A Novel Modal Representation of Battery Dynamics

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ABSTRACT

Electrochemical cells are complicated energy storage systems with nonlinear voltage dynamics. There is a need for accurate dynamic modeling of the battery system to predict its behavior over time when discharging. The study conducted in this paper developed an intuitive model for electrochemical cells based on a simple mechanical analogy. A three-degree-of-freedom, spring-mass-damper system was decomposed into modal coordinates that represent the overall discharge, mass transport, and double-layer effect of the electrochemical cell. The developed model was experimentally demonstrated through pulsed discharge tests of commercially available lithium-ion and nickel metal hydride cells. The modal parameters of the natural frequency and damping ratio for each mode were determined by numerically minimizing the error in the time responses. Additionally, the mechanical analog was applied to two datasets developed by the Center for Advanced Life Cycle Engineering (CALCE). The first dataset was used to optimize the modal parameters whereas the second dataset was utilized to validate the tuned parameters. It was found that the modal representation of the mechanical analog could accurately predict the time-response dynamics of all the cells considered. Additionally, by considering the discharge modal coordinate, the open-circuit voltage was determined and validated to that measured experimentally from the voltage relaxation peaks.

INDEX TERMS

Batteries, dynamic system modeling, mechanical equivalent system, mechanical analog, modal representation.

I. INTRODUCTION

Electrochemical cells for energy storage are becoming increasingly important in the industry and everyday life [1]–[3]. To optimize the power and energy that can be delivered by a battery, it is necessary to predict the behavior of the cell under different loading conditions. However, electrochemical cells are complicated dynamic systems with time-varying current and voltage output. Therefore, to predict and optimize the usage of cells, modern engineering requires simple, intuitive dynamic models that accurately describe the input and output relationship.

Numerous studies have been conducted to better understand the nonlinear response behavior of electrochemical cells [4]–[10]. A common technique for characterizing battery dynamics is electrochemical impedance spectroscopy (EIS) [11], [12], which is employed by applying a small sinusoidal excitation current to the cell at a typical frequency range of 1 mHz to 10 kHz and measuring its voltage response. The dynamics of the battery are then characterized in the frequency domain through the Randles equivalent circuit model using Nyquist and/or Bode plots to identify the internal impedances of the battery. Although valuable insights can be obtained from this technique, it cannot predict the run time of the cell and evaluates the dynamic behavior of the battery at a fixed state of charge. It is critical to portray the nonlinear dynamics of the battery throughout the entire discharge period. It is also regarded as complicated and nonintuitive for engineering applications such as battery management systems.

Considering this, Chen and Rincon-Mora [13] proposed an electrical circuit model to capture the dynamic characteristics...
of batteries. The circuit consisted of a resistor in series with two resistor-capacitor networks. The input to the circuit is the current at which the battery is discharged and the output is the voltage response of the system, which is then compared to the experimentally measured terminal voltage output of the battery tested. The model was utilized to predict the runtime, steady state and transient response of three batteries with different chemical compositions. In addition to that, the circuit captured significant dynamic electrical characteristics of batteries such as the usable capacity and the open-circuit voltage over the entire state of charge range.

Furthermore, several studies have focused on enhancing the parameter estimation method used in equivalent circuit models. Hau et al. [14] optimized passive circuit components as a function of the state of charge and different temperature levels. In addition, they were able to evaluate these parameters for different input current profiles to capture the different time constants that a lithium-ion battery cell exhibits during underload operation and compare them with the relaxation period. Zhang et al. [15] proposed a new decoupled weighted recursive least-squares method to separately estimate the battery’s slow and fast dynamics. Through this method, they were also able to estimate the SOC of the cell tested. Hariharan et al. [16] developed a nonlinear equivalent circuit model for lithium-ion cells, in which the circuit elements were evaluated based on the charge transfer reaction and variable resistance. Their state-space model was used to resolve the overall cell potential into potential components and recompenses the noise effect so that the model parameters can be extracted without bias.

Moreover, Zheng et al. [23] established two state of charge estimators based on two open-circuit voltage (OCV) tests, a low-current (OCV) test, and an incremental OCV test. The open-circuit voltage and state of charge relationship were determined to be dependent upon the operating temperature. This was accomplished by comparing the accuracy of both state of charge estimators suggested. It was found that the estimator based on the incremental OCV test showed higher accuracy at 25°C and 45°C; however, the estimator based on the low-current OCV test provided a higher resolution at 0°C.

