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Modeling of Li-ion Battery Thermal Runaway: Insights into Modeling and Prediction

Modeling of Li-ion Battery Thermal Runaway: Insights into Modeling and Prediction

by Paul T. Coman, Andrew Weng, Jason Ostanek, Eric Darcy, Donal P. Finegan, Ralph E. White

Complexities of Thermal Runaway

Lithium-ion battery safety has become one of the most discussed topics in recent years, not only as a subject of debate but also as a mandatory requirement driven by industry standards for deploying high-reliability battery power systems across all market applications. As more batteries enter the market in various applications, there is a strong incentive to improve safety and to mitigate associated consumer concerns to accelerate the adoption of electric vehicles (EVs) and other devices. The cornerstone of battery safety lies in understanding and mitigating thermal runaway (TR)—a failure mode characterized by a rapid, self-heating, and uncontrollable increase in temperature and pressure within a battery cell. This can lead to the venting of toxic gases, fires, or explosions, posing severe risks to both users and manufacturers.[1,2] Determining whether a Li-ion battery meets industry safety requirements, or assessing the severity of a TR event, requires advanced knowledge of TR phenomena and relevant experimentation.

Despite advances in battery technology, the chaotic nature of TR makes it a complex phenomenon to model and, more critically, to predict its impact on battery pack design. Variability in manufacturing processes, material properties, and usage conditions means that even cells from the same batch can exhibit significantly different characteristics during TR.[3-6] This unpredictability is compounded by the fact that TR is influenced by a multitude of interconnected factors, including electrochemical reactions, thermal dynamics, electrical configuration, and mechanical stresses.

Understanding the complexity of TR requires sophisticated experimentation, empirical data, and robust modeling and simulation approaches that capture the phenomenon's essential features. Physics-based mathematical models are often indispensable for elucidating TR mechanisms. However, they must balance detailed accuracy with computational efficiency, often requiring assumptions, mathematical constructs, and simplifications, especially for battery packs. Cell-level TR understanding is insufficient; as batteries scale to modules and packs, the risk of TR propagation escalates. Therefore, modeling must extend to the pack level, incorporating cell interactions and the overall thermal management system. Ensuring battery pack safety is critical, as a single cell failure can trigger a cascade of exothermic decomposition reactions, potentially leading to pack failure.

The most significant challenge, however, remains the accurate prediction of TR events both in single cells and battery packs. Future research must focus on refining these models and developing advanced predictive tools that integrate probabilistic methods. Machine learning (ML) and artificial intelligence (AI) also offer promising data-driven avenues for enhancing predictive capabilities.[7]

This article discusses the dual challenges of modeling and predicting TR in li-ion batteries. It explores the current challenges of TR modeling, the methods for progressing from single cells to battery packs, and future directions involving the use of probabilistic methods and ML/AI to tackle this multifaceted issue. Accurate prediction of TR events remains a major challenge, especially because of the cell-to-cell variability, but also due to parametrization, which requires complex experimentation or exhaustive experimental data for training data-driven ML models. Continued research and innovation in modeling and predictive techniques are essential for ensuring safer and more reliable battery systems.

Physics-Based Modeling Approaches

TR models often include detailed representations of the battery's internal reactions and structural changes in a full-order modeling (FOM) setting using different models, including mechanical models; electrochemical, electrical, thermal, and models that include TR propagation; fire propagation, reactive flow, pressure change models; mechanical response; and decomposition reactions.[8] These reactions involve the decomposition of the SEI (solid-electrolyte interphase) layer, anode, cathode, electrolyte, salt, binder, and other materials within the battery which can react with the electrolyte or with the other gases generated during TR.[9,10] These reactions can be modeled and used to calculate the thermal energy within a cell or pack, but such an approach often lacks mechanical or gas flow, for example. Some advanced models include thermodynamic equations to calculate the amount of gas vented from the cell and to measure the mass of each battery component to provide important parameters for analyzing TR numerically.[11] High-speed tomography has shown that TR can lead to the collapse of the electrodes and the structure, as well as the melting of the current-collecting materials, which also indicates that mechanical effects need to be included.[12] These insights are vital for creating accurate and representative numerical models. Accounting for all the reactions and phenomena in a model is an extremely complex process which is not practical with current computational capabilities. Such a model requires many measured parameters and knowledge of the reactions that occur for each chemistry of interest.[13] A typical physics-based model used for predicting single-cell TR behavior can be described with the equations in Table I.

