A Coupled Thermo-Mechanical Dynamic Characterization of Cylindrical Batteries

KHALED I. ALSHARIF1, ALEXANDER H. PESCH1, VAMSI BORRA1, (Senior Member, IEEE), FRANK X. LI1, (Member, IEEE), PEDRO CORTES1, ERIC MACDONALD2, (Senior Member, IEEE), AND KYOSUNG CHOO1

1Rayen School of Engineering, Youngstown State University, Youngstown, OH 44455, USA
2Department of Electrical Engineering, The University of Texas at El Paso, El Paso, TX 79902, USA

Corresponding authors: Alexander H. Pesch (ahpesch@ysu.edu) and Kyosung Choo (kchoo@ysu.edu)

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ABSTRACT Lithium-ion batteries have complicated dynamics and temperature behavior. In this paper, a dynamic system previously developed to characterize the voltage response was extended to estimate the heat generation rate due to the electrochemical reactions that a battery undergoes as being discharged. The dynamic system based on a modally decomposed three-degree-of-freedom, spring-mass-damper analogy was used to estimate the cells terminal voltage, open-circuit voltage and the mass transfer and boundary layer effects. The modal parameters were determined by minimizing the error between the experimental and simulated time responses. Then, these estimated parameters were coupled with a lumped thermal model to predict the temperature profiles of two cylindrical lithium-ion batteries. To capture the dynamic voltage and temperature responses, hybrid pulse power characterization (HPPC) tests were conducted with thermocouples. It was found that the dynamic model was able to accurately estimate the nonlinear dynamics of the batteries; therefore, the electrochemical heat generation rate was successfully able predict the surface temperature profile at 1C and 2C discharge rates.

INDEX TERMS Lithium-ion batteries, dynamic system modeling, heat generation, electric vehicles, mechanical analog.

I. INTRODUCTION

The demand for electric vehicles has been continuously growing as a promising solution for the energy and environmental issues caused by internal combustion engine vehicles [1]. Lithium-ion batteries have been extensively utilized as a major source of power in electric vehicles due to their high energy density, light weight, long lifespan, charge efficiency, minimal memory effect and design flexibility [2]. A battery pack in an electric vehicle may consist of thousands of cells connected in series/parallel in packs to meet the energy demands of the vehicle.

To optimize the power delivered by a battery cell, ensure safe application and improve the driving range, researchers have been developing models to monitor the state-of-health, state-of-charge, state-of-power the battery [3]—[10].

Hu et al. [11] developed an aging-robust and disturbance-immune ISC diagnostic method for lithium-ion batteries. The authors incorporated a multi-state-fusion ISC resistance estimator and a RTLS-VF-based bias compensator within a universal model switching. Their proposed model was able to accurately estimate the ISC resistance and outperform the state-of-the-art techniques in the noise immunity. She et al. [12] established a technique of applying the incremental capacity analysis (ICA) method for battery pack-level state-of-health (SOH) estimation in real-world situations. It was found that the study they conducted provided a scheme of applying the ICA-based method to accurately predict the SOH in a pack-level battery. Wang et al. [13] proposed a data-driven method for charging capacity diagnosis based on real-world EV operating data. The input to their three-based prediction model were the charging rate, temperature, state-of-charge and accumulated driving mileage. The battery charging capacity abnormality is diagnosed through a statistics-based method by analyzing the error distribution.
of large sets of data. Hu et al. [14] presented an SOC and SOH co-estimation scheme based on the fractional-order calculus. They used the fractional-order equivalent circuit model to predict the voltage response utilizing a Hybrid Genetic Algorithm/Particle Swarm Optimization method. Then, a fractional-order extended Kalman filter was used to estimate the SOC and SOH. It was found that this technique demonstrated high accuracy with a steady-state error of 1% for both SOC and SOH.

Thermal management of battery systems is also a critical factor to consider in the design of a battery pack as it impacts the performance of the cells and can lead to catastrophic fire incidents if not managed appropriately. The heat generated from a battery is due to the complicated electrochemical reactions taking place in the cell [15]. These reactions vary with time, temperature and current distribution; therefore, there is a need for a simple and intuitive dynamic model to predict the heat generated by a battery to obtain essential thermal parameters under dynamic discharging conditions.

Various studies have been conducted to develop accurate thermal models to estimate the heat generation rate and the temperature profile of batteries [16], [17]. Chiew et al. [18] developed a pseudo three-dimensional coupled electro-thermal model to investigate the thermal behavior of a cylindrical LFP battery under various discharge rates and temperatures. They used a series of regression models to quantify the thermal behavior of the battery and demonstrated how the performance of the battery differs at lower ambient temperatures and discharge rates. Mahamud and Park [19] proposed a thermal management method utilizing a reciprocating air flow for cylindrical Li-ion cells. They numerically analyzed their model utilizing a two-dimensional computational fluid dynamics (CFD) model and a lumped thermal-capacitance model. Their numerical results indicated that the reciprocating flow yielded to a 72% temperature drop in the battery system.

Furthermore, Zhang [20] investigated the heat generation characteristics of a cylindrical lithium-ion battery by using a coupled electro-thermal model. He analyzed the thermal characteristics of the battery by employing the finite volume numerical method that considered the electrolyte transport properties as a function of temperature and Li-ion concentration. It was found that the Ohmic heat contributed to 54% of the total heat generation in the battery, whereas the heat generated from the electrochemical reactions yielded to almost 30%.

In addition, Panchal et al. [21] presented a mathematical model to predict the transient temperature distribution of a prismatic battery under four constant current discharge rates. Their mathematical model was able to predict the surface temperature within close proximity compared to the experimental measurements. Ye et al. [22] developed an electro-thermal cycle life model by accounting for the thermal and capacity fading effects. With their model, they were able to predict the capacity lost and the temperature at different cycle number and the effects the temperature had on the capacity. Haung et al. [23] established a co-simulation thermolectric model for a Lithium-ion battery. They combined the equivalent circuit model with CFD to characterize the thermal and electrical behavior of the battery. Their results indicate that their method with the temperature correction has higher accuracy than the traditional thermal simulation without the temperature correction. Wang et al. [24] proposed a finite element thermal model for cylindrical Lithium-ion battery to address the inconsistency issues of temperature distribution among battery cells in a battery pack. Through their model, they were able to characterize the discharge thermal behavior and predict the temperature profile within a small proximity at varied ambient temperatures.

