Methodology to Assess the Impact of Electrochemical Model Parameters Based on Design of Experiments

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Abstract

Current and emerging energy storage devices need to be enhanced to cope with the energy and power density requirements of different applications. Electrochemical models are helpful tools for the development and redesign of existing Li-ion batteries as well as to support more innovative concepts, since they can provide useful information related to the internal mechanisms occurring in these devices.

In the present study, a methodology based on design of experiments (DOE) is proposed to evaluate the response of a cell when internal design parameters are changed. A physics-based battery model implemented in COMSOL Multiphysics® simulation software and developed by G. Plett et. al. [1] is used for the analysis. This electrochemical model is linked using the LiveLink™ for MATLAB® in order to analyse the effects and interactions of internal battery parameters by means of DOE. The mathematical framework of this model is based on the work of Newman et.al [2] and the cell parameters used for the validation of this methodology are taken from Doyle et. al. [3 - 4]. The cell is constructed with Carbon and Lithium Manganese Oxide (LMO) electrodes and the electrolyte is a mixture of lithium hexafluorophosphate salt (LiPF6) and commonly used organic carbonate solvents (Ethylene Carbonate (EC) and Dimethyl Carbonate (DMC)).

For this case study, a full factorial design is proposed. The effect and interactions of internal parameters such as the solid volume fraction, the thickness and the particle radius of the positive and negative electrodes are evaluated based on the response of the internal variables of the cell (electrolyte concentration, solid particle concentration, electric potential, electrolyte potential) and other cell characteristics (capacity, energy and power density). The procedure implemented in this work is shown in Figure 1.

This methodology can be applied to evaluate the performance of real cells in which internal parameters are experimentally obtained using the most suitable characterization techniques. In addition, this tool can help in the design of new cells, as it provides highly valuable insights on the response of the internal variables as a function of design parameters.

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Figures used in the abstract

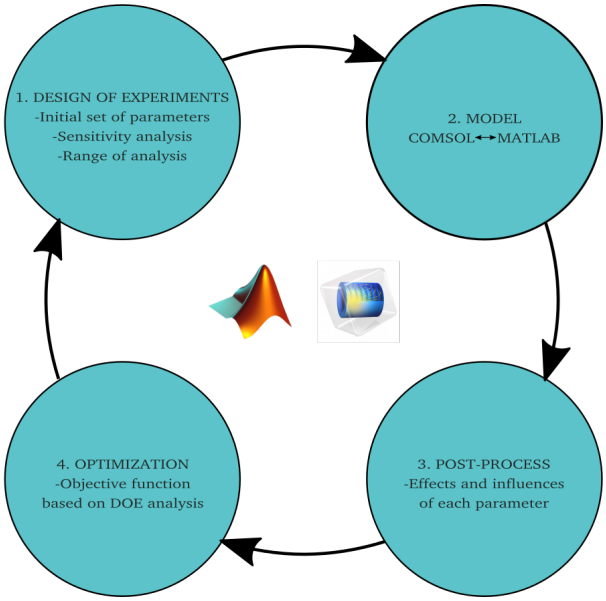

Figure 1: Methodology applied in this work.