Towards Understanding Thermal Runaway of Lithium Batteries

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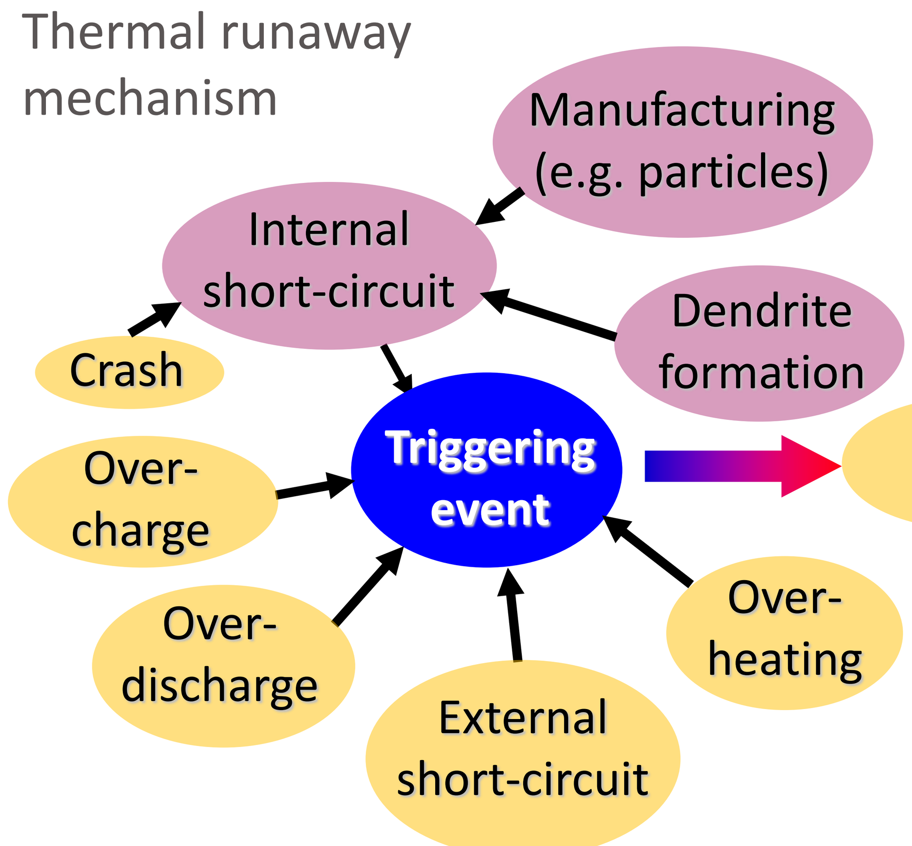
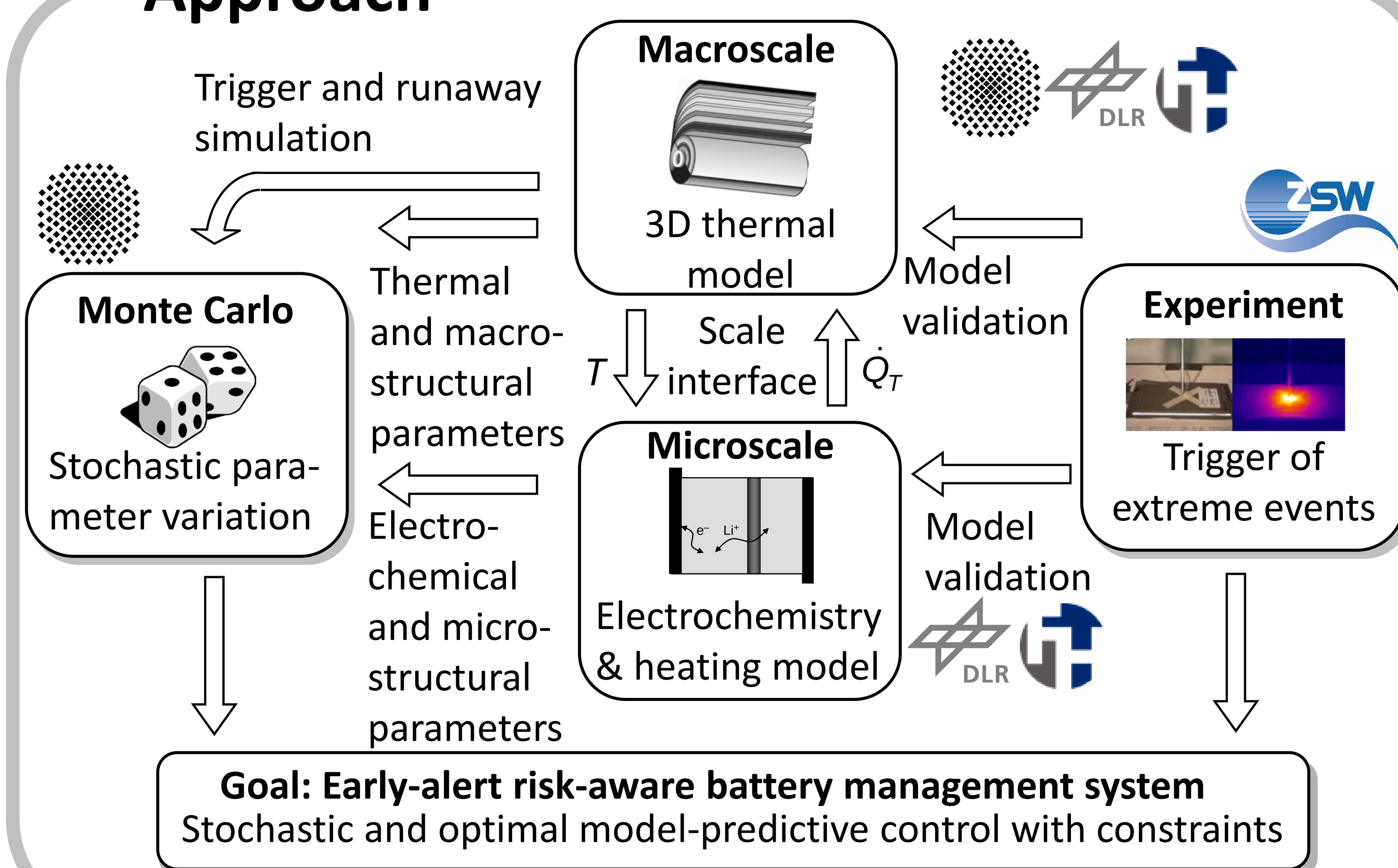
Motivation

