Numerical Simulation and Experimental Validation for Thermal Runaway on Lithium-ion Cells

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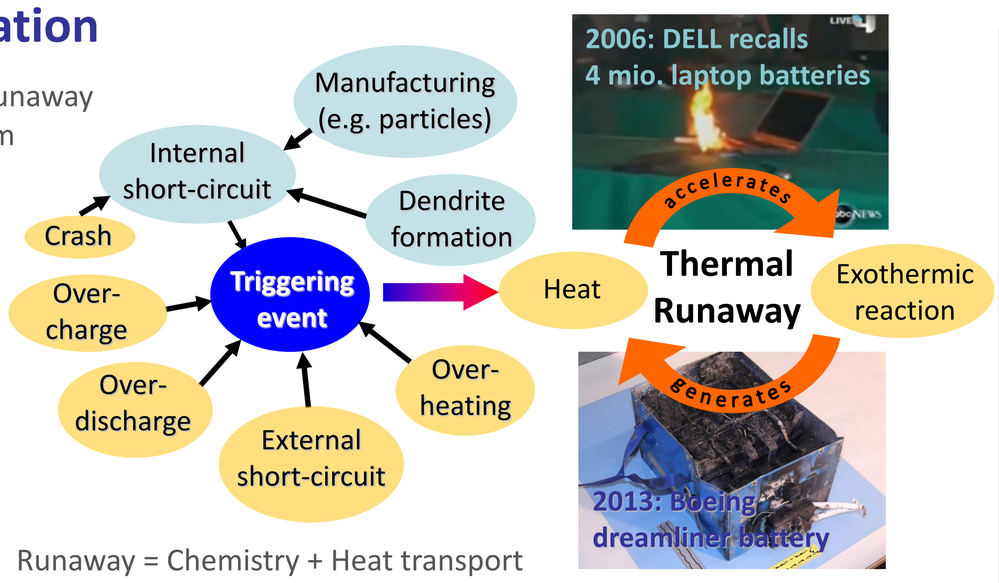
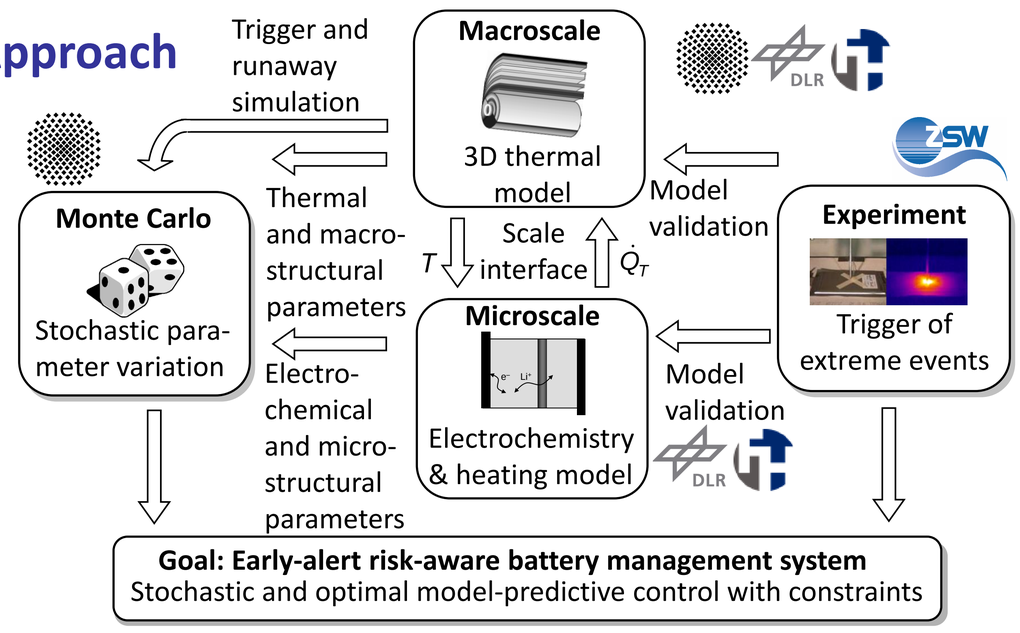
Motivation