Furthermore, Li et al. [25] established a computationally efficient state estimation method for lithium-ion batteries. Their technique is based on a degradation-conscious, high-fidelity, electrochemical-thermal model for battery management systems. They were able to significantly improve the state estimation by employing an ensemble-based state estimator using the singular evolutive interpolated Kalman filter.

The study conducted in this work proposes a novel coupled thermo-mechanical model to predict the dynamic and thermal behavior of cylindrical lithium-ion batteries. The dynamic system is an analogy based on a three-degree-of-freedom mass-spring system with damping. The system was decomposed into modal coordinates which represented the discharge of the battery, mass transport effect, and double-layer dynamic effect. Furthermore, the electrochemical heat generation rate was computed from the output states of the dynamic system and utilized as an input to a lumped thermal model. The thermal model was used to predict the surface temperature of the battery during dynamic discharging conditions. Models in this form were developed for two batteries: Panasonic NCR21700 for electric vehicles and a Samsung INR18650-25R. Both cells were experimentally tested utilizing the hybrid pulse power characterization (HPPC) test at two constant-current discharge rates of 1C and 2C. Moreover, the modal dynamic and lumped thermal parameters of each battery model were tuned to the experimental measurements using an error-minimization algorithm to ensure accurate results.

This work is structured as follows. Next, Section II is a literature review of the current electrochemical models which have been utilized to characterize the dynamic and thermal response of batteries. Section III details the theory of the proposed coupled thermo-mechanical model. Section IV details the experimental setup and equipment employed to demonstrate the method for the battery methods considered. Next, Section V presents the experimental results showing the ability of the coupled model to predict the voltage and temperature responses. Finally, the paper is concluded with closing remarks.

II. CURRENT STATE-OF-THE-ART

Several electrochemical models have been developed to estimate the heat generated by a battery at different discharge
rates and loading conditions. This section presents a brief review of the current state-of-the-art electrochemical models.

Lithium-ion battery modeling is complex due to its multi-domain, multi-physics nature. To compute the temperature distribution at the battery’s length scale, the governing transport equations that occur in the anode-separator-cathode layers are solved [26].

The multi-scale, multi-domain electrochemical solution method computes the battery’s thermal field through (1).

$$\frac{\partial \rho C_p T}{\partial t} - \nabla \cdot (k \nabla T) = \sigma_+ |\nabla \varphi_+|^2 + \sigma_- |\nabla \varphi_-|^2 + \dot{q}_{ECh}$$  

(1)

where \( \rho \), \( C_p \), \( T \), \( t \) and \( k \) are the density, heat capacity, temperature, time and thermal conductivity, respectively. Additionally, \( \sigma_+ \) and \( \sigma_- \) are the positive and negative electrodes electrical conductivity, respectively. \( \varphi_+ \) and \( \varphi_- \). Also, \( \dot{q}_{ECh} \) is the electrochemical reaction heat generation. Furthermore, the current flux is governed by (2)-(3), where \( j \) is the volumetric current density.

$$-j = \nabla \cdot (\sigma_+ \nabla \varphi_+)$$  

(2)

$$j = \nabla \cdot (\sigma_- \nabla \varphi_-)$$  

(3)

Three electrochemical models have been widely reported in literature to estimate the heat generation and the temperature distribution of a battery, which are briefly discussed in the following subsections.

A. NTGK MODEL

The Newman, Tiedemann, Gu, and Kim model (NGTK) is a semi-empirical electrochemical model proposed by Kwon et al. [27]. This method is regarded as the simplest electrochemical model as it requires the least inputs.

The volumetric current transfer rate is obtained utilizing the relationship displayed in (4).

$$j = \frac{Y [U - V]}{Vol}$$  

(4)

where \( Vol \) denotes the volume of the battery. In addition, \( V \) is the terminal voltage which can be measured experimentally or calculated from by \( \varphi_+ \) and \( \varphi_- \). Furthermore, \( Y \) and \( U \) are the model parameters obtained experimentally as a function of the battery’s depth of discharge (DoD) and temperature. The DoD is expressed through (5). Where \( Q_{nom} \) is the nominal capacity of the battery.

$$\text{DoD} = \frac{\text{Vol}}{3600Q_{nom}} \int_0^t j \, dt$$  

(5)

From the testing measurements, the relationship between \( Y \) and \( U \) and DoD and temperature is established through the \( 5^{th} \) order polynomial equations (6)-(7).

$$U = \left( \sum_{n=0}^{5} a_n (\text{DoD})^n \right) - C_2 (T - T_{ref})$$  

(6)

The equivalent circuit model established by Chen and Rincon-Mora [28] is presented in Fig. 1.

![FIGURE 1. Equivalent circuit model.](image)

$$Y = \left[ \sum_{n=0}^{5} b_n (\text{DoD})^n \right] \exp \left[ -C_1 \left( \frac{1}{T} - \frac{1}{T_{ref}} \right) \right]$$  

(7)

where, \( a_n \) and \( b_n \) are the polynomial coefficients and \( C_1 \) and \( C_2 \) are the NTGK model constants for a specific battery to be determined experimentally. Also, \( T_{ref} \) is the reference temperature set at 298K. Additionally, the electrochemical heat generation is computed through (8).

$$\dot{q}_{ECh} = j [U - V - T \frac{dU}{dT}]$$  

(8)

The first term in (8) describes the heat generated due to overpotential, whereas the second term is due to the entropic heating.

B. THE EQUIVALENT CIRCUIT MODEL

The equivalent circuit model established by Chen and Rincon-Mora [28] is presented in Fig. 1.

The voltage source characterizes the open-circuit voltage (\( V_{OCV} \)). The \( V_{OCV} \) describes voltage across the battery terminals when the cell is not loaded and at rest. The resistor \( R_s \) is the Ohmic resistance, which accounts for the power dissipated by the battery as heating.

