Comparative Analysis On The Impact Of Electrode Morphologies On Lithium-Ion Battery Performance

A. Lombardo Pontillo[1], A. Querio[1], E. Buccafusco[1], G. Boccardo[1], D. Marchisio[1]

[1]Politecnico di Torino, Turin, Italy

Abstract

During the last three decades, lithium-ion batteries have become the choice of power source for most portable electronic devices. During a discharge process, intercalated lithium, which is initially stored in the anode, de-intercalates, diffuses out in the electrolyte, reaches the cathode-electrolyte interface, and intercalates into the cathodic material. At the same time, electrons will be taken from the anodic current collector thanks to the oxidation of the anodic material, and travel through the load to the cathodic current collector, where they will reduce the cathodic material.

On the other hand, during a galvanostatic charge cycle, the application of an external work will reverse the motion of Li+, which will de-intercalates from the cathode and intercalate into the anode, and of the electrons as well.

Across the years, several approaches have been adopted to model the electrochemical dynamics of a lithium-ion battery, the most common of which is the Pseudo-2-Dimensional (P2D) one [1]. Anyways, this physics-based approach is rather simplified itself because it considers the electrodes to be composed of a monodisperse population of spherical particles. This limitation gives us the opportunity to conduct analysis by using more complex and computationally expensive approaches, that improve the description of the impact of different electrode morphologies on the battery performance.

To do so, the authors have developed a script adopting the Java API of COMSOL Multiphysics 6.3: the code reads the dimension, position, and rotation of each particle and reproduce it in the COMSOL environment. Then it recreates automatically the electrode and setup all the parameters needed to run the simulation.

The initial cloud of particles was generated with a discrete element method (DEM) coupling two open-source software: Yade and Blender. The first, creates a package of dispersed spheres with a specific particle size distribution, the second transform each sphere in an arbitrary shape and completes the rigid body simulation.

In the present work, the script was adopted to create and compare the discharge behaviour of three different electrode morphologies, as shown by Fig. 1, with increasing complexity: monodisperse spheres, polydisperse spheres, and polydisperse ellipsoids. Here, the idea is to show that modelling deviations from spherical shape is crucial to correctly predict battery performance [2].

The use of a code which can easily reproduce random package of active material particles is determining in producing dataset of simulation. A future alternative is the development of a surrogate model based on the use of Convolutional Neural Networks (CNN) [3]. The idea is based on the launch of several simulations of the 4D model under different operating conditions. Their outputs will then be used to create a dataset, which will subsequently be used to train the CNN. The goal is to reproduce, and subsequently predict, the electrochemical dynamics described by the 4D model but without the necessity of heavy computational efforts.

Reference

[1] M. Doyle, et al., Modeling of Galvanostatic Charge and Discharge of the Lithium/Polymer/Insertion Cell, Journal of The Electrochemical Society 140, 1526, (1993).

[2] A. Lombardo Pontillo, et al., Comparative Analysis via CFD Simulation on the Impact of Graphite Anode Morphologies on the Discharge of a Lithium-Ion Battery, Batteries, 11, 252, (2025).

[3] A. Marcato, et al., A computational workflow to study particle transport and filtration in porous media: Coupling CFD and deep learning, Chemical Engineering Journal, 417, 128936, (2021).