Uncertainty Assessment and Sensitivity Analysis of Heat Generation Within a Lithium-Ion Battery

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Abstract

Dedicated work in modeling, simulation and design optimization of Lithium-ion Battery (LIBs) was done in the past decades, and still, the most widely used one for electrochemical processes is the Newman model. [1] The underlying parameters are treated deterministically, but the impact of uncertainty due to experimental accuracy limitations and cell-to-cell variations have an undeniable impact on battery performance. [2] In this approach the analysis of uncertainty related to heat generation is the mayor focus due to its impact on safety and battery performance on a systems level.

At DLR VE a P2D-3D electrochemical-thermal battery model is established[3] and used in order to simulate the deterministic behaviour of a virtually represented commercial lithium-ion pouch battery cell, introduced to event based constant current and constant power charge and discharge profiles. The model uses the Heat Transfer in Solids interface and the Batteries and Fuel Cells Module of COMSOL Multiphysics® to implement the multiscale and multiphysic setting of the battery cell. Moreover it benefits from using the CAD Import Module and LiveLink™ for MATLAB® in order to virtually create CAD data with Autodesk Inventor® and process the statistical analysis in the MATLAB® programming environment.
In this approach the nature of uncertainties and inhomogeneities of the electrochemical sub model are mainly hidden within the electrochemical parameters and geometric interface relations of the cell materials. As such, with an emphasis on geometrical parameters, carefully selected uncertainty distributions of material parameters are defined to quantify the sensitivity of heat generation in a statistical Monte-Carlo approach. While geometric aspects are simplified in the electrochemical sub model, the thermal sub model strongly depends on an accurate complex representation of the cell design.
The thermal characteristics of the cell components (active layers, current collectors, separator, etc.) were experimentally determined using Laser Flash Analysis by LFA 447/2-4/InSb and Differential Scanning Calorimetry by DSC 204F1 Phoenix from NETZSCH, and geometrical measurements were performed with a µ-CT Skyscan 1172 from Bruker in our laboratories. Battery cycling is performed on multiple commercial cells in separate test branches under defined electrical test conditions by a Maccor Series 4000 potentiostat and environmental conditions maintained by a Vötsch VC7034 climate chamber in order to compare and validate simulated results of the quantity of interest for the given battery performance strategies.

Accurate distributions of material parameters will be proposed in accordance with the

measurements performed in our laboratories. The experimental battery behaviour is expected to be in good agreement with simulation data for low C and P-rates, mandatory in case of battery friendly management, and we are able to realistically predict the heat generation inside the battery cell.

Uncertainty of material parameters of a LIB cell model has a big influence on the battery performance. Therefore, a new test setup was developed to propose uncertainty distribution of input parameters, predict the impact of uncertainty for battery performance and derive accurate behaviour of the quantity of interest: heat generation. We will further utilize the model for comparative studies of commercial cell variants.

Figures used in the abstract

Literature:

[1] M. Doyle, T.F. Fuller, J. Newman, Modeling of galvanostatic charge and discharge of the Lithium/polymer/insertion cell, J. Electrochem. Soc., 1993

[2] Hadigol, M., K. Maute and A. Doostan, On uncertainty quantification of lithium-ion batteries: Application to an LiC 6 /LiCoO 2 cell, J. Power Sources, 2015

[3] Lundgren, H., P. Svens, H. Ekström, C. Tengstedt, J. Lindström, M. Behm and G. Lindbergh, Thermal Management of Large-Format Prismatic Lithium-Ion Battery in PHEV Application, J. Electrochem. Soc, 2015

Instruments:

[1] Determination of Heat Capacity (Cp)

Instrument	Netzsch DSC 204F1 Phoenix
Temperature measurement range	-20°C to 80°C
Heating rate	5 K/min
Active cooling purge gas	Nitrogen

[2] Determination of Thermal Conductivity (k)

Instrument	Netzsch LFA 447/2-4/InSb
Temperature measurement range	25°C to 80°C
Measurement area	0.785 cm²

Density (g/cm³) and thickness (mm) of each individual sample was provided as input.

[3] Qualitative Imaging and Current Collector Thickness

Instrument	Skyscan micro CT 1172
Resolution	1.5 µm/pixel
Rotation step	1.5°
Average Framing	6

[4] Determination of Impedance

Method	Instrument	Operating Parameters
Electrochemical impedance spectroscopy	Princeton Applied Research VersaSTAT 4	Potentiostat EIS: voltage amplitude 10 mV RMS

[5] Realization of Electrical and Thermal parameters

Method	Instrument	Operating Parameters
Potentiostatic cycling	Maccor Series 4000	Voltage 0-8 V (0.02 % accuracy), current 0-150 A (0.05 % accuracy)
Voltage and temperature measuring	Agilent 34972A + 34901A Multiplexer module	Voltage 0-100 mV (0.009 % accuracy)
Current measuring	Weigel current shunt resistor	60 A - 60 mV (0.2 % accuracy)

[6] Realization of Environmental Conditions

Method	Instrument
Temperature control	VC7034, Vötsch Industrietechnik GmbH

Figure 1: List of Literature References and Used Equipment.