The study conducted in this paper proposes a novel mechanical analogy for modeling battery dynamics. The analog is based on a three-degree-of-freedom, mass-spring-damper system. The system was decomposed into modal coordinates which represented the discharge of the battery, mass transport, and double-layer dynamic effects. Models in this form were developed for three commercially available batteries: Energizer Lithium Ultimate, Duracell Nickel Metal Hydride, and a Samsung INR18650-20R. First, experiments were conducted in which the Energizer Ultimate Lithium and the Duracell Nickel Metal Hydride batteries were discharged using repeated current pulses with a consistent duty cycle. Thereafter, the modal parameters for each battery model were fitted to the experimental measurements using an error-minimization algorithm. Finally, the models were simulated using the experimental input, and the simulated output was compared with the experimental output. For further validation of the model, two independent experimental datasets developed [23]–[24] for the Samsung INR18650-20R battery were utilized. The first dataset was a low current pulsing test that was used to fit the simulated modal parameters onto the measured output voltage. Moreover, the second dataset was a constant current discharge test and the measured output voltage was used to validate the optimized modal parameters obtained from the first dataset.

The remainder of this paper is structured as follows: Section II is a literature review on current state-of-the-art models utilized to characterize electrochemical cells dynamics. Section III details the proposed novel mechanical analogy. Section IV presents the experimental setup and methods used. Section V presents the results of the experiments, which
demonstrates the ability of the model to predict these results, and validates the optimized parameters. Finally, the paper is concluded with closing remarks.

II. CURRENT STATE-OF-THE-ART

Various models have been established to advance the accuracy of characterizing electrochemical cells by considering different factors that may affect the performance of a battery cell. This section presents a literature review of the current state-of-the-art models.

A. ELECTROCHEMICAL IMPEDANCE SPECTROSCOPY

An electrochemical cell can be considered simply an impedance to a small sinusoidal excitation. The equivalent electrochemical circuit represents the performance of a battery cell through a network of resistors and capacitors that pass current with the same amplitude and phase angle that an actual battery cell does under a given excitation. This technique is known as Electrochemical Impedance Spectroscopy (EIS) [25]. Shown in Fig. 1 is the Randles equivalent circuit utilized to characterize the battery in the frequency domain.

The impedance of the cell at a given sinusoidal excitation and frequency range is described theoretically through (1) and (2) and graphically on a Nyquist plot [25].

\[
Z_{Re} = R_\Omega + \frac{R_{ct} + \sigma \omega^{-1/2}}{(C_d \sigma \omega^{1/2} + 1)^2 + \omega^2 C_d^2 (R_{ct} + \sigma \omega^{-1/2})^2} \tag{1}
\]

\[
Z_{Im} = R_\Omega + \frac{\omega C_d (R_{ct} + \sigma \omega^{-1/2})^2 + \omega \sigma^{-1/2} (C_d \sigma \omega^{1/2} + 1)}{(C_d \sigma \omega^{1/2} + 1)^2 + \omega^2 C_d^2 (R_{ct} + \sigma \omega^{-1/2})^2} \tag{2}
\]

where \(\omega\) is the angular frequency, \(R_\Omega\) is the electrolyte resistance, \(R_{ct}\) is the charge transfer resistance that accounts for the voltage drop over the electrode-electrolyte interface, \(C_d\) is the double-layer capacitance that represents the effect of charges building up in the electrolyte at the electrode surface, and \(Z_w\) is the Warburg impedance. The Warburg impedance represents the diffusion of lithium ions in the electrodes and the resistance to mass transfer.

B. EQUIVALENT CIRCUIT MODEL

The equivalent circuit model developed by Chen and Rincon-Mora [13] is shown in Fig. 2.

The electrical circuit consists of a voltage source that represents the open-circuit voltage \(V_{OCV}\), which describes the voltage across battery terminals when the cell is unloaded and in equilibrium. The resistor in series, \(R_e\), is regarded as the ohmic resistance, which accounts for the power dissipated by the battery as heat. Additionally, the two resistor-capacitor sub circuits \((R_1, R_2, C_1 & C_2)\) represent the time constants in the circuit, which account for the diffusion dynamics of the battery [26].