The input to the system is the current drawn from the battery. Thus, the relationship between \( Y \) and \( U \) and DoD and temperature is established through the \( 5^{th} \) order polynomial equations (6)-(7).

$$\text{SOC} = \text{SOC}_0 - \int_{0}^{t} \frac{I(t)}{Q_{nom}} \, dt$$  

(9)

where \( \text{SOC}_0 \) is the initial state-of-charge of the battery, which is computed using (9).

$$\frac{dV_1}{dt} = -\frac{1}{R_1SOC + C_1SOC} V_1 - \frac{1}{C_1SOC} I(t)$$  

(10)

$$\frac{dV_2}{dt} = -\frac{1}{R_2SOC + C_2SOC} V_2 - \frac{1}{C_2SOC} I(t)$$  

(11)
where solid and electrolyte phase, respectively. $D$ fraction of the electrolyte phase in electrode. Also, $\varepsilon$ of the lithium ion, F is Faraday constant and $\sigma$ diffusion coefficients of the Li and the Li$^+$

FIGURE 2. Electrode and particle domain [29].

And, the heat generation rate of the battery is computed through (13).

$$\dot{q}_{ECh} = \frac{I(t)}{Vol} [V_{OCV} - V - T \frac{dU}{dT}]$$

(13)

Analogs to the NTGK model, the equation accounts for the heat generated due to overpotential and entropic effects.

C. NEWMAN’S P2D MODEL

The P2D model is a physics-based electrochemical model that can accurately capture the Li-ion migration utilizing the porous electrode and concentration solution theories. Fig. 2 illustrates the electrode and particle domain in the P2D model [26].

Lithium diffuses from the surface of the negative to the positive electrode during discharge, which endures an electrochemical reaction. This reaction releases electrons and transfers the lithium into the electrolyte phase. A similar reaction takes place which transfers the lithium from the electrolyte phase to the solid positive electrode phase.

The charge and mass conservation laws govern the lithium-ion transport phenomena. The lithium conservation equations solved in the $r$-dimension of the spherical particles in solid and electrolyte phases are described in (14)-(15).

$$\frac{\partial c_s}{\partial t} = \frac{D_s}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial c_s}{\partial r} \right)$$

(14)

$$\frac{\partial (\varepsilon_s c_s + \varepsilon_e c_e)}{\partial t} = \frac{\partial}{\partial x} \left( \frac{D_e \varepsilon_e}{\partial x} \frac{\partial c_e}{\partial x} \right) + \frac{1 - \varepsilon_s^0}{F} j^{Li}$$

(15)

where $c_s$ and $c_e$ are the phase concentrations in the solid and electrolyte phase, respectively. $D_s$ and $D_e$ are the diffusion coefficients of the Li and the Li$^+$ in solid and electrolyte phase. Additionally, $\varepsilon_s^0$ is the Bruggeman porosity exponent. Additionally, the charge conservation in solid and electrolyte phases are computed through (16)-(17),

$$\frac{\partial}{\partial x} \left( \sigma_s^e \frac{\partial \phi_s}{\partial x} \right) - j^{Li} = 0$$

(16)

$$\frac{\partial}{\partial x} \left( \sigma_e \frac{\partial \phi_s}{\partial x} \right) + \frac{\partial}{\partial x} \left( \frac{\sigma_e \frac{\partial \ln \varepsilon_e}{\partial x}}{\partial \phi_s} \right) + j^{Li} = 0$$

(17)

here $\varepsilon_s$ is the volume fraction of the active material in the electrode. Additionally, $k_{De}^eff$ is the electrolyte diffusional conductivity and is defined through (18).

$$k_{De}^eff = \frac{2RTk_s^}\beta}{F}(t_s^0 - 1)(1 + \frac{d\ln \varepsilon_s}{d\ln \phi_s})$$

(18)

Moreover, the volumetric current transfer rate is expressed as a function of the overpotential, $\eta$, through the Butler-Volmer equation displayed in (19).

$$j^{Li} = \frac{3\lambda_e}{t_s} \int \left\{ \exp(\frac{\alpha_a F}{RT} \eta) - \exp(\frac{\alpha_c F}{RT} \eta) \right\}$$

(19)

where $\alpha_a$ and $\alpha_c$ are the charge transfer coefficients at the anode and cathode, respectively. The exchange current density, $i_0$ is defined through (20).

$$i_0 = k_m(c_e)_{max} - c_s$$

(20)

From equation (20), $k_m$ is the reaction rate constant and $c_{s,max}$ is the maximum concentration of lithium in solid phase.

Furthermore, the volumetric current transfer rate due to the electrochemical reactions is expressed through (21),

$$j_{ECh} = -\frac{i_p}{Vol}$$

(21)

where $i_p$ is the transverse current density and computed through (22).

$$i_p = \int_{l_s}^{l_p} j^{Li} dx$$

(22)

Finally, (23) is utilized to compute the heat generation rate in the battery during the charge/discharge process.

$$\dot{q}_{ECh} = \frac{i_p V + \int_{l_p}^{l_s} j^{Li}(T_{Ref} \frac{dT}{dt} - U_{Ref}) dx}{l_p + l_s + l_n}$$

(23)

where $l_p$, $l_s$ and $l_n$ are the thicknesses of the positive electrode, negative electrode and the separator.

III. COUPLED THERMO-MECHANICAL CELL CHARACTERIZATION

The three methods discussed in the previous section all estimate heat generation in different ways which may be used to estimate temperature. The method developed in this paper and detailed in this section discusses a mechanical analog for battery dynamics which is useful because of its ability to achieve accurate predictions for heat generation and is intuitive to work with despite being higher order. Furthermore, since the system is modally decomposed, each degree of freedom can be analyzed independently adhering to the different dynamic effects. The estimated heat is used in a lumped mass thermal model to predict temperature.
The mechanical battery analog developed by Alsharif et al. [30] was used to estimate the steady-state and transient responses of two different cylindrical batteries. Additionally, the open-circuit voltage, boundary layer effect and mass transfer effect were obtained from the outputs of the model. To estimate the temperature profile of the cells under dynamic discharge conditions, the model was coupled with a lumped thermal system as shown in Fig. 3, here, \( V_Q \) is the overpotential voltage by the dynamic model. The following subsections outline the theory and derives the governing equations of the coupled models.

### A. MECHANICAL SYSTEM ANALOGY OF BATTERY DYNAMICS

The dynamic model used to characterize the dynamics response of a battery is shown in Fig. 4.

