Effect of a cell undergoing thermal runaway on the temperature of an adjacent cell

Group 9

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Overview

Thermal runaway occurs in situations where an increase in temperature changes the conditions in a way that causes a further increase in temperature, often leading to a destructive result

In other words, "thermal runaway" describes a process which is accelerated by increased temperature, in turn releasing energy that further increases temperature.

References

- **Modeling and Simulation of the Thermal Runaway in Cylindrical 18650 Lithium-Ion Batteries**;
  Andreas Melcher, Carlos Ziebert, Magnus Rohde, Boxia Lei, Hans Jürgen Seifert
- **Modeling and Simulation of the Thermal Runaway Behavior of Cylindrical Li-Ion Cells—Computing of Critical Parameters**;
  Andreas Melcher, Carlos Ziebert, Magnus Rohde and Hans Jürgen Seifert
- **Experimental Analysis of Thermal Runaway and Propagation in Lithium-Ion Battery Modules**;
  Carlos F. Lopez, Judith A. Jeevarajan and Partha P. Mukherjee

Literature Review

Modeling and Simulation of the Thermal Runaway in Cylindrical 18650 Lithium-Ion Batteries

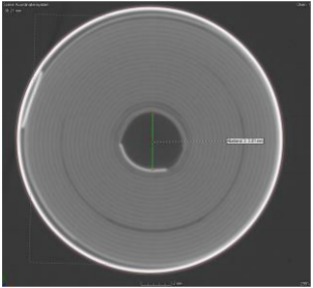
The coupled electrochemical-thermal model for a Lithium-ion battery (LIB) based on porous electrode theory has been extended with contributions coming from exothermic side reactions based on an Arrhenius law to model abuse mechanisms, which could lead to a thermal runaway.

Scheme :

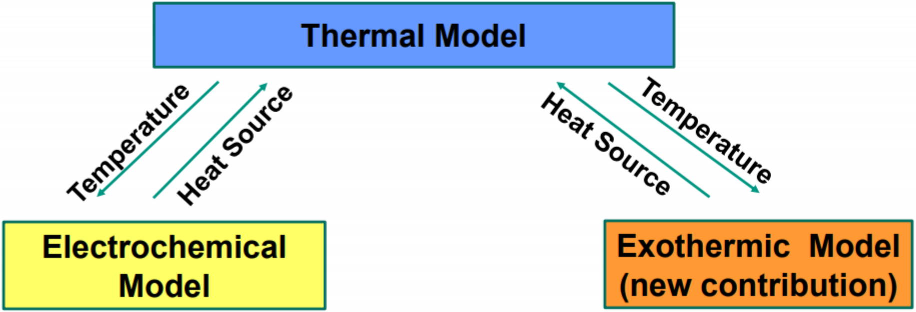
1. The thermal modelling is briefly described.
2. The thermal model is formulated and all heat sources are identified. Mathematical models corresponding to these heat sources are given.
3. The electrochemical heat source is modeled and is implemented in the Battery and Fuel Cell Module in COMSOL Multiphysics.
4. Discussion of exothermic kinetic reactions leading to a thermal runaway.
5. The implementation and the simulation using COMSOL Multiphysics are described. Simulation results for an oven test are shown. Moreover the different stages of the thermal runaway have been classified.

Geometry and Configuration of the Cell :

- Geometry : Cylindrical 18650 cell
- Cathode : LiCoO_2
- Anode : Li_xC_6
- Electrolyte : 1:1 EC : DEC with LiPF_6 salt



General scheme of the modeling of the thermal runaway of a Li-ion cell



Under general working conditions, LIB are exposed to an electrical and/or a thermal load. As consequence, heat is generated inside the cell due to several electrochemical and chemical processes.

- If the heat generation inside the cell is smaller than the ability of the cell to dissipate heat to the environment, the cell is in a thermally stable state.
- If more heat is generated in the cell than can be dissipated to the environment the cell is in a thermally unstable state. The worst case scenario in this second case is the occurrence of a thermal runaway.