The input to this circuit is the current drawn from the battery. The output of the system is the measured voltage drop across the passive components of the circuit subtracted from \(V_{OCV}\) to obtain the voltage delivered by the battery. An important parameter to evaluate and estimate in an electrochemical cell is the state of charge (SOC). The SOC is defined as the ratio of the available capacity to the maximum possible charge that can be stored in a battery [27]. SOC is computed using (3).

\[
SOC (t) = SOC_0 - \int_{t_0}^{t} \frac{I(t)}{Q_{nom}} dt \tag{3}
\]

where \(SOC_0\) is the initial state of charge of the battery tested, \(I(t)\) is the measured current, and \(Q_{nom}\) is the nominal capacity of the battery. Furthermore, the voltage-current relationship is established through (4)-(6).

\[
\frac{dV_1}{dt} = - \frac{1}{R_1 SOC C_1} V_1 - \frac{1}{C_1} I(t) \tag{4}
\]

\[
\frac{dV_2}{dt} = - \frac{1}{R_2 SOC C_2} V_2 - \frac{1}{C_2} I(t) \tag{5}
\]

III. PROPOSED MECHANICAL ANALOG MODEL

When a battery is discharged, the current is drawn out and the voltage that the battery can supply degrades over time. However, when the current load is removed, a portion of the voltage can recover, depending on the internal characteristics and properties of the cell. A mechanical system that behaves similarly is shown in Fig. 3.
motion represents the battery discharge. If the external force is removed, the compressed springs can decompress and recover a portion of the \( m_1 \) and \( m_2 \) displacements, although the overall displacement has moved negatively and does not recover. Note that each mass is connected to another mass by a spring; however, there is no spring-to-ground connection. This phenomenon mirrors the dynamic discharge characteristics of the electrochemical cells. Furthermore, each mass was damped by a viscous damping component to the ground. This term limits the discharge rate and stops discharging when there is no load applied. To model this system, free-body diagrams were developed, in which all physical contacts were severed and replaced by forces, as shown in Fig. 4.

FIGURE 4. Free-body diagram of the mechanical system under external load.

The equations of motion for each nodal point were based on Newto’s second law of motion. The equations of motion were assembled in a coupled system (7),

\[
\begin{align*}
\begin{bmatrix} m_1 & c_1 & k_1 \\ m_2 & c_2 & k_2 \\ m_3 & c_3 & k_3 \\ \end{bmatrix}
\begin{bmatrix} \ddot{x}_1 \\ \ddot{x}_2 \\ \ddot{x}_3 \\ \end{bmatrix}
&= - \begin{bmatrix} f \\ 0 \\ 0 \\ \end{bmatrix} \\
\begin{bmatrix} m_1 & 0 & 0 \\ 0 & m_2 & 0 \\ 0 & 0 & m_3 \\ \end{bmatrix}
\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \\ \end{bmatrix}
&= \begin{bmatrix} \dot{c}_1 \\ \dot{c}_2 \\ \dot{c}_3 \\ \end{bmatrix} \\
\begin{bmatrix} m_1 & 0 & 0 \\ 0 & m_2 & 0 \\ 0 & 0 & m_3 \\ \end{bmatrix}
\begin{bmatrix} \ddot{x}_1 \\ \ddot{x}_2 \\ \ddot{x}_3 \\ \end{bmatrix}
&= - \begin{bmatrix} -k_1 & 0 & 0 \\ 0 & -k_2 & 0 \\ 0 & 0 & -k_3 \\ \end{bmatrix}
\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \end{bmatrix}
\end{align*}
\]

where \( m_1, m_2, \) and \( m_3 \) are the masses, respectively. In addition, \( c_1, c_2, \) and \( c_3 \) are the damping coefficients, and \( k_1, k_2, \) and \( k_3 \) are the spring stiffnesses. Furthermore, \( f \) denotes the load externally applied to the system. Finally, \( x, \dot{x}, \) and \( \ddot{x} \) are the position, velocity, and acceleration, associated with each mass, respectively. The system of equation (7) is expressed in matrix form (8).