The system is excited when the external force \( f \) is applied on the mass \( m_1 \), which translates the spring-mass-damper assembly to the right. The dynamic response of the system to the excitation induced by the external force represents the dynamic voltage discharge characteristics of an electrochemical cell. When the driving force is removed, the compressed springs \( k_1 \) and \( k_2 \) relax and recover a portion of the displacements of \( m_1 \) and \( m_2 \). The overall displacement of the three masses has moved to the right and will not recover. Additionally, the components below each mass are viscous damping to ground. The viscous damping \( c_1 \), \( c_2 \) and \( c_3 \) effect limits the discharge rate and stops discharging after the external force is removed. To analyze the mass system, free-body diagrams were drawn and shown in Fig. 5.

The three equations of motion were derived according to Newton’s Second Law of motion and assembled in a coupled system (24).

\[
\begin{align*}
\dot{x}_1 + c_1(\dot{x}_1) + k_1(x_1 - x_2) &= -f \\
\dot{x}_2 + c_2(\dot{x}_2) + k_2(x_2 - x_3) - k_1(x_1 - x_2) &= 0 \\
\dot{x}_3 + c_3(\dot{x}_3) - k_2(x_2 - x_3) &= 0
\end{align*}
\]

Here \( m_1, m_2 \) and \( m_3 \) are the masses, \( c_1, c_2 \) and \( c_3 \) are the damping coefficients, and \( k_1 \) and \( k_2 \) are the spring stiffnesses. The terms \( x, \dot{x}, \ddot{x} \) are the position, velocity, and acceleration of each respective mass. The equations of motion can be stated in matrix form (25):

\[
\begin{align*}
\begin{bmatrix} m_1 & 0 & 0 \\ 0 & m_2 & 0 \\ 0 & 0 & m_3 \end{bmatrix} \begin{bmatrix} \ddot{x}_1 \\ \ddot{x}_2 \\ \ddot{x}_3 \end{bmatrix} + \begin{bmatrix} c_1 & 0 & 0 \\ 0 & c_2 & 0 \\ 0 & 0 & c_3 \end{bmatrix} \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} &= \begin{bmatrix} -k_1 \dot{x}_1 - k_1 \dot{x}_2 \\ -k_1 \dot{x}_2 - k_2 \dot{x}_3 \\ -k_2 \dot{x}_3 \end{bmatrix} + \begin{bmatrix} k_1(x_1 - x_2) \\ k_2(x_2 - x_3) \\ 0 \end{bmatrix}
\end{align*}
\]

\[
\begin{bmatrix} \ddot{x}_1 \\ \ddot{x}_2 \\ \ddot{x}_3 \end{bmatrix} = \begin{bmatrix} -1 \\ 0 \\ 0 \end{bmatrix} [f] \tag{25}
\]

A multiple-degree-of-freedom system of this form can be transformed into modal coordinates [31]. The system in modal representation can be thought of as three independent single-degree-of-freedom systems. To conveniently make the transformation, the system is written as the single matrix equation (26).

\[
\begin{align*}
\mathbf{M} \ddot{\mathbf{x}} + \mathbf{C} \dot{\mathbf{x}} + \mathbf{K} \mathbf{x} &= \mathbf{B} [f] \\
\mathbf{M}, \mathbf{C}, \text{ and } \mathbf{B} \text{ are the mass, damping coefficient, spring stiffness, and input matrices, as shown in (27)-(30).}
\end{align*}
\]

\[
\mathbf{M} = \begin{bmatrix} m_1 & 0 & 0 \\ 0 & m_2 & 0 \\ 0 & 0 & m_3 \end{bmatrix} \tag{27}
\]

\[
\mathbf{C} = \begin{bmatrix} c_1 & 0 & 0 \\ 0 & c_2 & 0 \\ 0 & 0 & c_3 \end{bmatrix} \tag{28}
\]

\[
\mathbf{K} = \begin{bmatrix} k_1 & -k_1 & 0 \\ -k_1 & k_1 + k_2 & -k_2 \\ 0 & -k_2 & k_2 \end{bmatrix} \tag{29}
\]

\[
\mathbf{B} = \begin{bmatrix} -1 \\ 0 \\ 0 \end{bmatrix} \tag{30}
\]

The position, velocity and acceleration of each mass can be expressed in terms of an intermediate coordinate system.
the coordinate system \( \mathbf{q} \) via (31).

\[
\mathbf{x} = \mathbf{M}^{(-1/2)} \mathbf{q}
\]

(31)

To allow the diagonalization of the modal equations of motion, the damping matrix is defined by a linear combination of the mass and stiffness known as the proportional damping expressed in (32).

\[
\mathbf{C} = \alpha \mathbf{M} + \beta \mathbf{K}
\]

(32)

Here, \( \alpha \) and \( \beta \) are scalar constants. Examining matrices (27)-(29), no mass is connected to ground by a stiffness term; therefore, to achieve proportional damping, the term \( \beta \) is taken as zero. Equation (33) can be reduced to (33).

\[
\mathbf{C} = \alpha \mathbf{M}
\]

(33)

Then, the equation of motion can then be written in terms of the coordinate system \( \mathbf{q} \) via (34).

\[
I \ddot{\mathbf{q}} + \mathbf{C} \dot{\mathbf{q}} + \mathbf{K} \mathbf{q} = \mathbf{M}^{(-1/2)} \mathbf{B} \{f\}
\]

(34)

Here, \( I \) is the identity matrix. Also, \( \mathbf{K} \) and \( \mathbf{C} \) are the mass-normalized stiffness and damping matrices, as shown in (35) and (36), respectively.

\[
\mathbf{\tilde{K}} = \mathbf{M}^{(-1/2)} \mathbf{K} \mathbf{M}^{(-1/2)}
\]

(35)

\[
\mathbf{\tilde{C}} = \mathbf{M}^{(-1/2)} \mathbf{C} \mathbf{M}^{(-1/2)}
\]

(36)

Finally, to express the system in modal coordinates, the coordinate \( \mathbf{q} \) can be written in terms of the modal coordinate via (22).

\[
\mathbf{q} = \mathbf{P} \mathbf{r}
\]

(37)

Here, \( \mathbf{P} \) is the matrix of the eigenvectors which are orthonormal of \( \mathbf{\tilde{K}} \) and \( \mathbf{\tilde{C}} \) multiplied by the \( \mathbf{P}^T \). The mass-normalized stiffness and damping matrices can be represented as shown in (38) and (39), respectively.

