Numerical Simulation of the Lithium-Ion Battery Cell Discharge Characteristics

NEXT ENERGY
EWE-Forschungszentrum für Energietechnologie e.V.

Z. Umar , D. Ledwoch, L. Komsiyska, S. Vasić

NEXT ENERGY · EWE Research Centre for Energy Technology at the University of Oldenburg, Germany, www.next-energy.de
Stanislav.vasic@next-energy.de

Introduction

In general battery cells are charged/discharged using constant current or constant power expressed as C-Rates and P-Rates respectively. We are developing a single cell-level Li-Ion battery model in order to simulate the performance and the physico-chemical phenomena under power 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).

Modeling Approach

The studies are performed by using the Equations Based Model with the following equations:

- **Fick's Law:** Diffusion of lithium-ions in active particles and electrolyte

$$\Gamma_{Li,Li^+}^{mass} = -D_{Li,Li^+} \cdot \nabla C_{1,2}$$

- **Ohm's Law:** Electrical potential (electron, ion fluxes) distribution

$$\Gamma_{e^-,i}^{current} = \sigma_{e^-,i} \cdot \nabla \Phi_1$$

- **Nernst Equation:** Concentration-dependence of electrode potentials

$$U_j^0 = \phi_j^0 + \frac{RT}{zF} ln \frac{c_{ox}}{c_{red}}$$

- **Butler-Volmer (modified):** Electrode kinetics (i. e. dependency of current on the charge transfer overpotentials) [1, 2]

$$i_{nj} = i_o \left[(c_2')^{-\alpha_{a,j}} \cdot \exp\left(\frac{\alpha_{a,j}F}{RT}\eta_j\right) - (c_2')^{\alpha_{c,j}} \cdot \exp\left(-\frac{\alpha_{c,j}F}{RT}\eta_j\right) \right]$$

- **Power density:** Power density defined as multiple of the current density and the cell's nominal voltage

$$P_d = i_c \cdot V_{nom}$$

Modeling with COMSOL Multiphysics®

- Modeling in 2-D Li-Ion cell geometry
- Five different cell components/boundaries: anode current collector, anode, separator, cathode, cathode current collector, electrolyte
- Visualization of particle size effects: active material particle for lithium (de)intercalation depicted as circles
- Solving of charge transfer reactions and transport processes described by set of partial differential equations
- Results: e. g. discharging profile, local anode/cathode SOC, effect of particle size, current-voltage-characteristics

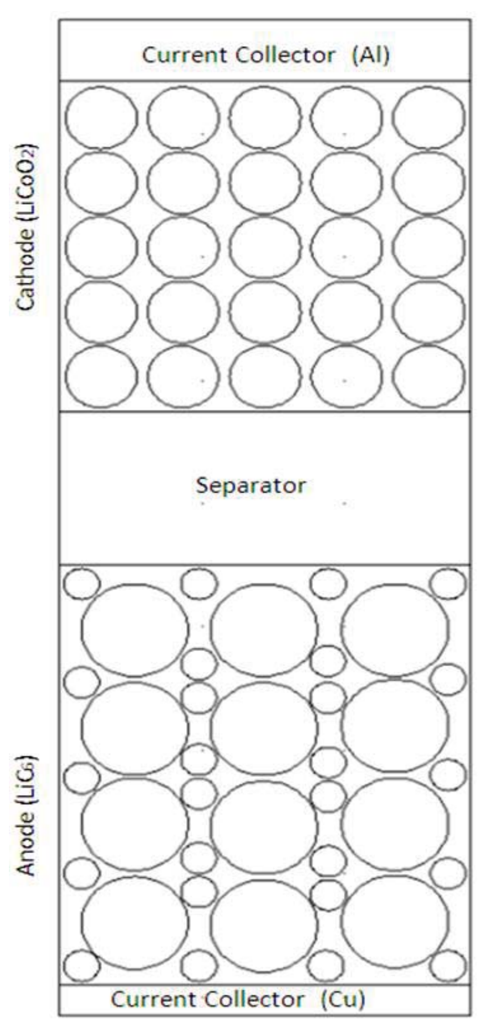

Figure 1: 2 D-Model of Li-Ion Cell.