\[
\begin{bmatrix} m_1 & 0 & 0 \\ 0 & m_2 & 0 \\ 0 & 0 & m_3 \\ \end{bmatrix}
\begin{bmatrix} \ddot{x}_1 \\ \ddot{x}_2 \\ \ddot{x}_3 \\ \end{bmatrix}
+ \begin{bmatrix} c_1 & 0 & 0 \\ 0 & c_2 & 0 \\ 0 & 0 & c_3 \\ \end{bmatrix}
\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \\ \end{bmatrix}
+ \begin{bmatrix} k_1 & -k_1 & 0 \\ -k_1 & k_1 + k_2 & -k_2 \\ 0 & -k_2 & k_2 \\ \end{bmatrix}
\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \end{bmatrix}
= \begin{bmatrix} -1 \\ 0 \\ 0 \\ \end{bmatrix}f
\]

The forced response of a multiple-degree-of-freedom system can be computed using modal analysis [28]. To make the transformation convenient, the system is written as the matrix (9).

\[
M\ddot{\mathbf{X}} + C\dot{\mathbf{X}} + K\mathbf{X} = \mathbf{B}[f]
\]

\[
M, C, K, \text{ and } B \text{ are the mass, damping coefficient, spring stiffness, and input matrices, as expressed in (10), (11), (12), and (13).}
\]

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

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

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

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

The position of each mass, velocity and acceleration can be defined in terms of an intermediate coordinate system \( \mathbf{q} \), as shown in Eqs. (14), (15), and (16).

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

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

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

The damping matrix is a linear combination of the mass and stiffness matrices, known as proportional damping (17).

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

where \( \alpha \) and \( \beta \) are the scalar constants. The damping of the proportional form allows for decoupling of the modal equations of motion. Inspecting the forms of (10)-(12) no mass has stiffness to ground; therefore, to achieve proportional damping, the constant \( \beta \) is assumed to be zero. Equation (17) can be simplified to (18).

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

Furthermore, the equation of motion can be written in terms of the coordinate system \( \mathbf{q} \), as shown in (19).

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

where \( I \) is the identity matrix. In addition, \( \mathbf{\dot{K}} \) and \( \mathbf{\ddot{K}} \) are the mass-normalized stiffness and damping matrices, as illustrated in (20) and (21), respectively.

\[
\mathbf{\ddot{K}} = \mathbf{M}^{-1/2}\mathbf{K}\mathbf{M}^{-1/2}
\]

\[
\mathbf{\dot{C}} = \mathbf{M}^{-1/2}\mathbf{C}\mathbf{M}^{-1/2}
\]

Additionally, to decompose the system into a modal coordinate representation, the coordinate \( \mathbf{q} \) can be written in terms of the modal coordinate, as shown in (22).

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

where \( \mathbf{P} \) is the matrix off the orthonormal eigenvectors of \( \mathbf{\dot{K}} \) and \( \mathbf{\ddot{K}} \) multiplied by the \( \mathbf{P}^T \). The mass-normalized stiffness
and damping matrices can be represented as shown in (23) and (24), respectively:

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

where \( \mathbf{C}_m \) and \( \Lambda \) are the damping and stiffness matrices, for the modal coordinates. Finally, the equations of motion can be decomposed into the modal coordinate representation, as shown in (25).

\[ \ddot{\mathbf{r}} + \mathbf{C}_m \dot{\mathbf{r}} + \mathbf{\Lambda} \mathbf{r} = \mathbf{D}^T \mathbf{M}^{-1/2} \mathbf{B} \{ \mathbf{f} \} \]  

The terms of the matrices are explicitly expressed in (26). After modal decomposition, for the proposed syste, the stiffness and damping matrices are diagonalized, and the significance is that it can be considered as three independent single-degree-of-freedom systems.

