Towards Understanding Thermal Runaway of Lithium Batteries

**Motivation**

Thermal runaway mechanism
- Internal short-circuit
- Crash
- Over-charge
- Over-discharge
- External short-circuit

**Approach**

Trigger and runaway simulation
- Monte Carlo
- Stochastic parameter variation

**Micro Model**

Degradation models at high temperature include:
- Solid electrolyte interface (SEI) decomposition
  \[ \text{CH}_3\text{OCO}_3\text{Li}_x \rightarrow \text{Li}_x\text{CO}_3 + \text{C}_2\text{H}_6 + \text{CO}_2 + 0.5 \text{O}_2 \]
- SEI formation (Electrolyte decomposition)
  \[ 2 \text{C}_2\text{H}_6\text{O}_4 (\text{EC}) + 2 \text{e}^- + 2 \text{Li}^+ \rightarrow (\text{CH}_3\text{OCO})_2\text{Li} + \text{C}_2\text{H}_4 \]
- Electrolyte evaporation
  \[ \text{C}_6\text{H}_6\text{O}_3 \text{(liquid)} \rightarrow \text{C}_6\text{H}_5\text{O}_3 \text{(gas)} \]

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

**Stochastic Model**

Bayesian filtering
\[ x_t \rightarrow \text{model state at time } t \]
\[ y_t \rightarrow \text{measurement at time } t \]

System model:
\[ x_t = f(x_{t-1}, u_t) + \mu_t \rightarrow \text{model error} \]

Measurement model:
\[ y_t = g(x_t, v_t) + \nu_t \rightarrow \text{measurement error} \]

Update of uncertain model predictions with measurements via Bayes' theorem:
\[ p(x_t|y_{0:t}) = \frac{p(y_t|x_t) \cdot p(x_t)}{p(y_t)} \]

Complete sequential procedure (simplified):
- Information loss
- Information gain
- Update

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

**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

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**Battery cycling**

Operation characteristics of SONY US26650VT

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

Experiment
deesof2006.dell.com

Thermal runaway = Chemistry + Heat transport