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Title:

Parametrization of a Newman P2D model for a commercial 37Ah Li-ion battery and validation with incremental capacity peaks

Authors:

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Abstract:

Physico-chemical modeling is seen as a very interesting way to simulate the performance and the aging of Li-ion batteries. The parametrization of such models is crucial for an accurate representation of the internal state of the cell. In the case of commercial batteries, the parametrization procedure is hardly ever entirely undergone, leaving room for parameters tweaking and inaccurate simulation results. In the framework of this work, over 70% of the parameters were measured for a commercial 37Ah Li-ion prismatic battery for PHEV applications (Graphite || NMC111). A DFN P2D physics-based model is chosen based on the work of Dufour et al. [1]. The major electrochemical characterization technics and measurement results for every component in the cell will be presented. The cells were opened in the ante-mortem procedure [2], materials were identified, geometrical parameters were measured and samples were taken for coin-cell experiments. A small portion of the electrolyte was recovered and studied to conclude that it was made of EC-DMC-EMC at 1:1:2 portions. A similar solution was synthesized in order to conduct ionic conductivity measurements at temperatures ranging from -30 to 60°C. Samples from the separator were taken both for effective ionic conductivity measurements under the same temperature range and for porosity measurements. The tortuosity of the electrodes was calculated via an EIS spectrum with a blocking-electrodes configuration and finally the diffusion factor in the active particles was estimated via GITT experiments. A very slow current regime was used to lithiate and de-lithiate the active materials in a half-cell experiment in order to balance the electrodes. The model was compiled using COMSOL Multiphysics 5.5, and results were compared to validation experiments conducted on the full-setup prismatic cell. The charge curve was validated under different current and power regimes at 25°C, and the Incremental Capacity (IC) curve showed a reasonable accuracy. With this in hand, the following step would be to couple this performance model to an aging model and to compare the evolution of the IC peaks with the experimental aging.

References:

- [1] N. Dufour, M. Chandesris, S. Geniès, M. Cugnet, and Y. Bultel, "Lithiation heterogeneities of graphite according to C-rate and mass-loading: A model study," *Electrochimica Acta*, vol. 272, pp. 97–107, 2018.
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