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# Modelling a Li-ion battery separator using effective properties: is an invariant scalar value of tortuosity appropriate?

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## Résumé

When simulating lithium-ion batteries, the separator is often homogenised and modelled using a single scalar value of tortuosity. However, real separator materials can be highly anisotropic, thus using a scalar tortuosity value may lead to large errors – Lagadec's dataset for a Celgard PP1615 separator has a tortuosity tensor with diagonal components differing by over an order of magnitude (1). In this work, we calculate a full tortuosity tensor for this dataset, using a Bamberger method (2). Then, we compare cell simulations with two different effective separators: the first uses a single scalar value for tortuosity, and the second uses a diagonal tensor for tortuosity.

Additionally, heterogeneities in the separator structure may cause some distributions of mass and charge flux, which would be overlooked in a model with an invariant tortuosity tensor. In this work, a "semi-homogenised" model is presented, which strives to capture flux distributions whilst not requiring the large computational resources of direct numerical simulations (DNS). The method can serve as an intermediate between DNS and simplified homogenised models. In essence, a tomographic image of a real separator structure (1) is divided into small blocks, and effective property tensors are calculated for each block - these are determined by solving three steady-state diffusive transport simulations (one for each axis) (3). The result is a spatial field of effective properties, as opposed to the invariant properties used in a fully-homogenised model. Simulations of the fully-homogenised model, semi-homogenised model, and the DNS are compared by taking several slices of the domain. Average positive ion flux and the L2 norm are calculated for these slices, to evaluate how well flux distributions are represented.

(1) M. Lagadec, Microstructure of Celgard PP1615 Lithium-Ion Battery Separator, (2016).

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\*Intervenant

- (2) R. Guibert, A Comparison of Various Methods for the Numerical Evaluation of Porous Media Permeability Tensors from Pore-Scale Geometry, *Maths. Geosci.*, 48(3), (2016).
- (3) S. Cooper, TauFactor: An open-source application for calculating tortuosity factors from tomographic data, *SoftwareX*, 5, 203-210 (2016).