



A 3D thermal runaway propagation model for a large format lithium ion battery module



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ABSTRACT

In this paper, a 3D thermal runaway (TR) propagation model is built for a large format lithium ion battery module. The 3D TR propagation model is built based on the energy balance equation. Empirical equations are utilized to simplify the calculation of the chemical kinetics for TR, whereas equivalent thermal resistant layer is employed to simplify the heat transfer through the thin thermal layer. The 3D TR propagation model is validated by experiment and can provide beneficial discussions on the mechanisms of TR propagation. According to the modeling analysis of the 3D model, the TR propagation can be delayed or prevented through: 1) increasing the TR triggering temperature; 2) reducing the total electric energy released during TR; 3) enhancing the heat dissipation level; 4) adding extra thermal resistant layer between adjacent batteries. The TR propagation is successfully prevented in the model and validated by experiment. The model with 3D temperature distribution provides a beneficial tool for researchers to study the TR propagation mechanisms and for engineers to design a safer battery pack.

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1. Introduction

Fuel shortage and air pollution are among the big concerns of current and future energy [1,2]. New energy vehicles [3,4], especially the electric vehicles [5,6], are developed to face the challenge of the fuel shortage and air pollution. Lithium ion batteries are the promising choices to power the electric vehicles, given their high energy/power density and extended cycle life [7–10]. The safe operation of the new energy vehicle must be guaranteed [11], and the safety of the lithium ion battery must be secured in practical operations [12,13]. The safety issues of lithium ion batteries, especially those associated with thermal runaway (TR), have aroused much attention [14–24]. The thermal management system must guarantee the safe operation of lithium ion battery [25–27], considering extreme working conditions [28]. Modeling analysis is valuable for designing a battery thermal management system [29]. However, although models have been built to analyze the characteristics at normal condition [30], there are still few models that can simulate the behavior of the battery system under extreme conditions.

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Large format lithium ion battery is favored by manufacturers because they can provide reduced cell number and pack complexity in the battery pack design [31], associated with an improved reliability of the battery pack [32]. However, the large format lithium ion battery is more vulnerable to safety problems because it contains more stored energy. Additionally, cooling is less effective because of its lower surface/volume ratio, which leads to higher non-uniformity of temperature distribution within the cell [32].

To reduce the possibilities of safety problems, lithium ion batteries have to pass test standards [33–46] before sales. However, accidents occurred one after another [47–53], because the abuse conditions can be tricky and unpredictable in practical conditions [54]. Once the TR is triggered within a single cell, cell-to-cell TR propagation can result in catastrophic hazards [52,53,55]. Therefore the prevention of TR propagation must be considered in battery pack design [56,57].

Experimental study on TR propagation is essential, and we may need massive experiments on TR propagation to help design a safe battery pack. Some current literature provides experimental data related to TR propagation [57–60]. However, given that the experimental study on TR propagation within a battery pack costs much time and money, building an easy-to-use, verified abuse model that realistically captures the mechanisms of TR propagation in battery pack is beneficial to find efficient approaches to prevent

Nomenclature

Abbreviations, description

ARC	Accelerating Rate Calorimetry
BMS	Battery Management System
CATARC	China Automotive Technology and Research Center
DIN SPEC	The Specification made by the Deutsches Institute für Normung
DSC	Differential Scanning Calorimetry
PE	Polyethylene
PHEV	Plug-in Hybrid Electric Vehicle
PP	Polypropylene
TC	Thermocouple
TR	Thermal Runaway
VDA	Verband Der Automobilindustrie