Assumptions :

- The interior of the cell is separated from the environmental air due to the battery can, so the cell can be considered as a closed system.
- There is no heat convection inside the LIB
- the initial temperature at the boundary of the cell coincides with the environmental temperature at $t = 0$ s
- the concentration $c_i(\mathbf{x}, t)$ is constant (Constant Fuel model).
- All time-spatial dynamics of the concentrations are neglected.

Governing Equations :

Energy Conservation :

$$\rho c_p \frac{\partial T}{\partial t}(\mathbf{x}, t) = \kappa \Delta T(\mathbf{x}, t) + Q_{gen}$$

for the temperature T : ($\mathbf{x}$, t) $\epsilon\ \Omega \times \Re+ \mapsto \Re$ of the cell in K.
The corresponding initial and boundary conditions are:

$$T(\mathbf{x}, 0) = T(\mathbf{x})\ ,\ \forall\ \mathbf{x}\ \epsilon\ \Omega_o$$

$$\mathbf{n}(\kappa \nabla \mathrm{T}) = -\mathrm{h}(\mathrm{T} - T_{env}) - \varepsilon\, \sigma(T^4 - T_{env}^4)\ ,\ \forall\ \mathbf{x}\ \epsilon\ \partial\Omega$$

For Q_{gen}, contributions come from the heat generated by reversible and irreversible thermodynamic effects, which are represented by the electrochemical heat source $Q_{el-chem}$ and from exothermic kinetic side reactions $Q_{exotherm}$:

$$Q_{gen}(\mathbf{x}, \mathrm{t}) = Q_{el-chem}(\mathbf{x}, \mathrm{t}) + Q_{exotherm}(\mathbf{x}, \mathrm{t})$$

Electrochemical Heat sources :
heat generated inside the cell is due to the reversible and irreversible processes in the cathode, anode and the electrolyte of the LIB. The total electrochemical heat source is given by:

$$Q_{el-chem} = Q_{rev} + Q_{irrev} + Q_{ohm} + Q_{joule}$$

$$Q_{rev} = \mathrm{I.T.}\frac{dU_{eq}}{dT}$$

$$Q_{irrev} = \mathrm{I(U\ -}\ U_{eq})$$

$$Q_{ohm} = I^2 R_{in}$$

$$Q_{joule} = \mathrm{U.I}$$

Thermal runaway can be described with respect to rising temperature in four main stages as follows:

1. SEI decomposition reaction: At T > T1 the solid-electrolyte interface (SEI) will decompose in an exothermic reaction $\implies$ heat source Q_{SEI}.
2. Negative solvent reaction: At T > T2 an exothermic reaction between the intercalated Li-ions and the electrolyte will start $\implies$ heat source Q_{NE}.
3. Positive solvent reaction: For T > T3 an exothermic reaction between the positive material and the electrolyte takes place under the evolution of oxygen inside the cell $\implies$ heat source Q_{PE}.
4. Electrolyte decomposition: In a final exothermic reaction the electrolyte will decompose at T > T4 $\implies$ heat source Q_{Ele}.

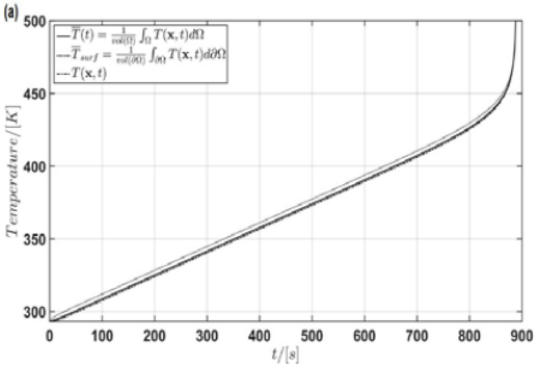
The exothermic heat source is given as:

$$Q_i(\mathbf{x},t) = c_i q_i A_i exp(-\frac{E_{a,i}}{RT(\mathbf{x},t)})$$

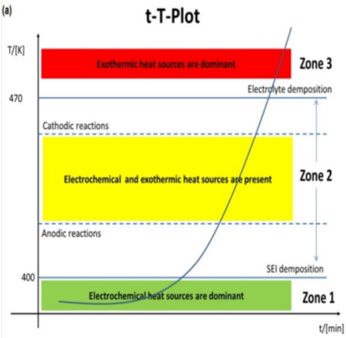
Simulation Results and Discussion :

