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3D-Electrochemistry: Designing and resolving the microstructure of an electrode



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With the rise of portable appliances, hybrid & electric cars and storage systems for renewable energy sources, Li-ion batteries have proven to be the most relevant storage device for these applications.

As a consequence of this increased interest, the need for more efficient, safer and longer life cells is clear. However, designs and test methods for new products are very expensive. A trend is emerging towards simulation, which represents a very cost and time effective alternative or compliment to design and test processes. Simulation solutions already exist for 1D models, such as Newman* type formulations. However, the complexity of the electrochemical phenomenon involved would benefit from a more detailed understanding by characterising the three-dimensional structure of the electrode within this system. This is now possible with STAR-CCM+'s new 3D electrochemistry model. This new feature accounts for transportation and reaction processes inside the resolved electrode in order to simulate the overall cell behaviour. This talk presents the formulation and status of this model and compares results with 1D solutions produced using Battery Design Studio (Battery Design LLC).

Reference * Fuller, Doyle, Newman ?Simulation and Optimization of the Dual Lithium Ion Insertion Cell?, JECS, 1994.

Author Company:

CD-adapco

Author Name:

Gaëtan Damblanc

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