Thermal runaway mechanism



Runaway = Chemistry + Heat transport

Approach

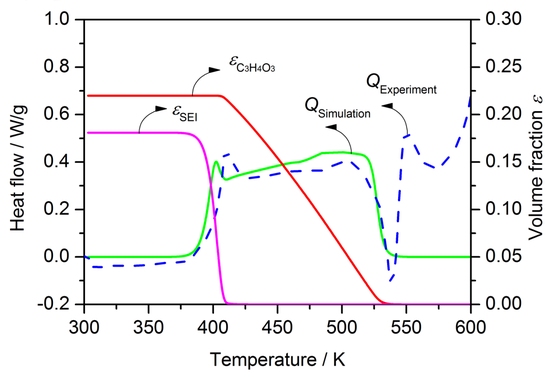


Micro Model

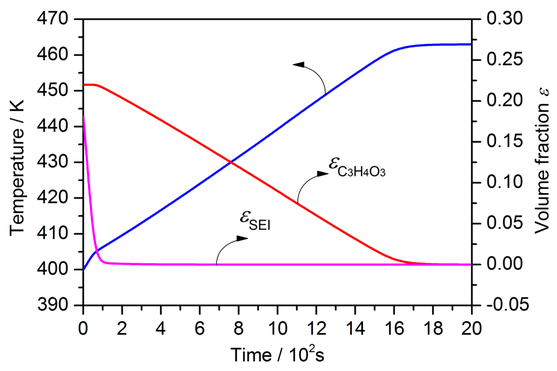
Degradation models at high temperature include:

- **Solid electrolyte interface (SEI) decomposition**
  $(CH_2OCO_2Li)_2 \rightarrow Li_2CO_3 + C_2H_4 + CO_2 + 0.5\ O_2$
- **SEI formation (Electrolyte decomposition)**
  $2\ C_3H_4O_3\ (EC) + 2\ e^- + 2\ Li^+ \rightarrow (CH_2OCO_2Li)_2 + C_2H_4$
- **Electrolyte evaporation**
  $C_3H_4O_3\ (liquid) \rightarrow C_3H_4O_3\ (gas)$

Simulation of **differential scanning calorimetry (DSC)** for SEI decomposition and formation. Dash line : experiments by Pasquier et al.* , Solid line s: simulation. Heat rate : 5K/min.



Simulation of **self-accelerating heat** with SEI decomposition and formation reaction at adiabatic condition. The initial temperature is 400 K.



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Stochastic Model

Bayesian filtering

$x_t \cdots$ model state at time t
$y_t \cdots$ measurement at time t
$\mu_t \cdots$ model error
$\nu_t \cdots$ measurement error

System model: $x_t = f(x_{t-1}, \mu_t)$
Measurement model: $y_t = g(x_t, \nu_t)$

Update of uncertain model predictions with measurements via Bayes' theorem:

$$p(x_t|y_0, \cdots, y_t) = \frac{p(y_0, \cdots, y_t|x_t)}{p(y_0, \cdots, y_t)}$$

Complete sequential procedure (simplified):

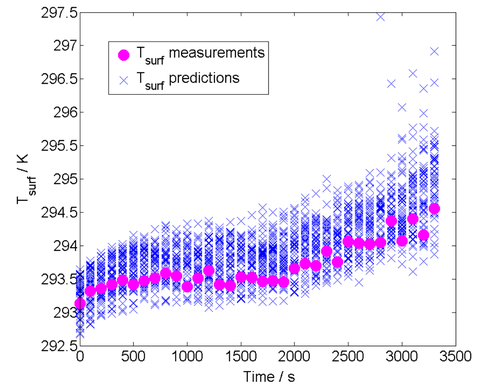
$$p(x_{0,\ldots,t-1}|y_{0,\ldots,t-1}) \xrightarrow[\text{prediction}]{\text{information loss}} p(x_{0,\ldots,t}|y_{0,\ldots,t-1}) \xrightarrow[\text{update}]{\text{information gain}} p(x_{0,\ldots,t}|\, y_{0,\ldots,t})$$

$$t = t + 1$$

Solution of model equations with a particle filter:

- Continuous probability density is discretized by particles (individual model runs)
- Measurement update via reweighting of the particles

Monte Carlo prediction of surface temperature over time



Macro Model

3D, 2D and 1D model of single cell will be investigated using COMSOL

Temperature distribution of 3D cell model

3D simulation is compared with 1D simulation under nominal discharge operation in 1 hour (1C rate).

Experiment

General characterization

cell type	weight [g]	volume [l]	VN [V]	C [Ah]	E [Wh]	spec C [Ah/kg]	C density [Ah/l]	spec E [Wh/kg]	E density [Wh/l]
A123 ANR26650	72,90	0,0345	3,3	2,45	7,75	33,5	70,9	106,2	224
Sony US26650VT	90,52	0,0345	3,7	2,67	9,57	29,5	77,4	105,7	277
Panasonic CGR-26650B	93,35	0,0345	3,6	3,36	11,9	36,0	97,4	127,8	346

Battery cycling
Operation characteristics of SONY US26650VT

Abuse experiments such as short circuit, nail penetration and overcharge will be conducted.

DLR Deutsches Zentrum für Luft- und Raumfahrt
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