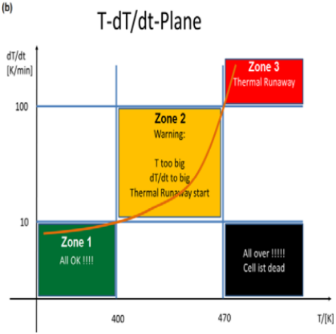
To classify the different stages of a thermal runaway in the phase-space τ the overall spatial mean cell temperature T and their first $\frac{d}{dt}T$ and second $\frac{d^2}{dt^2}T$ time derivative are considered.

Figure: Thermal Runaway during an oven test



From Figure, one can identify three zones during the rise of the temperature T towards the thermal runaway depending on both cases.





Since we have some electrochemical and some exothermic heat sources in the thermal model, the results have the following physical meaning :

- Zone 1: In this zone the electrochemical heat sources represented by the reversible and irreversible part are dominant. The exothermic heat sources can be neglected. This zone corresponds to a thermal stable state of the LIB.
- Zone 2: to the rise in the temperature the exothermic heat sources start to become more active. This zone can be considered as a transient zone on the way from a thermal stable to a thermal unstable state of the cell.
- Zone 3: In this zone the exothermic heat sources are dominant and the electrochemical heat sources can be neglected. This zone corresponds to a thermal unstable state of the LIB which represents the thermal runaway.

Cell Model

Objectives :

1. Temporal variation of temperature for the cell undergoing thermal runaway.
2. Temporal variation of temperature for the adjacent cell.
3. Comparison of temperature profiles of both cells for different values of applied current.
4. Comparison of temperature profiles of both cells for different values of inter-cell distances.

Assumptions :

1. Spatial variation of temperature is not considered
2. Constant specific heat capacity is considered
3. Thermal Runaway under adiabatic conditions
4. Constant Fuel model is used for modeling exothermic reactions
5. Constant volume for the battery
6. Heat convection inside the battery is neglected.
7. Only Ohmic heat is considered for electrochemical heat generation.
8. Constant internal resistance of the battery is considered
9. Inter-cell medium is assumed to be air.

Governing Equations for Modeling Thermal Runaway :

$$mc_p \frac{dT}{dt} = I^2 R_{in} + q_{exotherm}$$

Initial Condition :

$$T(0) = T_{env} = 293K$$

The $q_{exotherm}$ depends on the temperature of the cell.

Governing Equations for Modeling the Neighbouring Cell :

$$mc_p \frac{dS}{dt} = KA(\frac{T - S}{l}) + \sigma A(T^4 - S^4)$$

Initial Condition :

$$S(0) = T_{env} = 293K$$

Parameters Considered :

Mass of the cell (m) = 50 gms

Short-circuit Current (I) = 9, 12, 15, 20 A

Internal Resistance (R_{in}) = 38 mΩ

Specific heat capacity (c_p) = 1189 J/Kg. K

Distance between the cells (l) = 2 mm

Volume of the cell (Vol) = 0.0011 m^3

Surface area of the cell (A) = 0.0018 m^2

Thermal conductivity of the medium between the cells (K) = 0.022 W/mK

Constants for exothermic reactions are directly taken from the reference.