\[
\mathbf{C}_m = \mathbf{P}^T \mathbf{\tilde{C}} \mathbf{P}
\]

(38)

\[
\mathbf{A} = \mathbf{P}^T \mathbf{\tilde{K}} \mathbf{P}
\]

(39)

where \( \mathbf{C}_m \) and \( \mathbf{A} \) are the damping and stiffness matrices, for the modal coordinates. Finally, the equations of motion can be decomposed in modal representation, as shown in (40).

\[
\mathbf{\tilde{r}} + \mathbf{C}_m \mathbf{\tilde{r}} + \mathbf{A} \mathbf{\tilde{r}} = \mathbf{P}^T \mathbf{M}^{(-1/2)} \mathbf{B} \{f\}
\]

(40)

The terms of the matrices are shown directly in (41). After the modal decomposition, the stiffness and damping matrices become diagonalized.

\[
\begin{bmatrix}
\mathbf{\tilde{r}}_{OCV} \\
\mathbf{\tilde{r}}_{MT} \\
\mathbf{\tilde{r}}_{DL}
\end{bmatrix} +
\begin{bmatrix}
c_{OCV} & 0 & 0 \\
0 & 2\xi_{MT}\omega_{n,MT} & 0 \\
0 & 0 & 2\xi_{DL}\omega_{n,DL}
\end{bmatrix}
\begin{bmatrix}
\mathbf{\tilde{r}}_{OCV} \\
\mathbf{\tilde{r}}_{MT} \\
\mathbf{\tilde{r}}_{DL}
\end{bmatrix} =
\begin{bmatrix}
b_{OCV} \\
b_{MT} \\
b_{DL}
\end{bmatrix} \{f\}
\]

(41)

Furthermore, Fig 6 demonstrates the three-independent single-degree-of-freedom systems in modal representation. The significance of this transformation is that each mode can be considered individually to reflect the different dynamic effects of the battery.

Here, \( r_{OCV} \) is the modal displacement which represents the actual discharge of the battery. The natural frequency of this mode is zero which appears as zero in the top left term of the \( \mathbf{A} \) matrix. Consequently, this is a rigid body mode which does not vibrate such that the open-circuit voltage does not recover after the cell delivers amperage. The corresponding term of the modal damping matrix is \( c_{ocv} \). Modes \( r_{MT} \) and \( r_{DL} \) represent the mass transfer and double-layer dynamic effects, respectively. The associated stiffness terms are the squared natural frequencies \( \omega_{n,MT} \) and \( \omega_{n,DL} \). These control the rate at which each mode responds.

The damping matrix terms are expressed in standard form in relation to the natural frequency and damping ratios. These influence the relative rate at which each degree of freedom’s oscillations degrades. The external force \( f \), acts upon \( m_1 \) but excites all three modes through the modal input matrix \( \mathbf{B} \). The gains of the input matrix become \( b_{OCV}, b_{MT} \) and \( b_{DL} \). These are the amounts the single input current excites each mode. The modally transformed system is shown in the block diagram in Fig. 7. Each mode, which is SISO and 1DoF, is indicated by a dashed box. Generally, the \( r_{MT} \) signal is associated with a slower frequency effect, and the \( r_{DL} \) signal is associated with a faster frequency effect. The output signal \( V_{out} \) is a modal superposition of all the frequency components. The input to the system was the current at which the battery was discharged. \( V_{out} \) is the voltage measured across the battery terminals. Furthermore, \( V_{OCV} \) is an internal signal related to the SOC and \( V_Q \) is the voltage signal utilized as an input to the thermal model.

The OCV and terminal voltages obtained by the dynamic model were coupled with the lumped thermal model to estimate the temperature response of the batteries. The next subsection outlines the governing equations utilized to thermally analyze a cylindrical battery.
The Nusselt number equations for a horizontal cylinder are a function of the surface temperature for a specific geometry. Prandtl numbers \[32\]. Here, the heat transfer coefficient is of Nusselt number, which is a function of the Rayleigh and coefficient obtained from the natural convection equations \(h\) of the battery. Additionally, \(\text{FIGURE 7.} \) Here, \(\nu\) is the kinematic viscosity. Furthermore, the energy balance relationship between buoyancy and viscosity in the fluid and \(\nu\) is Prandtl number which establishes the relationship between the Rayleigh number is obtained through \(45\), \(\text{where} \(g\) \text{is the gravitational acceleration,} \(k\) \text{is the thermal conductivity,} \(\beta\) \text{is the coefficient expansion,} \(L_e\) \text{is the characteristic length of the geometry and} \(\nu\) \text{is the kinematic viscosity. Furthermore, the energy balance equation of a single cell can be expressed as shown in} (46). \[ \rho V C_p \frac{dT}{dt} = \dot{Q}_{ECh} + \dot{Q}_{conv} + \dot{Q}_{rad} \] (46) where \(\rho\) is the density of the battery, \(C_p\) is the heat capacity, \(V\) is the volume and \(T\) is the temperature. Furthermore, \(\dot{Q}_{ECh}\) is the heat power generated from the battery due to the overpotential and entropic heating. Bernardi and Newman [33] established this term as displayed in \(47\). \[ \dot{Q}_{ECh} = I(V - V_{OCV}) + IT \frac{\partial V_{OCV}}{\partial T} \] (47) This expression neglects the uneven heat generation and phase change heat generation of the battery reactants. For further simplification, the entropic heating was neglected \[34\]. Furthermore, \(\dot{Q}_{conv}\) is the convection heat transfer term and is defined through \(48\), where \(A\) is the surface area of the battery and \(T_{amb}\) is the ambient temperature. \[ \dot{Q}_{conv} = h A (T - T_{amb}) \] (48) Additionally, the last term from \(46\) incorporates the heat transfer due to radiation effects. \(\dot{Q}_{rad}\) is defined through \(48\), where \(\varepsilon\) is the emissivity constant and was set to 0.80 \[20\] and \(\sigma\) is Stefan-Boltzmann’s constant equivalent to \(5.6710^{-8}\). \[ \dot{Q}_{rad} = \varepsilon \sigma A (T^4 - T_{amb}^4) \] (49) Fig. 8 displays the block diagram employed to compute the temperature profile from the lumped thermal model.