Simulation Results and Validation

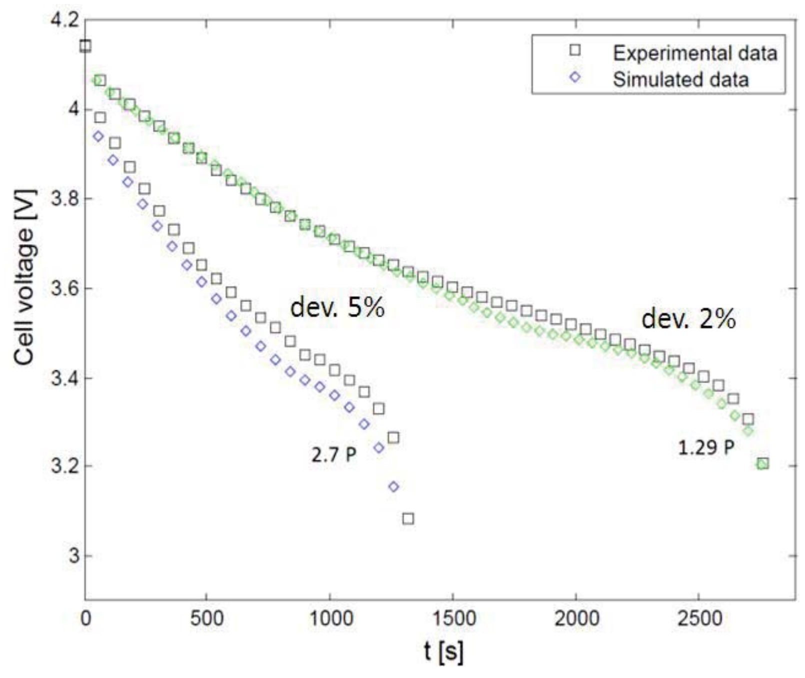

Figure 2: Comparison of simulated and experimental voltage discharge profiles. Deviations of 2-5 % between both validate the model's applicability for different P-Rates.

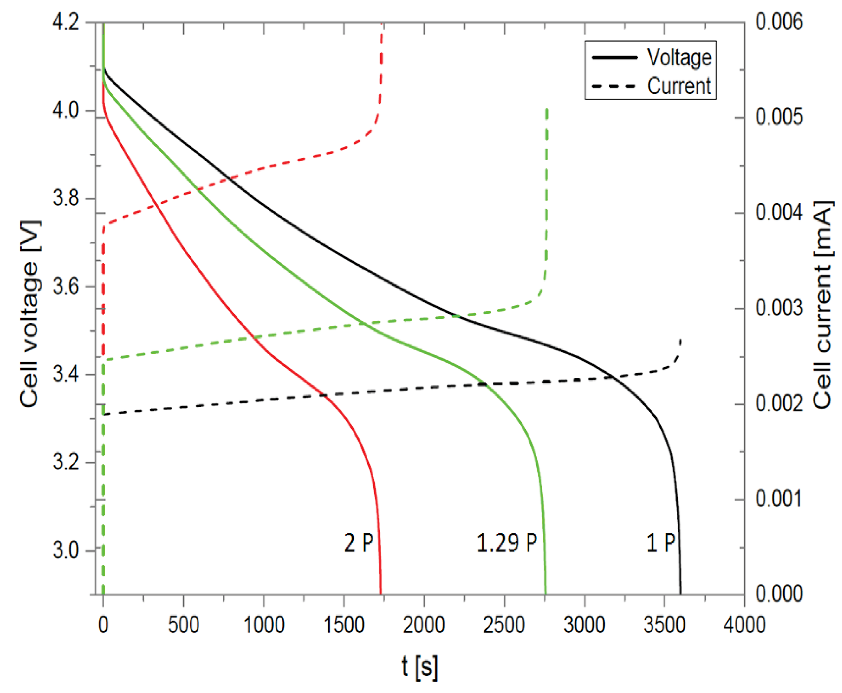

Figure 3: Simulated behaviour of the current and voltage profiles during discharging at different P-Rates.