As can be seen from Table I, the model describes the reactions that occur inside a cell during TR, but even this basic model requires at least 15 parameters that require complex experimental data. For instance, accelerating rate calorimetry (ARC) or differential rate calorimetry (DSC) is needed to determine the activation energy (the E-terms in the Table) and pre-exponential factor (the A-terms) for each cell under different conditions. This comprehensive physics-based modeling can lead to accurate temperature predictions, but it lacks some critical phenomena that are essential for understanding the real dynamics of TR.

Another key aspect of TR that needs to be incorporated is the venting of gas and ejecta. Venting plays a significant role in the overall TR process, as it involves the release of gases and materials from the cell, impacting the thermal, electrical, and mechanical behavior of the battery, but, in this specific case, adds at least 12 extra parameters that need experimentation, as seen in Table II.

But venting is also a complex phenomenon, which can be divided into two assumptions: 1) considering vapor-liquid equilibrium (VLE) assumption,[15] and 2) considering conditions of non-equilibrium. In the latter approach,[16] a non-equilibrium model using porous drying theory can be introduced. This evaporation process is described by the constant rate drying period (CRDP) and the decaying rate drying period (DRDP). This is important because evaporative cooling affects the time between venting and thermal runaway.[17] Gas is also generated from decomposition reactions. The gas generation rate can be modeled in several ways. Simple constant rate assumptions are commonly employed, while other approaches include an analogy where heat

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Table I. Set of equations describing the decomposition reactions modeled in typical physics-based models.[10,11,14]

EQUATION	DESCRIPTION	VARIABLES	PARAMETERS
$\frac{dx_c}{dt} = A_c x_c (1-x_c) \exp\left(-\frac{E_c}{k_{bT}}\right)$	Cathode decomposition rate	x_c	A_c, E_c, T
$\frac{dx_a}{dt} = -A_a x_a \exp\left(-\frac{E_a}{k_{bT}}\right)$	Anode decomposition rate	x_a	A_a, E_a
$\frac{dx_{SEI}}{dt} = -A_{SEI} x_{SEI} \exp\left(-\frac{z}{z_0}\frac{E_{SEI}}{k_{bT}}\right)$	Anode SEI decomposition rate	x_{SEI}	A_{SEI}, E_{SEI}
$\frac{d\theta_e}{dt} = -A_e \theta_e \exp\left(-\frac{E_e}{k_{bT}}\right)$	Electrolyte decomposition rate	θ_e	A_e, E_e
$\frac{dx_{SoC}}{dt} = -A_{ec}(1-x_c)x_a \exp\left(-\frac{E_{ec}}{k_{bT}}\right) + \left(\frac{dx_c}{dt} - \frac{dx_a}{dt}\right) SoC$	Electrochemical reaction	SoC	A_{ec}, E_{ec}
$\dot{Q}_c = m_c h_c \frac{dx_c}{dt}$	Heat-generation cathode decomposition	$\dot{Q}_c$	h_c, m_c
$\dot{Q}_a = m_a h_a \frac{dx_a}{dt}$	Heat-generation anode decomposition	$\dot{Q}_a$	h_a, m_a
$\dot{Q}_s = m_a h_s \frac{dx_x}{dt}$	Heat-generation SEI decomposition	$\dot{Q}_s$	h_s
$\dot{Q}_{ec} = (m_a - m_c) h_{ec} \frac{dSoC}{dt}$	Heat generation due to electrochemical reactions	$\dot{Q}_{ec}$	h_{ec}

generation and gas generation are proportional. For example, in Refs.[11,15] it was assumed that the electrolyte decomposition reaction rate is proportional to the rate of electrolyte evaporation. The authors in Ref.[16] made a similar assumption for the vent gas mixture.

Models can incorporate the venting of the electrolyte by setting up burst conditions for the trigger pressure of the battery relief mechanism, simulating venting. This approach includes the partial ejection of the jelly roll, where the amount of ejecta is measured and incorporated into the model.

The processes involved in the electrolyte are complex and include evaporation, boiling, and venting, which can be accompanied by explosions of ejecta. In terms of boiling and evaporation, knowledge about the electrolyte composition is also required, because it influences the energy output.

