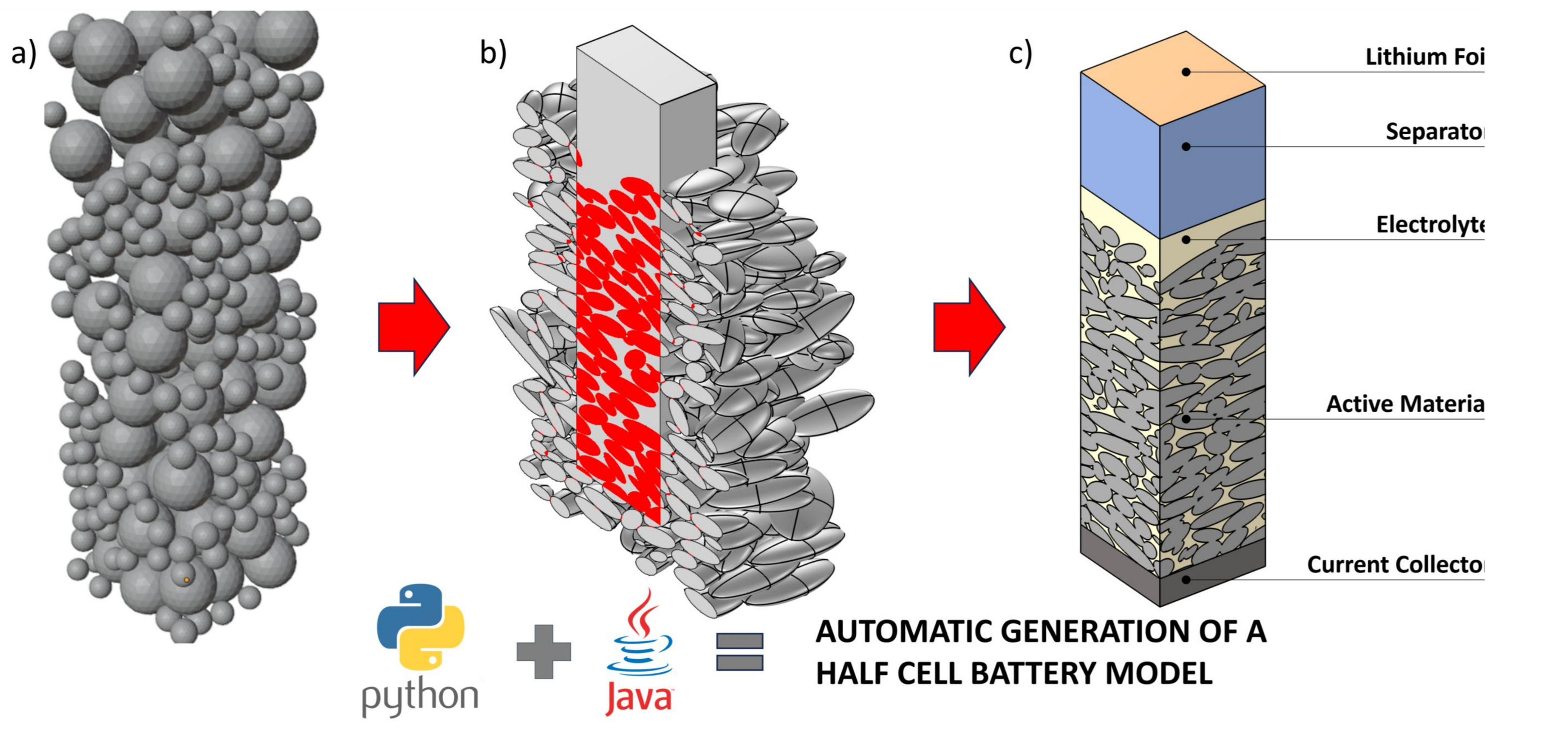

Figure 1. Main steps of the automatic script in Python and Java. a) Pre-packing cloud of spheres. b) Packed ellipsoids. c) Electrode

Methodology

The framework is divided in two parts. In the first one, a python code generates a cloud of polydisperse spheres replicating the chosen experimental particle size distribution. Then, each sphere is transformed into an ellipsoid. After, a discrete element simulation compacts the particle layer, and the geometrical information (position, size, and orientation, for each particle) is saved. In the next step, a Java script imports these data to reconstruct the entire particle layer directly in COMSOL®. Then, the central portion is extracted to generate the half-cell battery electrode. The code automatically detects the different domains and sets up the corresponding PDEs, from Battery Design Module and Chemical Species Transport, to solve mass and charge transport in the two phases. Finally, the material properties and the initial conditions are defined.