### B. LUMPED THERMAL MODEL

For a body to be considered as a lumped system, the Biot number criteria expressed in \(42\) was confirmed \[32\].

\[ \text{Bi} = \frac{hD}{k_b} \leq 0.1 \] (42)

Here, \(D\) and \(k_b\) are the diameter and the thermal conductivity of the battery. Additionally, \(h\) is convection the heat transfer coefficient obtained from the natural convection equations of Nusselt number, which is a function of the Rayleigh and Prandtl numbers \[32\]. Here, the heat transfer coefficient is function of the surface temperature for a specific geometry. The Nusselt number equations for a horizontal cylinder are given by \(43\)-(44).

\[ Nu = \frac{hD}{\nu} \] (43)

\[ Nu = \left\{ 0.6 + \frac{0.387 R_a D^{1/6}}{1 + (0.559/Pr)^{9/16}} \right\}^2 \] (44)

From \(44\), \(R_a D\) is Rayleigh number which describes the relationship between buoyancy and viscosity in the fluid and \(Pr\) is Prandtl number which establishes the relationship between the momentum diffusivity and thermal diffusivity. Moreover, the Rayleigh number is obtained through \(45\),

\[ R_a D = \frac{g \beta (T - T_{amb}) L_e^3}{\nu^2} \] (45)

The circuit was constructed from a DC electronic load (BK Precision 8601) to discharge the battery at consistent current level, a relay to actuate when the current is drawn from the battery, a microcontroller (Arduino MEGA2560 R3) to trigger the relay at a consistent duty cycle and generate the current square waves. Additionally, two Digit multi-meters (Keysight 34465A 6) were utilized to measure the current and the voltage of the battery. The first multimeter was connected in series to record current, whereas the second one was connected in parallel to measure the voltage response across the battery. Furthermore, a K-type thermocouple connected to a data acquisition system (DAQ) (OMEG OM-CP-QuadTemp2000digital) was used to record the temperature values.

The sampling rate on the multimeters were set to 0.4 Sa/s, whereas the thermocouple DAQ was set to a sampling rate of 2 Sa/s. In addition, the microcontroller triggered the relay
at constant frequency of 2.8mHz. Fig. 10 shows the experimental instrumentation.

V. RESULTS & DISCUSSION
This section presents the experimental data and simulation results obtained from the dynamic system and the lumped thermal model for the two lithium-ion batteries considered. The dynamic model was utilized to match the terminal voltage and predict the OCV. Furthermore, the electrochemical heat generation computed from the OCV and the terminal voltage was used as an input to the lumped thermal model to obtain the temperature profile of the battery.

The model parameters for each battery case were numerically tuned to fit the measured terminal voltage by performing the method of nonlinear least squares through the Trust-Region-Reflective algorithm. Each parameter was optimized as a lookup table with breakpoints dependent on SOC as 20 discrete values from 0.05 to 1. This was done using the parameter estimation toolbox in MATLAB/Simulink. In addition, to capture the effects of the current drawn from the battery during discharge, the modal gains were tuned as a function of the C-rate and SOC.

The natural frequency terms were tuned according to the angular frequency ranges reported from the electrochemical impedance measurements. The mass transfer phenomenon is known to govern the lower-frequency dynamics of batter-
ies. Likewise, the double-layer phenomenon dominates the higher-frequency dynamics. Table 2 illustrates the angular frequency values reported in literature for the dynamic effects considered.

The damping ratios were bounded to be above unity as all the transient behaviors were assumed to be overdamped. Also, the modal input gains were constrained only to take any positive value. The initial $C_{OCV}$ range was not known;
however, it was found by iterating that an upper bound is required to achieve the optimizer convergence. The identified model parameters for the two battery cases can be referred in Appendix.
The convection heat transfer coefficient was estimated utilizing the Nusselt number relationships shown in (43)-(44). The value was optimized as a function of the temperature change independent of the dynamic model tuning. Initially, the density and specific heat of the battery were estimated by computing the summation of the assumed materials in the cell core (anode, cathode and separator), the positive and negative tab materials and the insulation film as reported in literature for cylindrical batteries [17]. These values were also optimized as a function of temperature and updated for the entire experimental history.

The purpose of the coupled dynamic-thermal model proposed in this paper is to accurately predict the steady-state and transient response of batteries. Also, the model has the ability to accurately predict the SOC-OCV nonlinear relationship. Furthermore, from the estimated OCV and the terminal voltage of the cells, the heat generated from the cells during a dynamic discharge can be obtained. Lastly, the energy balance equation (46) can be solved to predict the temperature response of an electrochemical cell at various discharge rates.

The following subsections illustrate the experimental data and the capability of the model to characterize two cylindrical lithium-ion batteries with different form factors.

### A. PANASONIC NCR21700

Figure 11 displays the measured current load for both discharge rates at which the battery was tested. The top plot shows data for 1C discharge rate and the bottom plot shows that for 2C discharge rate.
Furthermore, from the measured current data, the SOC for both discharge rates was computed utilizing (9) and displayed in Fig. 12.

As illustrated in Fig 13, the SOC of the battery began fully charged with an SOC of 1 and decreased by 0.05 after each current pulse at 1C, whereas at 2C, the SOC decreased by 0.1 over each pulse. The modal parameters were then fit as a function of this SOC computed to fit the corresponding experimentally measured battery terminal voltage.

Figure 12 displays the battery terminal voltage as predicted by the dynamic model compared to the measured terminal voltage. With each pulse of current, the electrical potential drops mainly due to the mass transfer effect and double-layer effect degrees of freedom, and when the current load is set to zero, most of the electrical potential is recovered from the vibration of these modes. However, a slight portion of the voltage is lost due to the static-discharge mode.

To statistically evaluate the fitment of the dynamic model to the measured terminal voltage, the error standard deviation was computed. It was found that the model was able to match the voltage response of the battery within 0.96% and 2.15% of standard deviation of the error, for the 1C and 2C discharge rates, respectively.