Variable or parameter, description, unit

A	The pre-exponential factor, s^{-1}
b	The reaction index, 1
c_{chem}	The normalized concentration for the chemical reactions, 1
c_{ele}	The normalized concentration of the electric energy, 1
$\frac{dc_{chem}}{d\tau}$	The reaction rate of c_{chem} , s^{-1}
$\frac{dc_{ele}}{d\tau}$	The reaction rate of c_{ele} , s^{-1}
C_{chem}	The constant for the reaction kinetics of c_{chem} , s^{-1}
C_{ele}	The constant for the reaction kinetics of c_{ele} , s^{-1}
C_p	The specific heat capacity of the component, $J\ kg^{-1}\ K^{-1}$
$c_{x,0}$	The initial normalized concentration of reactant x , 1
$D_{i,i+1}$	The duration of thermal runaway propagation from one battery to its neighbor, s
ΔE	The total increase of the internal energy, J
$\dot{\Delta E}$	The increase rate of the internal energy of the battery cell, W
h	The equivalent thermal contact resistance, or the convection coefficient, $W\ m^{-2}\ K^{-1}$
h_{conv}	The convective heat dissipation coefficient, $W\ m^{-2}\ K^{-1}$
ΔH_{chem}	The total chemical energy released throughout the thermal runaway process, J
ΔH_{ele}	The total electric energy released throughout the thermal runaway process, J
ΔH_x	The total heat generated during reaction of reactant x , measured by DSC test, J
L_{nail}	The length of the nail, m
M	The total mass of the battery, kg
Δm_x	The mass of the reactant x within the battery cell, kg
Q	The self-heat generation rate within the battery cell, W
Q_{chem}	The heat release rate by the chemical reaction, W
Q_{ele}	The heat release rate by the electric short circuit, W
q_v	The volumetric heat generation rate, $W\ m^{-3}$
q_{chem}	The volumetric chemical energy release rate caused by side reactions at high temperature, $W\ m^{-3}$
q_{ele}	The volumetric electric energy release rate after separator collapse and short circuit occurs, $W\ m^{-3}$
q_{nail}	The volumetric heat release rate due to short circuit at the nail, $W\ m^{-3}$
R_{add}	The thermal resistance of the added thermal resistant layer, $m^2K\ W^{-1}$
R_s	The thermal resistance perpendicular to the adjacent surface of the battery, $m^2K\ W^{-1}$

R_s^*	The thermal resistance perpendicular to the adjacent surface of the battery considering R_{add} , $m^2K\ W^{-1}$
T	The temperature, K, $^{\circ}C$
$\frac{dT}{d\tau}$	The temperature rise rate, $K\ s^{-1}$
T_0	The temperature at the surface of the solid component, K, $^{\circ}C$
T_1, T_2	The temperature at the surface of the component with the index of 1 or 2, K, $^{\circ}C$
T_{∞}	The ambient temperature, K, $^{\circ}C$
$T_{TR,ARC}$	The triggering temperature of thermal runaway, K, $^{\circ}C$
T_{chem}	The start temperature of chemical reactions, K, $^{\circ}C$
T_{ref}	The reference temperature to normalize the temperature T in Kelvin, K
ΔT	The total temperature rise, K, $^{\circ}C$
$\Delta T_{p_{i,i+1}}$	The temperature difference between the negative pole of Bat i and the positive pole of Bat $i+1$, $i \in \{1,2,3,4,5\}$, K, $^{\circ}C$
V	The volume of the component, m^3
V_{bat}	The total volume of the battery cell, m^3
V_{nail}	The total volume of the nail, m^3

Greek letters

α_{nail}	The proportion of the electric energy released within the nail, 1
γ	The proportion factor for ΔH_{ele} in modeling analysis, 1
δ	The thickness, m
δ_{add}	The thickness of the added layer, m
δ_{layer}	The thickness of the equivalent thermal resistant layer, m
ε	The emissivity constant, 1
λ	The heat conductivity of all solid components, $W\ m^{-1}\ K^{-1}$
λ_0	The heat conductivity of the solid component, $W\ m^{-1}\ K^{-1}$
λ_1, λ_2	The heat conductivity of adjacent component with the index of 1 or 2, $W\ m^{-1}\ K^{-1}$
λ_{add}	The heat conductivity of the added layer, $W\ m^{-1}\ K^{-1}$
λ_{layer}	The heat conductivity of the equivalent thermal resistant layer, $W\ m^{-1}\ K^{-1}$
λ_{nail}	The heat conductivity of the nail, $W\ m^{-1}\ K^{-1}$
$\lambda_x, \lambda_y, \lambda_z$	The heat conductivity in direction of x , y and z , $W\ m^{-1}\ K^{-1}$
ρ	The density of the component, $kg\ m^{-3}$
σ	The Stefan-Boltzmann constant, $W\ m^{-2}\ K^{-4}$
τ	Time, s
$\tau_{TR,i}$	The triggering time of thermal runaway for Bat i , $i \in \{1,2,3,4,5,6\}$, s
Φ_{ht}	The heat transfer intensity, W

Subscript, description

i	Denotes that the variable is for the Bat i , $i \in \{1,2,3,4,5,6\}$
x	Denotes that the variable is for reactant x , as listed in Table 2

Superscript, description

sim	The parameter with this superscript is adjustable in simulation
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