Upscaling of lithium-ion battery models: from the pore-scale to the cell-scale through homogenization.

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Lithium-ion batteries (LiBs) are currently the leading energy storage technology for applications ranging from portable devices to aerospace vehicles. They are also expected to play a significant role in net-zero energy buildings, with global battery demand projected to increase by approximately 27% annually until 2030. Their advantages include a high energy-to-weight ratio, low self-discharge, and decreasing production costs, making them a top choice for future non-fossil fuel-powered systems. However, understanding LiB performance and lifespan involves studying complex phenomena, such as non-uniform current distribution influenced by electrode morphology, which necessitates models that are both predictive and computationally efficient.

The purpose of this work is the identification of the microscopic equations of charge and mass transport within both liquid and solid phases in a LIB cell, and the macroscopic formulation of the same equations with a rigorous mathematical derivation. To do so, homogenization techniques were applied to derive macroscopic properties from microscopic behavior. This involved rewriting equations in dimensionless form to extract parameters like the Damköhler and Péclet numbers, which determines the feasibility of scale separation [1]. A closure problem was solved on a periodic unit cell to calculate effective diffusivity and conductivity values for both solid and liquid phases. These effective properties were then used to create and solve a homogenized model [2].

The derived homogenized model has been tested and validate with an accurate pore-scale numerical model. This technique produced results comparable, with a predictable error, to those of the computationally intensive pore-scale simulations while requiring significantly less time and resources. Therefore, homogenization enables the creation of fast and efficient models that facilitate experimental design and planning.

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