The OCV predicted by the steady-state component of the experimental data and the mode signal V_{OCV} are shown in Fig. 14. The experimentally based OCV was found by taking the peak voltage value during the regeneration period relative to the SO. This neglects any small remaining transient to steady-state due to the frequency and duty cycle that induced the current load. In general, good agreement is found; therefore, it can be deemed apt to use the predicted parameters from the model to estimate the heat energy generated by the battery.

Good agreement is found between the OCV predicted as a state within the dynamic model and that from the quasi-static component of the experiment. With the terminal voltage and OCV estimated, the overpotential heat generation was computed for both discharge rates from (43) and shown in Fig. 15.

With each current pulse, heat is generated from the battery due to the electrochemical reactions the battery undergoes as being discharged. On average, the overpotential power generated by the battery increased by 70.62% when discharged at 2C relative to 1C.

Then, the estimated heat generation history is used to predict the surface temperature profile of the battery over time through (42). Fig. 16 displays the temperature response measured experimentally relative to that predicted by the lumped thermal model for both discharge rates. The higher discharge rate results in the battery reaching a higher temperature in keeping with the greater heat generated as seen in Fig. 15.

The lumped thermal model was able to estimate the temperature profile for both discharge rates with 0.22% and 0.40% error standard deviation, which indicates a high level of accuracy. For a higher precision estimation, the entropic heating effect may be considered.

B. SAMSUNG INR18650-25R

The test was repeated for an 18650 battery. Fig. 17 illustrates the measured current load for both discharge rates. The top plot shows data for 1C discharge rate and the bottom plot shows that for 2C discharge rate.

Similarly, as in the Panasonic battery test, the amperage increases from 0 A to the designated discharge rate when the relay is triggered at the set switching period.

From the current load, the SOC was calculated again from (9) and is shown in Fig 18. Initially, the battery was fully charged and was discharged to almost 10%; therefore, the modal parameters lookup tables were tuned with SOC breakpoints in that range. Analogs to the 27100 battery, each 1C pulse corresponded to a 5% decrease in SOC, whereas each current pulse during the 2C test yielded to a 10% decrease.

Fig 18 shows the experimental terminal voltage and the simulated system response of the modally decoupled coordinates over the same time history shown in Fig 19. The dynamic model utilized in this study was able to match the voltage response of the battery within 0.41% and 0.82% standard deviation of the error, for the 1C and 2C discharge rates, respectively.

Fig. 20 displays the OCV predicted by the modal signal V_{OCV}, relative to the electrical potential measured at the peaks of the relaxation period. Again, the dynamic model estimated the OCV of the battery within high level of accuracy; therefore, the estimated can be used OCV to computed the overpotential heat generation rate.

The overpotential heat generation was for each current pulse was calculated from (42) and is displayed in Fig. 21. The pulsing current causes heat generation in the test battery. The overpotential power generated by the battery increased by approximately 71% when discharged at 2C compared to 1C. The heat generation prediction was used to predict the battery temperature and compared with experimental data in Fig 22. The model was able to estimate the surface temperature of the battery within 0.16% and 0.25% standard deviation of the error, for both discharge rates, respectively.

The overall temperature increase for the INR 18650 battery is less than that for the Panasonic battery due to the smaller form factor.

VI. CONCLUSION

This study extended the dynamic model proposed by Li et al. [25] to predict the electrochemical heat generated by a battery. The dynamic battery model was a mechanical analogy composed of a three-degree-of-freedom damped spring-mass system. The system was represented by three independent single-degree-of-freedom modes in modal coordinates to estimate the OCV and mass transfer effect and boundary layer effect of both batteries. Furthermore, the modal parameters of natural frequencies and damping ratios were tuned and optimized relative to the SOC utilizing the Trust-Region-Reflective algorithm to fit the measured terminal voltage for the tests conducted. The model was extended to predict battery surface temperature by using the predicted overpoten-
TABLE 3. Optimized modal parameters.

|   |   |   |   |   | bocv (1C) | bocv (2C) | bocv (1C) | bocv (2C) | bocv (1C) | bocv (2C) | bocv (1C) | bocv (2C) |
|---|---|---|---|---|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| 0.2 | 4.63e+04 | 1.95e-00 | 3.76e+01 | 4.18e+01 | 2.00e+00 | 9.70e+00 | 2.35e+00 | 1.70e-01 | 7.43e-02 | 4.20e+02 | 1.48e+02 |
| 0.25 | 1.91e+04 | 2.30e-00 | 3.51e+01 | 4.79e+01 | 2.00e+00 | 6.86e-01 | 8.25e-01 | 3.08e-01 | 7.69e-02 | 4.62e+02 | 1.48e+02 |
| 0.3 | 2.17e+04 | 3.61e-00 | 2.63e+01 | 8.02e+00 | 2.00e+00 | 3.54e+00 | 1.41e+00 | 3.77e-01 | 1.53e-01 | 3.71e+02 | 7.30e+01 |
| 0.35 | 1.81e+04 | 4.04e-00 | 4.26e+01 | 8.06e+00 | 1.04e+00 | 1.02e+00 | 9.31e-01 | 1.78e+00 | 1.30e+01 | 6.59e-01 | 2.21e+02 |
| 0.4 | 8.48e+03 | 4.87e-00 | 6.03e+01 | 3.28e+01 | 1.00e+00 | 1.91e+00 | 1.12e+00 | 2.03e+00 | 9.11e-02 | 4.95e-01 | 1.80e+02 |
| 0.45 | 1.52e+04 | 2.28e+00 | 4.75e+01 | 1.02e+00 | 3.13e+00 | 1.76e+00 | 1.13e+00 | 7.74e-01 | 2.01e-02 | 4.94e-01 | 1.80e+02 |
| 0.5 | 2.29e+04 | 4.37e+00 | 4.98e+01 | 1.01e+00 | 1.02e+00 | 4.70e+00 | 2.46e+00 | 1.41e+00 | 7.12e+00 | 7.02e+00 | 2.59e+00 |
| 0.55 | 2.21e+04 | 2.69e+00 | 5.27e+01 | 5.21e+00 | 1.02e+00 | 6.32e+00 | 3.70e-01 | 6.49e-01 | 9.84e-02 | 6.98e-02 | 3.51e+02 |
| 0.6 | 4.17e+04 | 3.49e+00 | 4.73e+01 | 8.47e+00 | 1.00e+00 | 7.19e+00 | 2.72e+00 | 3.34e+00 | 1.39e-01 | 6.02e-02 | 2.69e+00 |
| 0.65 | 1.91e+04 | 6.39e-01 | 5.06e+01 | 1.92e+00 | 1.01e+00 | 1.10e+00 | 6.57e+00 | 5.12e+00 | 6.42e-03 | 8.68e+00 | 3.32e+00 |
| 0.7 | 2.65e+04 | 8.01e-01 | 4.59e+01 | 2.11e+00 | 1.00e+00 | 7.51e+00 | 2.73e+00 | 5.33e+00 | 1.08e-02 | 1.01e-03 | 3.30e+00 |
| 0.75 | 1.87e+04 | 1.05e+01 | 2.35e+01 | 2.33e+00 | 1.19e+00 | 2.23e+00 | 8.43e-01 | 1.31e-01 | 2.31e-02 | 1.62e-02 | 7.39e-01 |
| 0.8 | 2.45e+04 | 2.25e+00 | 2.03e+01 | 4.79e+00 | 1.00e+00 | 5.67e-01 | 2.94e+00 | 5.16e-01 | 8.68e-02 | 3.38e+00 | 6.44e-01 |
| 0.85 | 1.36e+04 | 1.42e+00 | 5.31e+00 | 2.54e+00 | 1.02e+00 | 3.09e+00 | 3.08e+00 | 1.45e-01 | 3.32e+00 | 1.51e+00 | 3.36e+00 |
| 0.9 | 2.52e+04 | 3.37e+00 | 3.47e+00 | 7.40e+00 | 1.00e+00 | 1.95e+00 | 1.92e+00 | 2.05e+00 | 1.16e-01 | 4.72e+00 | 1.75e+00 |
| 0.95 | 1.60e+04 | 2.17e+00 | 2.44e+00 | 6.39e+00 | 1.00e+00 | 6.25e-01 | 3.44e+00 | 6.56e+00 | 8.53e-02 | 3.35e+00 | 9.43e-01 |
| 1 | 6.79e+03 | 2.17e+01 | 3.70e+01 | 6.85e+00 | 1.01e+00 | 5.08e+00 | 1.45e+00 | 1.87e+00 | 5.88e+00 | 1.52e+03 | 2.92e+00 |