Thermal runaway mechanism



Runaway = Chemistry + Heat transport

Approach

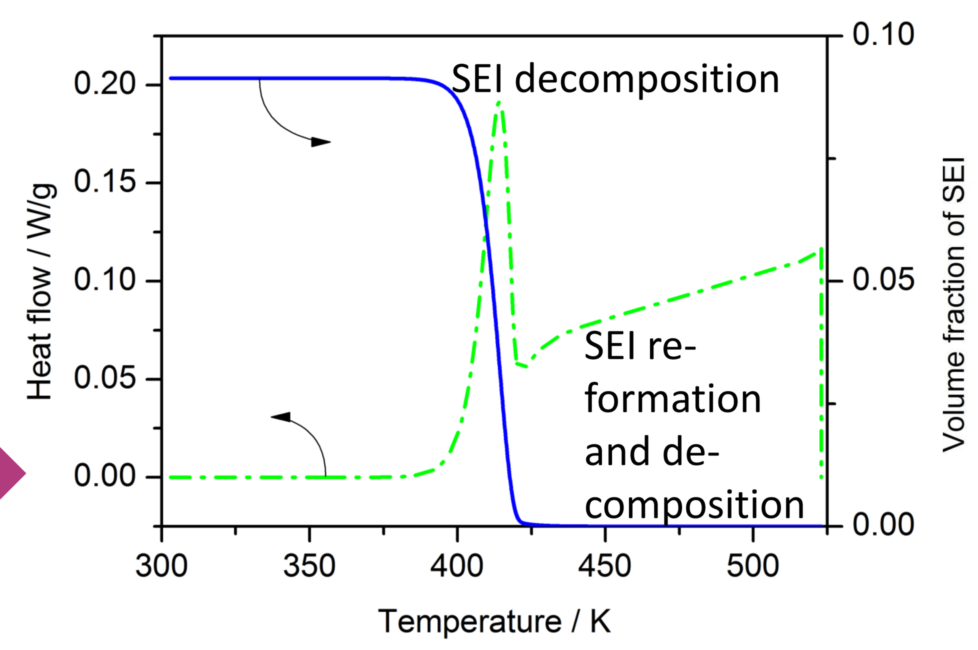


Micro Model

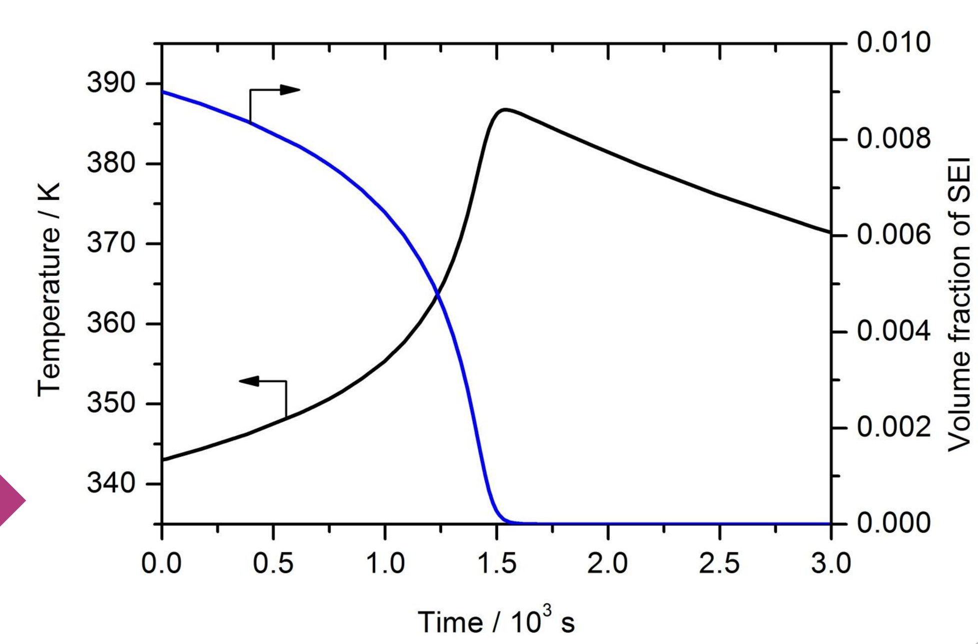
Degradation models at high temperature include:

- **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) → $C_3H_4O_3$ (gas)

Simulation of **differential scanning calorimetry (DSC)** for SEI decomposition and formation.
Heat rate is 5K/min.



Thermal runaway is successfully observed at extreme condition under low heat transfer coefficient and thermal conductivity.



Stochastic Model

Bayesian filtering

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

x_t ... model state at time t
y_t ... measurement at time t
μ_t .... model error
ν_t ... measurement error

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

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

Complete sequential procedure (simplified):