For modeling the electrolyte, mixtures with specific compositions need to be known, and venting is modeled by assuming the electrolyte behaves as an ideal gas flowing isentropically through an orifice, which opens at a critical pressure, but might be assumed to be a real gas during the VLE phase. The pressure and temperature during venting are defined by equations derived from the energy balance in a reversible system with compressible flow of an ideal gas passing through an orifice.

Additionally, another challenge is combustion outside the cell,[18,19] which, in fact, can impact the TR behavior inside the cell. By incorporating gas venting, electrolyte thermodynamics, and combustion, the models can provide a more comprehensive understanding of TR and help identify critical areas for improving battery safety. An example of modeling prediction using a comprehensive physics-based model using the venting equations can be seen in Fig. 1.

Such a model can predict the heat dynamics that can be observed by measuring the temperature of the housing of a cell and can provide

Table II. Equations describing the reactions modeled in a typical physics-based model with venting.[10,11,14]

EQUATION	DESCRIPTION	VARIABLES	PARAMETERS
$P = \frac{m_e RT(1-\theta_e - y)}{V_h M_e} + P_{amb}$	Pressure formulation	P	m_e, T, V_h, P_{amb}
$\frac{dy}{dt} = \frac{P_{vent} V_{vent} A_{vent} M_e}{RT_{vent} m_e}$	Fraction rate of vented electrolyte	y	$P_{vent}, A_{vent}, V_{vent}, T_{vent}$
$\dot{Q}_{vent} = -m_a h_s \frac{dx_x}{dt}$	Endothermic heat associated with venting of electrolyte	$\dot{Q}_{vent}$	h_s
$\dot{Q}_{boil} = -m_e h_{vap} \frac{dy}{dt} - m_e Cp_e T \frac{dy}{dt}$	Endothermic heat associated with boiling	$\dot{Q}_{boil}$	h_{vap}, Cp_e
$\dot{Q}_{ej} = -m_{ej} Cp_{ej} T \frac{dy}{dt}$	Endothermic heat associated with venting of solid ejecta	$\dot{Q}_{ej}$	m_{ej}, Cp_{ej}

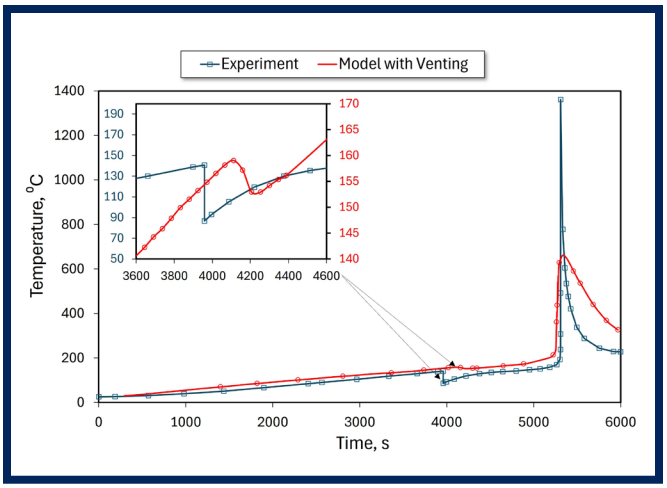

Fig. 1. *Comparison between modeling predictions using a comprehensive physics-based model and experimental data. Incorporating venting equations also captures the Joule-Thomson/evaporative cooling effect in the pre-onset phase.*[11]

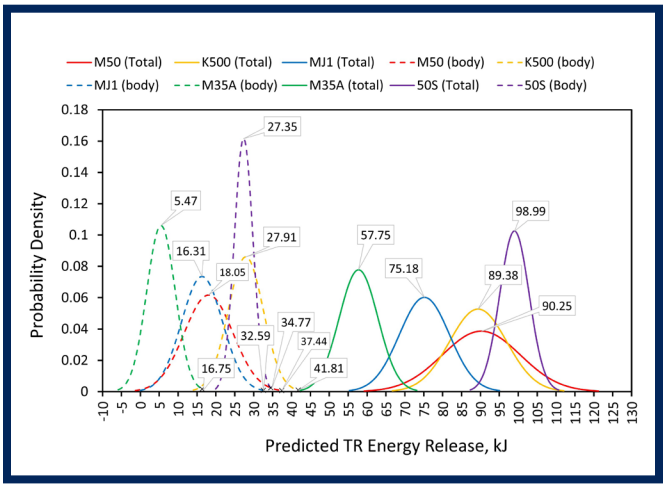

Fig. 2. *Distribution of energy released during TR through the cell body vs. total, for the same type of 18650-format cells and chemistry calculated using a fractional thermal runaway calorimeter (FTRC).*[21]

the energy released during various exothermic and endothermic reactions, including the gas-throttling Joule-Thomson/evaporative cooling effect[20] that might occur before the TR onset point.

