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A Multiphysics Informed TR Model for Estimation of Pressure Evolution Induced by Gas Formation of a Lithium-ion Battery

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This study proposes a multiphysics informed thermal runaway model of a lithium-ion battery for estimation of both temperature and pressure evolution under thermal abuse conditions. The proposed model comprises four sub-models: state estimation, thermodynamics, chemical reaction, and pressure estimation. In the model of sate estimation, thermal runaway dependency on both SOC and SOH is depicted by changing the kinetic parameters [1,2]. Specifically, activation energy and reaction factor of a cathode are used to replicate SOC dependency of chemical reaction on thermal runaway, whereas the thickness evolution of a SEI layer is addressed to reflect SOH dependency. Then, the model of thermodynamics calculates the heat propagation inside a cell and heat balance between a cell and environment as $\rho c_p \frac{\partial T}{\partial t} = \nabla k \nabla T + \dot{Q}_{abuse}$ *where* ρ, c_p, T, k, *and* $\dot{Q}_{abuse}$ *denote the cell density, heat capacity, temperature, thermal conductivity of a cell, and heat generation rate from chemical reaction of critical species, respectively [3]. Heat generation from the chemical reaction is also considered to account for chemical degradation of chemical components. The model of chemical reaction estimates the heat generation rate from the decomposition of major components inside a cell, including SEI layer, negative electrode, positive electrode, and electrolyte as* $\dot{Q}_{abuse\_*} = H_* W_* R_*$ *where* H_*, W_*, *and* R_* *denote heat release, specific active material content, and reaction rate of a cell component* $*$ *[4]. Hence, models of thermodynamics and chemical reaction iteratively solve the underlying physics to accurately estimate node-wise cell temperature. Finally, the model of pressure estimation accounts for underlying physics of major gas formation inside of a cell including CO,* C_2H_4, CO_2, *and* H_2, *which highly correlates to chemical reaction of chemical components. Specifically, CO and* C_2H_4 *are produced by reduction at the lithiated anode,* CO_2 *is originated from SEI decomposition, and* H_2 *is emitted from binders reacting with lithium, which has the identical melting point of the electrolyte [5]. The difference in reaction ratio of each component attributes to a different amount of gas generation and partial pressure. Parameters addressed in this model are optimized through experimental data under thermal abuse condition and the initial mass of each gas component is calibrated to fit the initial pressure. Specifically, the experimental data of a 26650, 18650 LFP cell and 18650 NMC cell is used to identify the parameters and validation of estimation of temperature and pressure evolution during thermal runaway [6,7]. The comparison between the experiment and estimation of temperature and pressure evolution proved they corresponds well each other, which demonstrates that this model with the identified parameters can depict the thermal runaway accurately. One outstanding feature of this model is that the model accounts for underlying physics of chain reaction and pressure evolution according to individual cell components. Also, the estimation of multiphysics phenomena in thermal runaway with the proposed model provides important considerations for diagnostic of thermal runway and establishing novel thermal management strategies. Specifically, the sensitivity of measuring temperature and pressure is analyzed, suggesting that both are needed to effectively detect thermal runway under a variety of heating conditions. Furthermore, the active gas detection system including active air sampling detection would be effective for accurate early detection of thermal runaway. Therefore, the proposed model established insight of understanding the underlying physics of gas generation and guideline for optimal battery management system for the early detection of thermal runaway. In addition, future work includes expansion to module and pack scale as a next step and developing novel thermal management strategies for lithium-ion batteries from the operational perspective.*

NOMENCLATURE

SOC = state of charge
SOH = state of health
LFP = lithium iron phosphate battery
NMC = lithium Manganese Cobalt battery
T_{Cell} = temperature of a cell
ρ = *denote the cell density*
c_p = *heat capacity*
k = *thermal conductivity of a cell*
$\dot{Q}_{abuse}$ = heat generation rate
H_* = *heat release*
W_* = *specific active material content*
R_* = *reaction rate*

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REFERENCES

1. E. Kwak, J. Kim, S. Hong, and K-Y. Oh, Detailed modeling investigation of thermal runaway pathways of a lithium iron phosphate battery, Int. J. Energy Res. 46 (2022) 1146-1167.
2. J. Chen, X. Rui, H. Hsu, L. Lu, C. Zhang, D. Ren, L. Wang, X.He, X. Feng, and M.Ouyang, Thermal runaway modeling of LiNi0. 6Mn0. 2Co0. 2O2/graphite batteries under different states of charge, J. of Energy Storage, 49 (2022) 104090.
3. Abada S, Petit M, Lecocq A, et al. Combined experimental and modeling approaches of the thermal runaway of fresh and aged lithium-ion batteries. J Power Sources. 2018;399:264-273.
4. Kim G-H, Pesaran A, Spotnitz R. A three-dimensional thermal abuse model for lithium-ion cells. J Power Sources. 2007;170(2):
5. L. Yuan, T. Dubaniewicz, I. Zlochower, R. Thomas, and N. Rayyan, Experimental study on thermal runaway and vented gases of lithium-ion cells, Process Safety and Environment Protection, 144 (2020), 186-192.