End-of-life prediction of a lithium-ion battery cell based on mechanistic ageing models of the graphite electrode

Serena Carelli[a], Christian Kupper[a], Wolfgang G. Bessler[a]
[a] *Institute of Energy Systems Technology (INES), Offenburg University of Applied Sciences, Badstr. 24, 77652 Offenburg, Germany*

E-mail: serena.carelli@hs-offenburg.de

Mathematical modelling and numerical simulation have become standard techniques in Li-ion battery research and development, with the purpose of studying the issues of batteries, including performance and ageing, and consequently increasing the model-based predictability of life expectancy.

We present an electrochemical model of a graphite-based lithium-ion cell that includes combined ageing mechanisms: (i) Electrochemical formation of the solid electrolyte interphase (SEI) at the anode, (ii) breaking of the SEI due to mechanical stress from volume changes of the graphite particles, causing accelerated SEI growth, (iii) gas formation and dry-out of the electrodes, (iv) percolation theory for describing the loss of contact of graphite particles to the liquid electrolyte. Also, first results on the integration of lithium plating are presented.

The electrochemistry is coupled to a multi-scale heat and mass transport model[1] based on a pseudo-3D approach. Heat transport in the through-cell direction is modelled as conductive process (1D, macroscale) while mass and charge transport on the electrode-pair scale as diffusion and migration (1D, mesoscale). Intraparticle transport of lithium atoms is modelled as Fickian diffusion with concentration-dependent diffusion coefficient (1D, microscale). A 0D model of the void cell volume is also added, allowing the description of gas-phase species concentration and pressure build-up during ageing.

A time-upscaling methodology is developed that allows to simulate large time spans (thousands of operating hours). The combined modeling and simulation framework is able to predict calendaric and cyclic ageing up to the end of life of the battery cells. The results show a qualitative agreement with ageing behavior known from experimental literature, in particular the dependence of temperature, current, cycling depth, and average SOC. The introduction of electrode dry-out to the model allows to capture for the first time the strong nonlinearity of ageing towards end of life (“sudden death”).

Acknowledgements:
This work was supported by DFG through the Research Training Group GRK 2218 SiMET (Simulation of Mechanical, Electrical and Thermal processes in lithium-ion batteries) and by Land Baden-Württemberg through the cooperative graduate college DENE (Dezentrale Erneuerbare Energiesysteme).

References:
[1] C. Kupper, W. G. Bessler, J. Electrochem. Soc. 164 (2017) A304-A320.
[2] J. Vetter, P. Novák, M. R. Wagner, C. Veit, K. -C. Möller, J. O. Besenhard et al., J. Power Sources 147 (1-2) (2005) 269–281.