APPENDIX

See Table 3.

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ALEXANDER H. PESCH received the B.S. degree in mechanical engineering from Ohio University, with a minor in economics, and the M.S. and Ph.D. degrees in mechanical engineering from Cleveland State University. After graduating with his bachelor’s degree, he worked in the jet engine overhaul industry as a Product Support Engineer. He is currently an Assistant Professor at Youngstown State University. Before joining Youngstown State University, he was an Assistant Professor at Hofstra University. His research interests include mechanical vibrations, controls, and active magnetic bearings.

VAMSI BORRA (Senior Member, IEEE) received the bachelor’s degree in electronics and communication engineering from Jawaharlal Nehru Technological University, the master’s degree in electrical and computer engineering from Youngstown State University, and the Ph.D. degree in electrical engineering from The University of Toledo. He is currently an Assistant Professor at YSU. Prior to YSU, he worked as an Assistant Professor and a Program Coordinator at the Department of Computer Science, Information Systems, and Engineering Technology, California University of Pennsylvania (CALU). Also, prior to CALU, he was a Visiting Assistant Professor with the Electrical Engineering and Computer Science (EECS) Department, The University of Toledo. He also worked as an Electrical Engineer at Valley Electrical Consolidated Inc., Girard, OH, USA, before starting his Ph.D. studies. His research interests include whiskers, material characterization, semiconductors, surface plasmon polariton, and thin films.

FRANK X. LI (Member, IEEE) received the B.S. degree in electrical engineering from The Ohio State University, in 1996, the master’s degree from Youngstown State University, in 1999, and the Ph.D. degree from Case Western Reserve University, in 2005. He joined the Department of Electrical and Computer Engineering, Youngstown State University, as an Assistant Professor, in August 2006, after serving ferrous and non-ferrous metal industry for 11 years. He advanced in academic rank to an Associate Professor and a Professor, in 2011 and 2016, respectively. He is currently working as the Acting Chair of the Rayen School of Engineering, YSU. His current research interests include autonomous power conversion, software engineering, RF engineering, wireless networks, VLSI, and applied magnetic fields.

PEDRO CORTES is currently an Associate Professor with the Department of Civil/Environmental and Chemical Engineering Program as well as the Materials Science and Engineering Program, Youngstown State University. He has served twice as a Faculty Fellow for the Wright-Patterson Air Force Base. His research work has been funded through the U.S. Department of Transportation, the Department of Defense, NASA, the National Science Foundation, and the Ohio Federal Research Network. He has published several articles in the area of composite structures and 3D printing. His research interests include the area of 3D printing, including smart and multifunctional materials, composite structures, and metal-ceramic systems.

ERIC MACDONALD (Senior Member, IEEE) received the Ph.D. degree in electrical and computer engineering from The University of Texas at Austin, in 2002. He held a Faculty Fellowship at the NASA’s Jet Propulsion Laboratory and U.S. Navy Research. He is currently a Professor of mechanical engineering and the Murchison Chair at The University of Texas at El Paso. His research interests include 3D printed multifunctional applications and process monitoring in additive manufacturing with instrumentation and computer vision for improved quality and yield. He is a member of ASME and ASEE and a Registered Professional Engineer, TX, USA. He was awarded the U.S. State Department Fulbright Fellowship in South America.

KYOSUNG CHOO received the B.S. degree in mechanical and control engineering from Handong University, South Korea, and the M.S. and Ph.D. degrees in mechanical engineering from the Korea Advanced Institute of Science and Technology (KAIST). He is currently an Associate Professor of mechanical engineering at Youngstown State University. Prior to joining YSU, he worked as a Postdoctoral Fellow at the Center for Environmental Energy Engineering, University of Maryland. He has published over 40 articles and papers in the field. His research interests include heat transfer for additive and advanced manufacturing, two-phase flow, jet impingement, energy efficiency of data centers and buildings, and electronics cooling. He is listed in Who’s Who in the World 2011 and a recipient of the Outstanding Research Award from Brain Korea 21 in 2010 and the Outstanding Academic Award from KAIST in 2011.