Results

For the present work, we generated three anodic half-cell batteries with morphologies of increasing complexity. Specifically, they are composed of monodisperse spheres, polydisperse spheres, and polydisperse ellipsoids. Each electrode was discharged under three different current values, expressed through the C-rate: C/5, C/3, and 1C. Then, we evaluated the intercalated lithium concentration within the active material. Electrodes with ellipsoidal particles show a high vertical concentration gradient at any current value and an almost zero radial gradient, reflecting experimental observations. In contrast, systems with spherical particles show radial gradients (polydisperse) or homogeneous distributions (monodisperse).

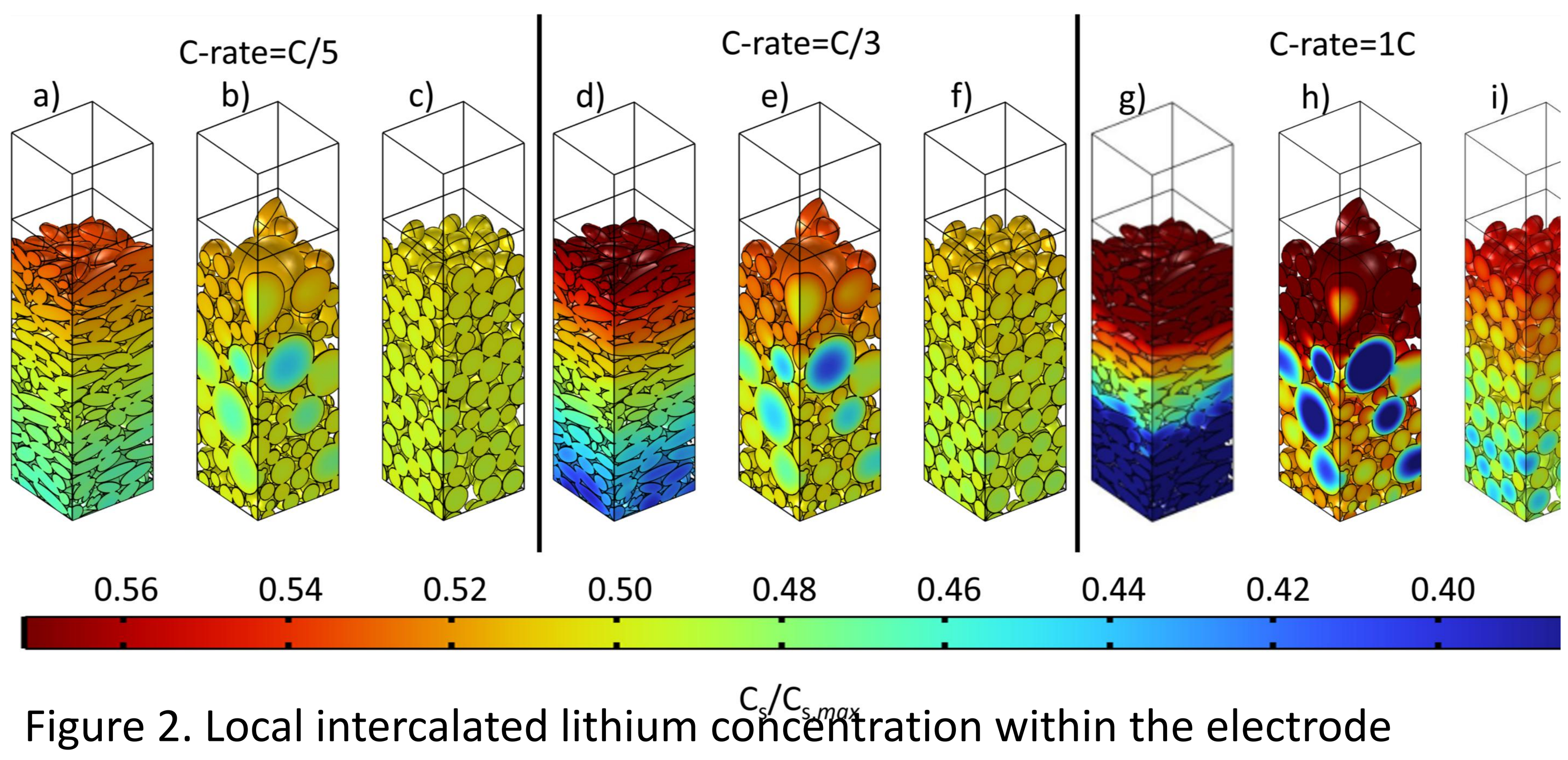

Figure 2. Local intercalated lithium concentration within the electrode (SoC=50%). Left (a, b, c): C-rate=C/5; Center (d, e, f): C-rate=C/3; Right (g, h, i): C-rate=1C.

REFERENCES

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