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On the use of tortuosity for modelling Li-ion battery separators

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Currently, the industry standard for modelling Li-ion batteries at cell scale is known as "Porous Electrode Theory."This approach has prevailed for about 50 years, and still undergirds the majority of commercial software and academic tools for this application. The macroscale equations employed in these models typically use a single tortuosity factor to estimate both effective diffusivity and ionic conductivity. Furthermore, it is standard practice to use the Bruggeman correlation to calculate this tortuosity factor, despite its validity for this application being the subject of some dispute [1]. In recent years, various authors have explored the versatility of the Bruggeman correlation for Li-ion battery electrodes [2, 3], but there has been comparatively little investigation of the battery separator. In this work, the pore-scale transport equations are upscaled using a volume-averaging method, giving insight into the possible structure of the macro-scale equations, and the nature of the effective properties, thus highlighting which assumptions are implicit in the use of a single tortuosity factor. Additionally, effective transport properties for a Celgard® PP1615 battery separator are derived directly from tomographic images, to evaluate if the Bruggeman correlation is appropriate, and to further clarify if using a single tortuosity factor is reasonable. To do so, concentrated-solution transport equations are solved over a reconstruction of the separator geometry whilst imposing various Dirichlet conditions on electrolyte concentration and potential. To give a benchmark for comparison, the pore-scale transport equations are solved for a separator sample under realistic discharge conditions, allowing evaluation of the accuracy gain offered by a macroscale model with tomography-derived transport properties.

Participation

In-Person

References

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