Local State of Charge (SOC)

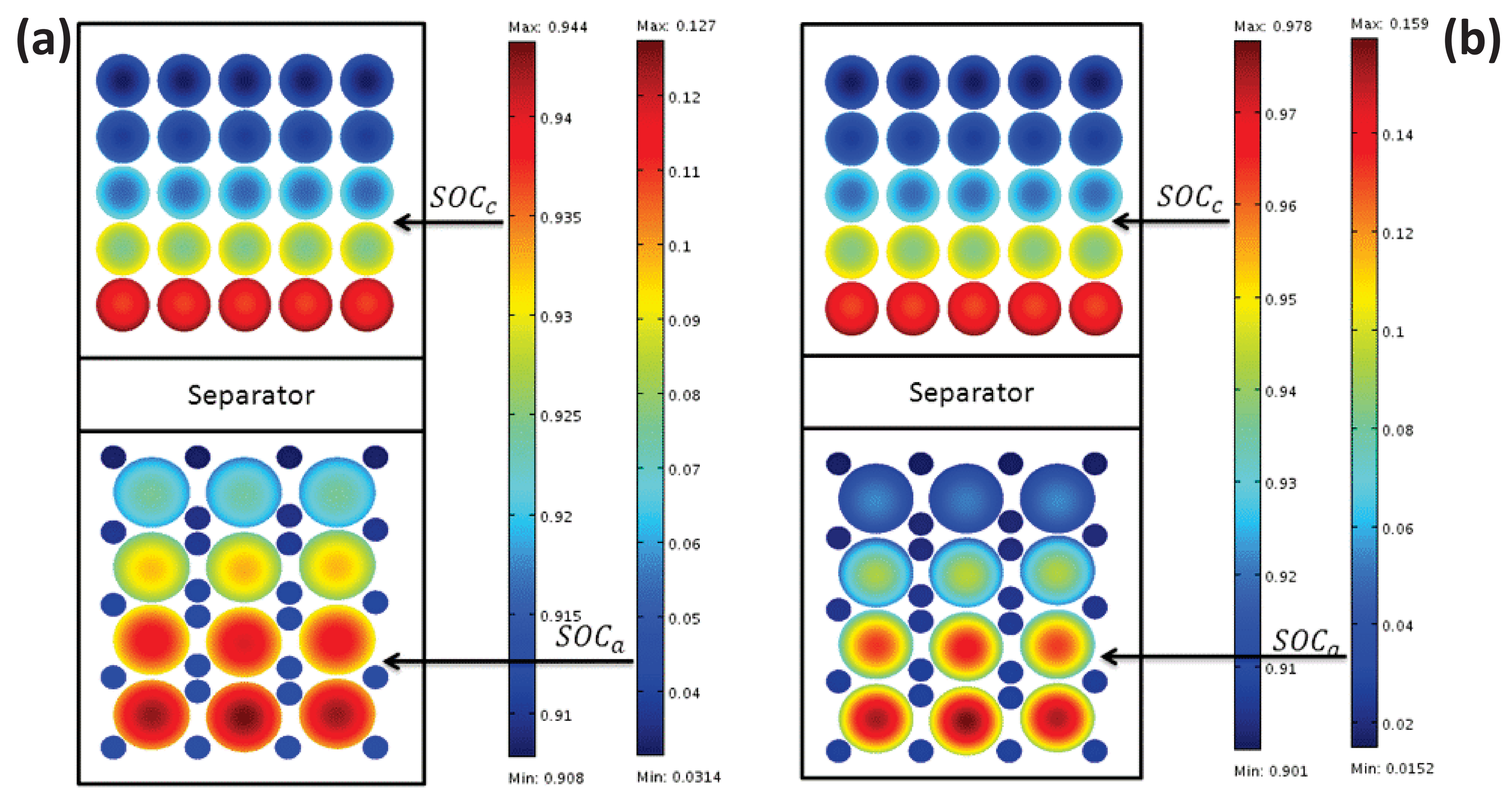

Figure 4: SOC distribution at anode and cathode at 3.2 V for (a) 1 P-Rate, (b) 2 P-Rate.

Conclusion and Outlook

- A physico-chemical model of a Li-ion battery, able to predict the discharging behaviour at different P-Rates, was developed and validated.
- A gradient in the particle SOC as a function of the distance from the separator is observed for both electrodes during discharge with constant power.
- At the anode particle SOC shows gradient in dependence of the particle size. Gradient increases at higher discharge powers.
- The model will be further developed in order to increase modeling accuracy and to predict battery ageing phenomena. In addition safety issues will also be addressed.

Acknowledgement

The Present work was conducted within the project LESSY (Lithium-Electricity-Storage-System) and we acknowledge the financial support of the German Federal Ministry of Education and Research. Additional thanks go to Sven Pueschel from Li-Tec Battery GmbH and Dr. Phillip Niehoff from University of Muenster.

References

[1] W. B. Gu *et al.*, ECS Proceedings 99(25), 2000, pp. 748
[2] M. Meyer *et al.*, Appl. Math. Model. 37, 2013, pp. 2016-2027