Although these FOMs offer a high fidelity in calculating temperatures and energy, they often require simplifications to manage computational efficiency while retaining essential details, while they also require a large number of parameters. Despite the complexity and the need for numerous parameters, these TR models can still be used to assist in the design of safe battery packs and to analyze various geometric designs. However, they cannot be used for prediction in their current form. Importantly, even when a physics-based model is set in place for a certain Li-ion chemistry, during TR, each cell yields different energy outputs even if they come from the same batch of cells. Consequently, there is a large distribution in terms of energy output during TR (Fig. 2).

Given the importance of ensuring battery safety, especially at the pack level, continuous research and development in TR modeling is crucial. Experimental data is essential for validating these models and for ensuring that they accurately reflect real-world behavior.

Reduced-order Thermal Runaway Models

One of the methods to model TR in battery packs is to find ways to reduce the computational burden. Reduced-order models (ROMs) are crucial for integrating detailed multi-scale simulations into practical engineering applications. These models aim to simplify the complex behaviors captured in multi-scale simulations while retaining the essential characteristics needed for accurate predictions. By reducing the number of parameters and computational requirements, ROMs provide a more efficient way to analyze TR and support the rapid prototyping and evaluation of battery systems, even when analyzing complex phenomena like the venting of gases and expansion.[22] They are instrumental in making advanced modeling techniques accessible for real-world applications, ensuring timely and cost-effective safety assessments. Some of the most common reduced-order methods, especially for battery packs, is to consider either reducing the thermal model and coupling with the electrochemical model[23] or reducing the number of equations by coupling decomposition reactions[24] (Fig. 3).

In Fig. 3, it can be seen that some of the reactions can be nested into a so-called efficiency factor, which greatly reduces the number of parameters that need to be fitted, estimated (for example by knowing the cell capacity), or measured. Another common reduction method is to downscale a model from a 3D to a 2D model. In Fig. 4, it can be seen that a 3D-2D reduced order model can still predict the temperature measured experimentally without much loss in terms of precision for a single cell.

However, when scaling from cells to packs, additional parameters are added to the model, associated with the cell dimensions, heat transfer coefficients, and others, which adds more uncertainty in modeling. Using 3D or 2D FEA reduced models is the most desirable approach for analyzing battery packs, due to the presence of pack design piece-part electrical, mechanical, and thermal components, etc. However, a physics-based FOM is almost impossible because there are so many unknowns and because of cell-to-cell variability. A recent reducing order approach, where the 3D thermal model was reduced to a 2D model with a heat-generation profile generated by empirical observation (Fig. 5(a) and (b)) and combined with an efficiency factor.

Adding an efficiency factor is a good approach to assist the design of battery packs, as seen when comparing simulation with experimental data (Fig. 5(c)). Modeling TR in lithium-ion batteries can be approached through physics-based models, reduced-order models, or multi-scale models, each with its own set of advantages and challenges. Physics-based models provide a detailed understanding of the electrochemical and thermal processes involved, while reduced-order models offer computational efficiency by simplifying complex interactions. Multi-scale models integrate phenomena across different scales to provide a comprehensive view of TR dynamics.

Accurately Predicting TR: What's Needed and Can AI Help?

