Numerical Simulation of the Lithium-Ion Battery Cell Discharge Characteristics

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Abstract

Introduction: In general battery cells are charged/discharged using constant currents expressed as current densities (C-Rates). We are developing a single cell-level Li-Ion battery model in order to simulate the performance and the physico-chemical phenomena under power density discharging mode (P-Rate). The P-rate is defined as the measure of the rate at which a battery charges/discharges relative to its maximum capacity under constant power (i.e. 1 P equals to the power needed to fully charge/discharge the battery in one hour).

Use of COMSOL Multiphysics®: The two-dimensional Li-ion model geometry consists of five different layers (Figure 1): anode current collector made of copper (a), graphite anode layer (LiC6, b), separator sheet (c), active cathode layer (LiCoO2, (d)) and cathode current collector aluminum (e). A set of partial differential equations (PDEs) describes the transport processes and the charge transfer reactions in the cell are solved with COMOL Multiphysics® 3.5 with no additional program modules. The PDEs were parametrized with data from discharging experiments with Li-Ion battery cells.
The redox reaction occurring at the electrode/electrolyte interfaces are assumed to follow the Bulter-Volmer equation [1], which can be reduced to the dependence of the Li-concentration at the anode and the cathode respectively [2].

Results: The developed model is able to predict the discharge profile (cell voltage) for different discharging P-Rates as shown in (Figure 2). Note that the current is increasing during discharge due to the decreasing cell voltage as shown in, which is especially distinct at end of discharge (fast voltage drop). This is a striking difference of the P-rate operation compared to C-rate operation (constant current). The simulation results reveal strong gradient in the local state of charge (SOC) of the single electrode particles in dependence of the particle position and size. Furthermore the model was validated with experimental discharging curves of Li-Ion batteries studied in the model. A good agreement between experimental and modeled cell voltage vs. discharging time curves was found with different P-rates with deviation of 2-5 % as shown in (Figure 3) .

Conclusion: The model is able to predict the discharging profiles for different P-rates at reasonable deviations compared to experimental profiles. From the comparison of simulated current and voltage, the increasing current behavior with decreasing voltage is characteristic for P-rate operation. Future activities will be devoted to further increase the modeling accuracy and

to examine the impact of the sharp current increase at the end of discharge on, e. g. battery ageing and safety questions.

Acknowledgements: The present work was conducted within the project LESSY (Lithium-Electricity-Storage-System) and we gratefully acknowledge the financial support of the German Federal Ministry of Education and Research. The authors would like to thank Sven Pueschel from Li-Tec Battery GmbH and Dr. Phillip Niehoff from University of Muenster for their valuable inputs regarding electrical and electrochemical characterization of the used Li-Ion battery cells.

Reference

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2.Macro Meyer, Study of the local SOC distribution in a lithium-ion battery by physical and electrochemical modeling and simulation, journal of applied mathematical modeling, 37, 2016-2027 (2013)

Figures used in the abstract

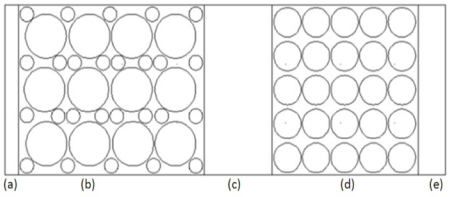

Figure 1: 2-D model geometry of Li-Ion battery consisting of circular intercalation particles at active layers, separator and current collector. [2]

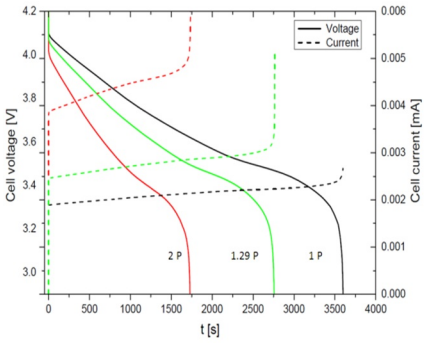

Figure 2: Discharging voltage profile of the model with different P-Rates.

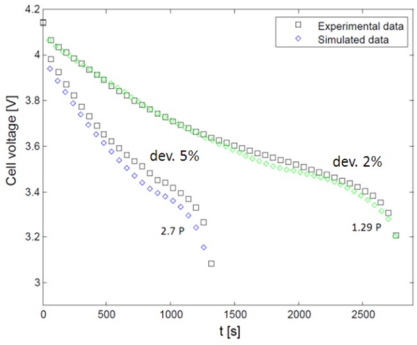

Figure 3: Comparison of discharge profile with experimental data.