$x \in \{sei, pe, ne, e\}$, $y \in \{c, p, e\}$	Reaction Heat $H_x / \left[\frac{J}{kg}\right]$	Frequency factor $A_x / \left[\frac{1}{s}\right]$	Activation Energy $E_A / \left[\frac{J}{mol}\right]$	Volume Content $W_y / \left[\frac{kg}{m^3}\right]$
SEI reaction	2.57×10^5	1.667×10^{15}	1.3508×10^5	1.39×10^3
Neg. solvent reaction	1.714×10^6	2.5×10^{13}	1.3508×10^5	1.39×10^3
Pos. solvent reaction	3.14×10^5	6.667×10^{13}	1.396×10^5	1.3×10^3
Electrolyte decomp.	1.55×10^5	5.14×10^{25}	2.74×10^5	5×10^2

Discretization of Governing Equations :

- Modeling different exothermic energy sources.

```
    if T(i)<378
        q=0;
    elseif T(i)>=378&&T(i)<393
        q=(a1*exp(-e1/(R*T(i))));
    elseif T(i)>=393&&T(i)<443
        q= (a1*exp(-e1/(R*T(i))))+ (a2*exp(-e2/(R*T(i))));
    elseif T(i)>=443&&T(i)<473
        q= (a1*exp(-e1/(R*T(i))))+ (a2*exp(-e2/(R*T(i)))) +(a3*exp(-e3/(R*T(i))));
    else
        q= (a1*exp(-e1/(R*T(i))))+ (a2*exp(-e2/(R*T(i)))) +(a3*exp(-e3/(R*T(i)))) + (a4*exp(-e4/(R*T(i))))
    end
```

- Modeling thermal runaway.

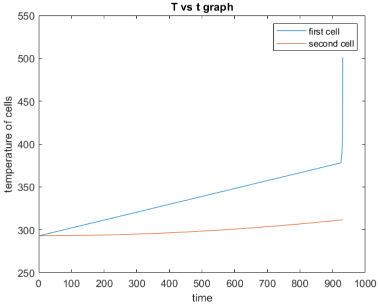
```
    T(i+1)=T(i)+(dt/(m*c))*(((I^2)*r)+q*(vol));
```

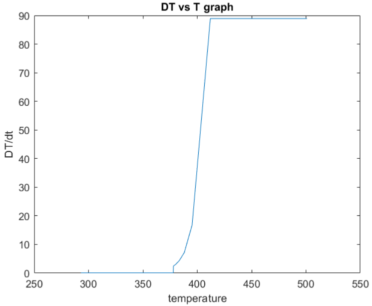
- Modeling governing equation for neighbouring cell.

```
S(i+1)=S(i)+(dt*a/(m*c))*(((k/l)*(T(i)-S(i)))+sigma*((T(i))^4-(S(i))^4));
```

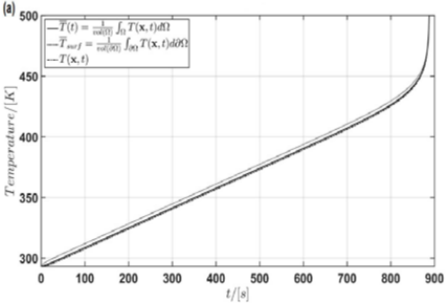
Results and Comparison

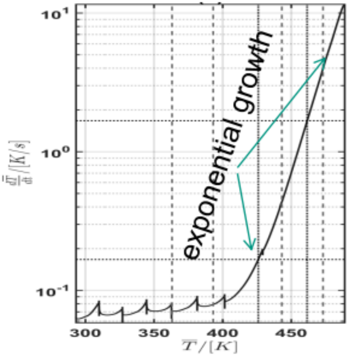
(For I = 12 A)
Temperature Variations w.r.t time. (On left)
Temperature rate Variation w.r.t temperature. (On right)



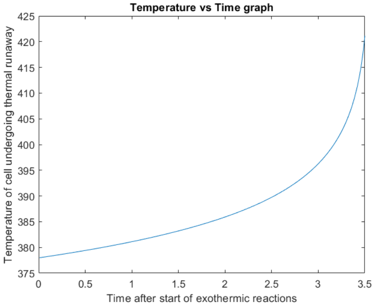


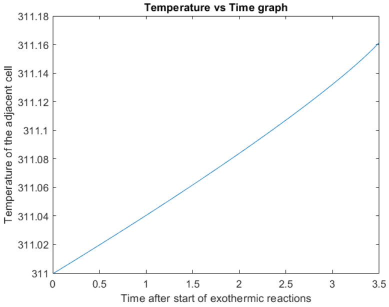
Experimental plots taken from the reference paper.