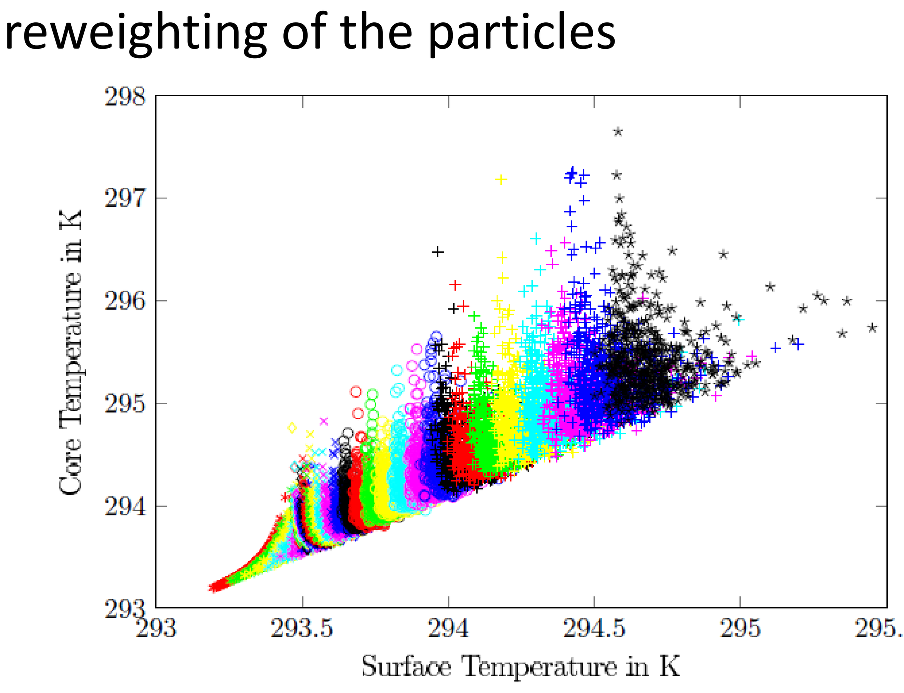
$$p(x_{0,\dots,t-1}|y_{0,\dots,t-1}) \xrightarrow[\text{prediction}]{\text{information loss}} p(x_{0,\dots,t}|y_{0,\dots,t-1}) \xrightarrow[\text{update}]{\text{information gain}} p(x_{0,\dots,t}|\,y_{0,\dots,t})$$

$$t = t + 1$$

Solution of model equations with a particle filter:

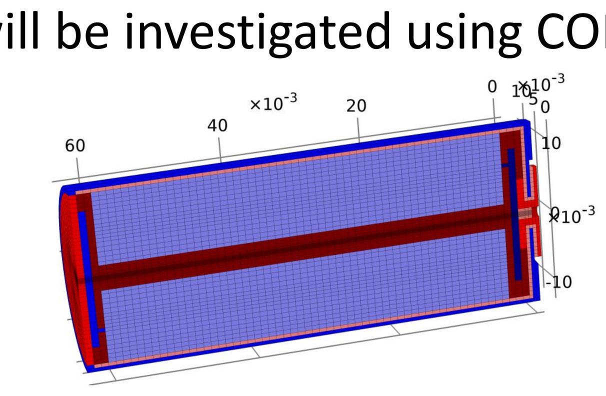
- Continuous probability density is discretized by particles (individual model runs)
- Measurement update via reweighting of the particles

Prediction of cell core temperature as a function of surface temperature for a number of simulation runs under uncertainty