Despite significant efforts in TR modeling, accurate TR predictions remain elusive. The main impediment to accurate predictions is the inherently stochastic nature of TR. Even cells from the same

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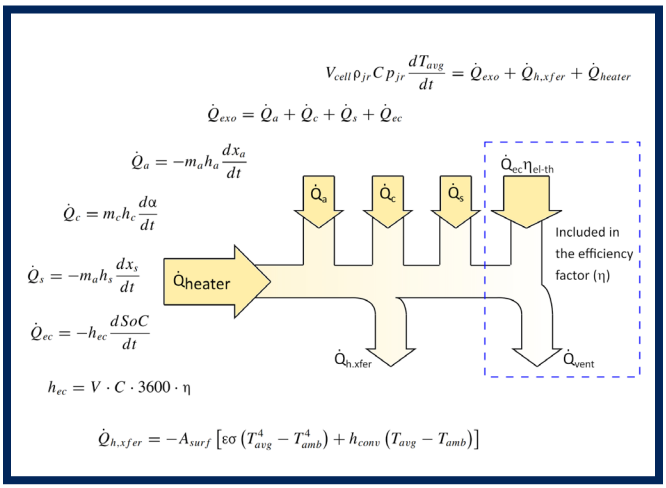

Fig. 3. *ROM by subtracting the energy due to venting of electrolyte and ejecta from the total electrochemical energy and introducing the efficiency factor (η).*[24]

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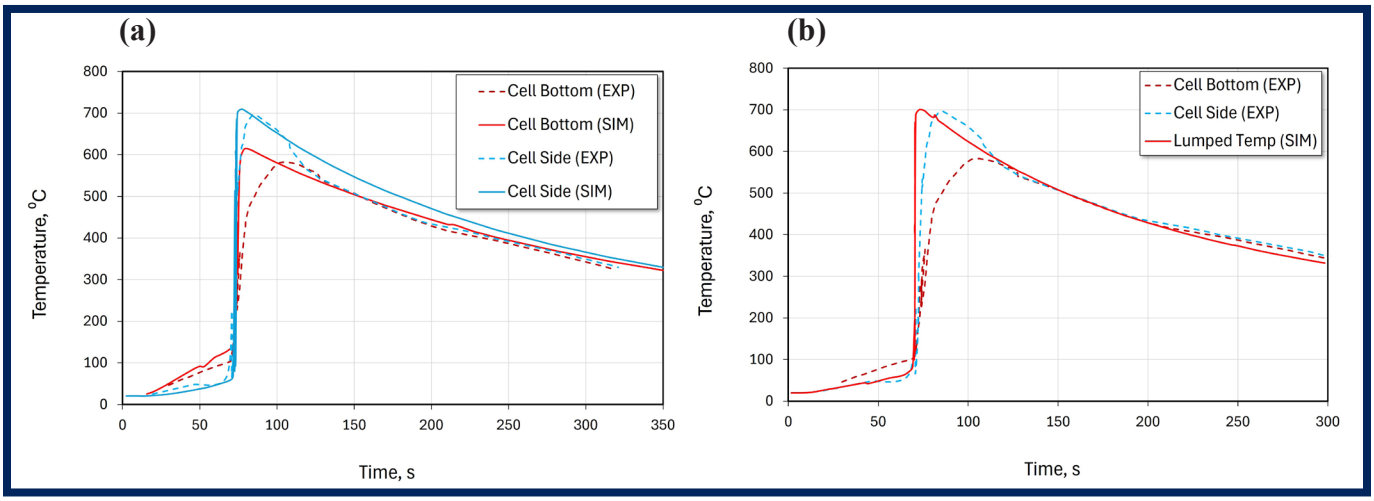

Fig. 4. *A 3D-2D reduced-order model which can fit experimental data (temperature measured on the side of the 18650-format cell steel can and at the bottom) without the burden of an FOM.*[24]

production batch from the same manufacturer with the same dimensions, same chemistry, and same capacities can exhibit different TR characteristics. For example, Fig. 6 shows the variability in total energy released through the cell casing for a variety of cell types. For some cell types, the energy released can vary from 2% to 30%, highlighting the extremely stochastic nature of TR. This high degree of variability in TR propagation is an inherent attribute of the system which exhibits high sensitivity to initial conditions.