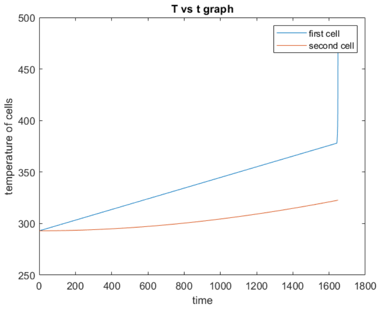


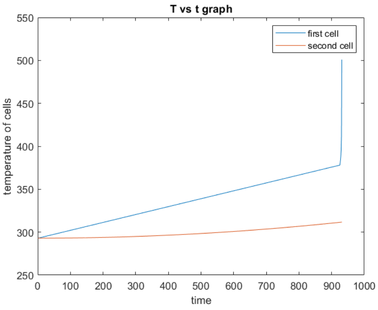
(For I = 12 A)
Temperature Variations w.r.t time in Zone 2. (On left)
Temperature Variations w.r.t time in Zone 2 for the Neighboring cell. (On Right)



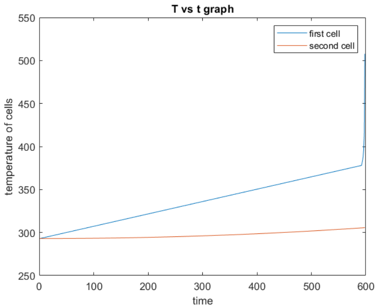


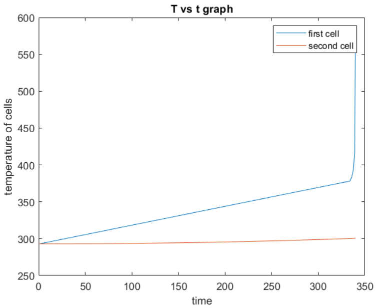
For I = 9 and 12 A



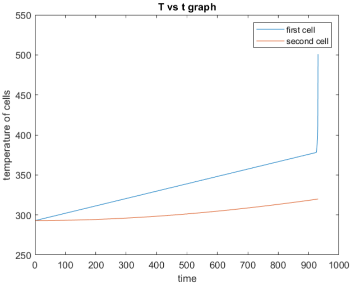


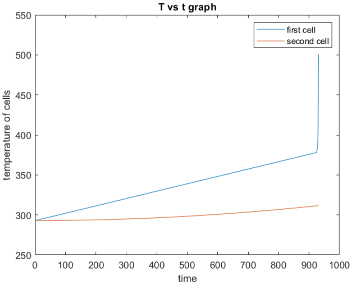
For I = 15 and 20 A

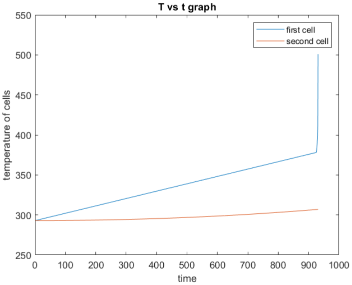




Comparison of temperature profiles for different inter-cell distance : (For 1mm, 2mm, & 4mm)







Future Objectives

- Modeling Spatial and Temporal Variations of temperature for both the cell undergoing thermal runaway and the neighbouring cell.
- Effect of distance between the cells on the temperature profile.
- Maximum temperature plot with time ,and its location for both cells
- Temperature contours at different times of both cells
- Extending the thermal model to other electrochemical heat sources for thermal abuse simulation.

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