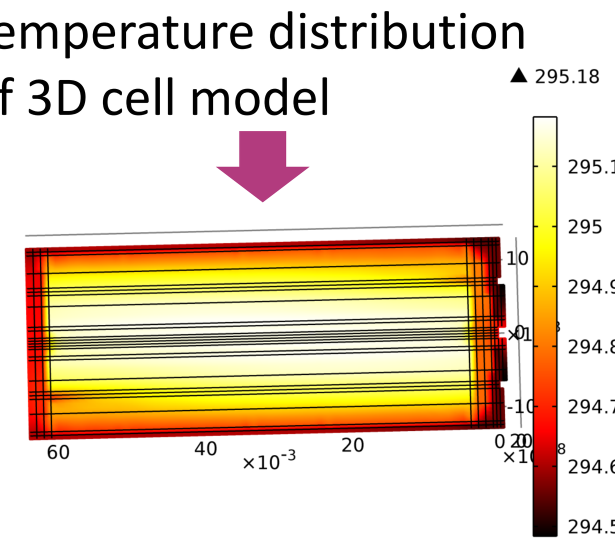


Macro Model

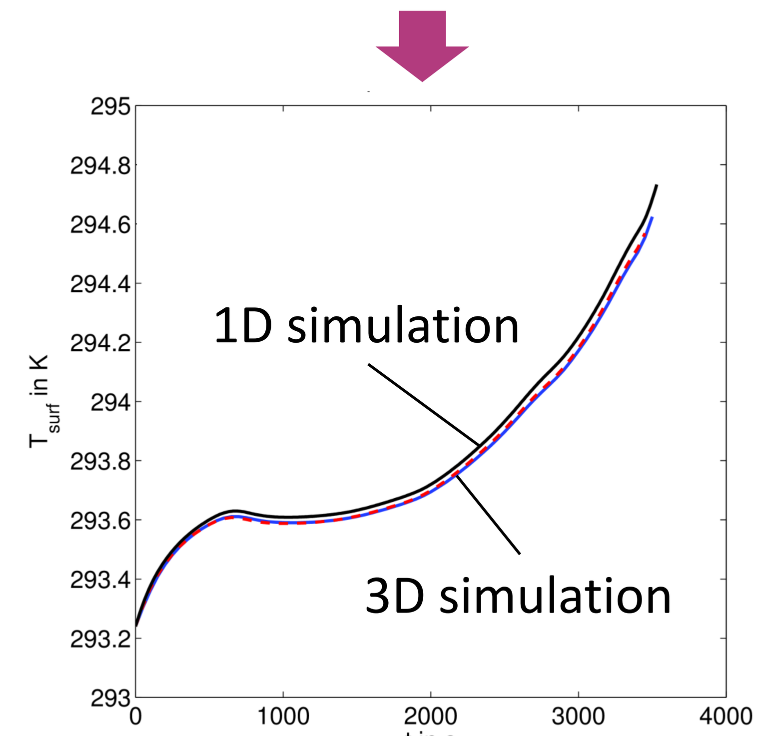
3D, 2D and 1D model of single cell will be investigated using COMSOL



Temperature distribution of 3D cell model



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



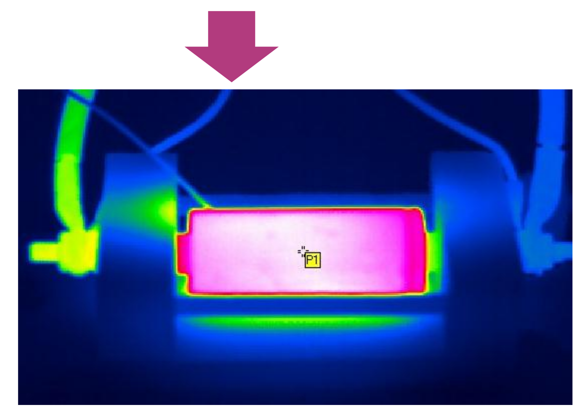
Experiment

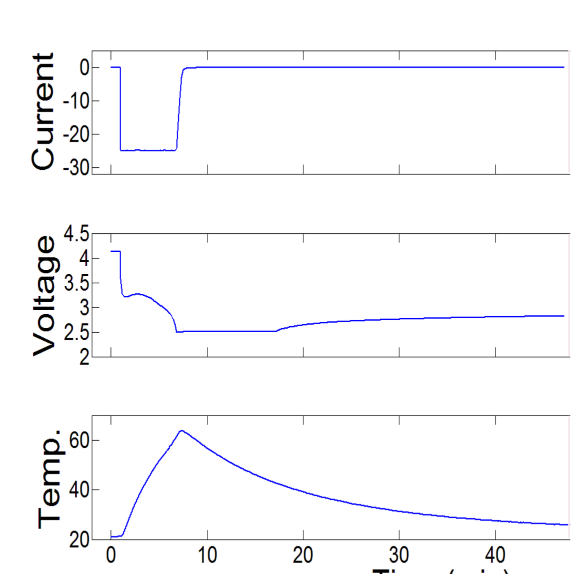
General characterization

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.

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