The stochastic nature of TR calls for the use of more probabilistic frameworks for TR prediction. Existing prediction methods tend to be deterministic and thus only predict a single TR outcome. This predicted outcome is not necessarily "wrong," but it can represent only one outcome when a range of different outcomes are possible. For physics-based TR models, a future approach could be to combine existing deterministic simulations with Monte Carlo simulation approaches in which the model is repeatedly run to generate a

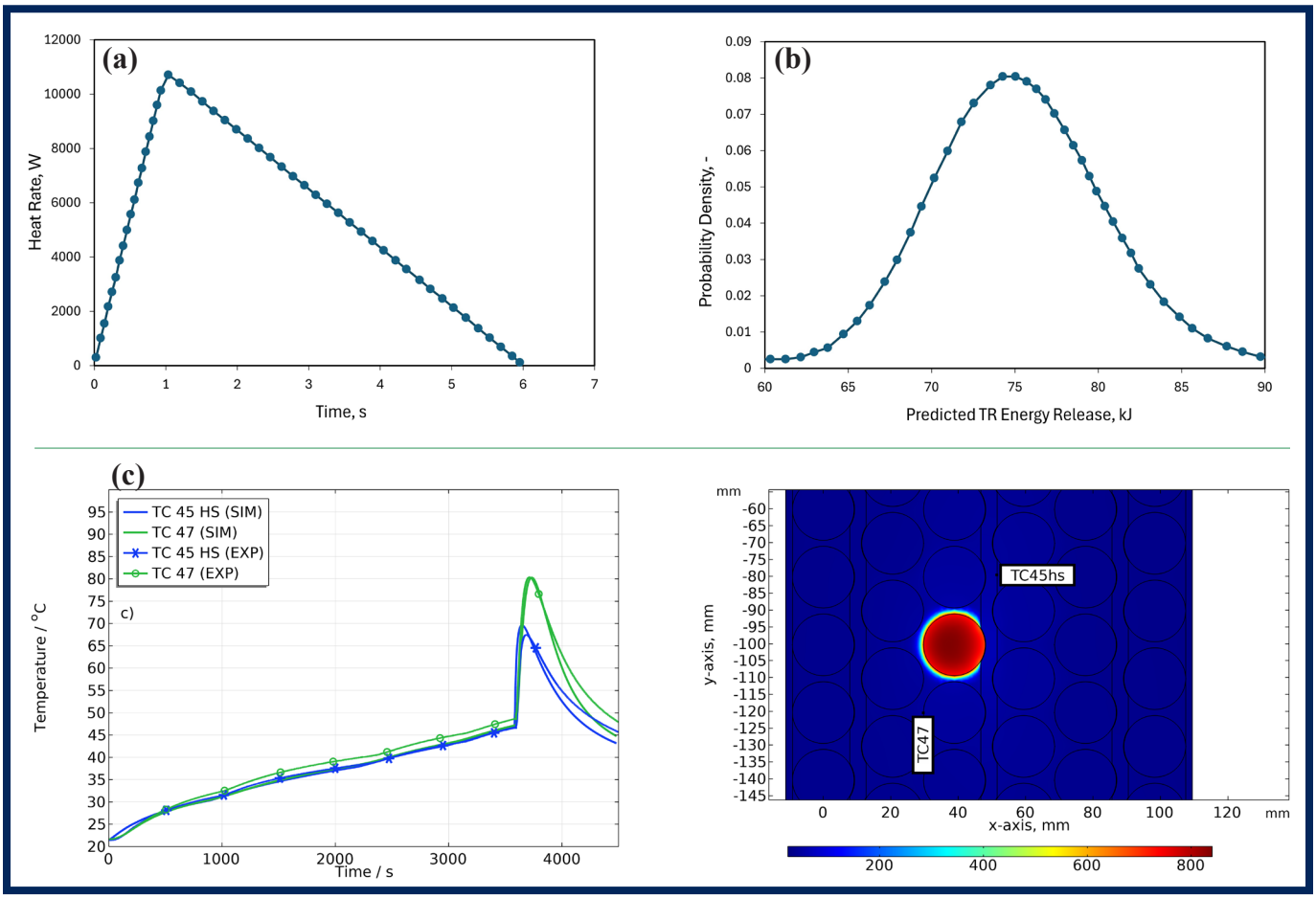

Fig. 5. *The results from the ROM depicting: (a) the empirically observed heat generation profile, (b) the thermal runaway energy (TR) released through the single-cell cans, and (c) left and right, the comparison between the modeling predictions and experimental data for a battery pack.*[25]

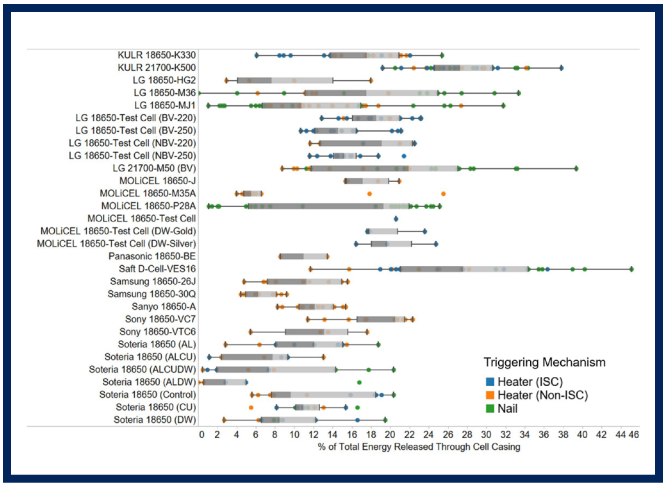

Fig. 6. *Variability in total energy released through cell casing. Dataset adapted from the Battery Failure Databank (NREL).*[3]

distribution of outcomes. Within each run, model parameters, such as those listed in Table I and Table II, are randomly sampled based on distributions of values that are either measured or assumed. It is not yet clear how many runs are necessary to accurately capture the failure distributions of typical commercial cells. When computation time becomes a bottleneck, ROMs can be used in place of FOMs. Thus, fast and accurate ROMs of TR may play an important role in enabling stochastic TR predictions.

AI/ML models, specifically artificial neural network (ANN) models, may still play a role in enabling accurate TR predictions, though many challenges remain. ANN models provide some inherent representation of stochasticity since the nodes in the layer can be interpreted as a probability (e.g., of TR occurrence). ANN models are also fundamentally data-driven without requiring knowledge of the complex, often intractable, multi-domain physics of TR. Recently, physics-informed neural networks (PINNs)[26] which combine the advantages of both types of models[27,28] have also been proposed. As of today, the literature on ANN models for TR prediction applications focuses on prediction of battery heat generation,[29] temperature estimation,[30,31] and surrogate modeling for FEM simulations.[32] These methods show the feasibility of physical-state predictions without the need to construct a physical model. However, the accuracy of such models when applied beyond the immediate dataset they were trained and tested on remains unclear.

Ultimately, the availability of reliable experimental TR data is the biggest impediment to building and validating any kind of TR model. Large amounts of experimental data are especially needed for AI/ML approaches whose accuracy and generalizability largely depend on the quality and volume of data used to train the model. Comparatively, AI/ML methods need the most data, followed by FOMs, followed by ROMs. The stochastic nature of TR further means that even more measurements are needed to resolve distributions of outcomes. Given the difficulty of TR experiments and the existing sparsity of data, community efforts are needed to build and curate large TR datasets for model training and validation. The NREL/NASA Battery Failure Databank[3] is the first effort of its kind and should be viewed as a promising beginning to an effort that must be continued and expanded.

Summary

Modeling TR in lithium-ion batteries can be approached through physics-based models, reduced-order models, or multi-scale models, each with its own set of advantages and challenges. Physics-based models provide a detailed understanding of the electrochemical and thermal processes involved, while reduced-order models offer computational efficiency by simplifying complex interactions. Multi-scale models integrate phenomena across different scales to provide a comprehensive view of TR dynamics. Despite these advancements, accurate prediction of TR events remains a major challenge due to the chaotic and highly variable nature of the phenomena.

Future research must continue to refine these models and explore the integration of probabilistic approaches and AI/ML to enhance predictive capabilities. These advanced techniques hold the potential to significantly improve battery safety and reliability. However, predicting the dynamics of TR in a battery pack from the beginning remains challenging and requires a large volume of data for both individual cells and packs. The continuous development of probabilistic approaches and AI/ML models, combined with comprehensive data collection and real-time monitoring, is essential for overcoming these challenges and ensuring the safe and efficient operation of lithium-ion batteries.

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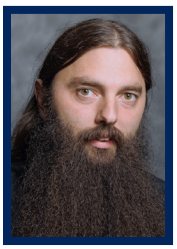

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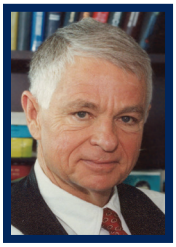

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