\[
\begin{cases}
\mathbf{r}_{OCV} \\
\mathbf{r}_{MT} \\
\mathbf{r}_{DL}
\end{cases}
\begin{bmatrix}
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
\mathbf{c}_{OCV} \\
\mathbf{2}\zeta_{MT}\omega_{n,MT} \\
\mathbf{2}\zeta_{DL}\omega_{n,DL}
\end{bmatrix}
\begin{bmatrix}
\dot{\mathbf{r}}_{OCV} \\
\dot{\mathbf{r}}_{MT} \\
\dot{\mathbf{r}}_{DL}
\end{bmatrix}
\]

\[
\begin{bmatrix}
0 & 0 & 0 \\
0 & (\omega_{n,MT})^2 & 0 \\
0 & 0 & (\omega_{n,DL})^2
\end{bmatrix}
\begin{bmatrix}
\mathbf{r}_{OCV} \\
\mathbf{r}_{MT} \\
\mathbf{r}_{DL}
\end{bmatrix}
\begin{bmatrix}
\mathbf{b}_{OCV} \\
\mathbf{b}_{MT} \\
\mathbf{b}_{DL}
\end{bmatrix}
\]

Here, \( \mathbf{r}_{OCV} \) is the modal displacement, which represents the degradation of the open-circuit voltage. The natural frequency of this mode is zero rad/s which manifests as zero in the first diagonal term of the \( \Lambda \) matrix. Therefore, this is a rigid body mode that does not oscillate and the open-circuit voltage never recovers after the current is drawn from the cell. The first diagonal term of the modal damping matrix is \( \mathbf{c}_{OCV} \), which limits the rate of change of the open-circuit voltage state, and stops the voltage drop when the cell is in equilibrium. Modes \( \mathbf{r}_{MT} \) and \( \mathbf{r}_{DL} \) represent the displacement of the mass transfer and double-layer degrees of freedom, respectively. The associated stiffness terms are the squared natural frequencies \( \omega_{n,MT} \) and \( \omega_{n,DL} \) and, which dictate the rate at which each mode responds.

By convention, the natural frequencies are ordered as the lowest first and the highest last. Therefore, the rigid-body mode is the first mode. The mass transfer phenomenon is known in electrochemistry to dominate the lower-frequency dynamics of batteries. Therefore, \( \omega_{n,MT} \) are in second order. Similarly, the double-layer phenomenon is associated with higher-frequency dynamics. Accordingly, \( \omega_{n,DL} \) are in the third order. Subsequently, these frequency-range dependencies are significant in the transient time responses.

Furthermore, the corresponding terms in the damping matrix are expressed in a standard form in relation to the natural and nondimensionalized damping ratios. The damping ratio dictates the relative rate at which each oscillation mode decays over time. The input force, which was assumed to only act upon \( n_1 \), contributed to the excitation of all three modes according to the modally transformed input matrix \( \mathbf{B} \).

The gains of the input matrix become \( \mathbf{b}_{OCV}, \mathbf{b}_{MT} \) and \( \mathbf{b}_{DL} \), which are the amounts at which the single input current affects each mode. The system in modal coordinates is shown graphically in the block diagram in Fig. 5. Each mode, which is the SISO single-degree-of-freedom, is indicated by a dashed rectangular box. In general, the \( \mathbf{r}_{MT} \) signal is associated with a lower dynamic frequency component, and the \( \mathbf{r}_{DL} \) signal is associated with a dynamic higher frequency component. The output signal \( \mathbf{V}_{out} \) is a modal summation containing all frequency components. The input to the system was the current at which the battery was discharged. \( \mathbf{V}_{out} \) is the voltage measured across the battery terminals. Furthermore, \( \mathbf{V}_{OCV} \) is an internal signal related to the SOC.

![Block diagram of the battery system in modal representation.](image)

FIGURE 5. Block diagram of the battery system in modal representation.

The purpose and unique benefits of this mechanical system are to accurately predict the runtime, steady state and transient response of the battery. In addition, the model has the capability to numerically quantify and graphically display the effects that the mass transfer and double-layer has on the battery for the entire SOC range, which were previously evaluated at a fixed SOC. Finally, the model is able to predict the nonlinear SOC-OCV relationship.

IV. EXPERIMENTAL PROCEDURES & APPROACHES

Two commercially available AA batteries were tested. The first cell was an Ultimate Lithium from Energizer® [29], and the second cell was a nickel metal hydride from Duracell® [30]. Table 1 lists the parameters for the batteries tested.

To conveniently and effectively measure the current and voltage responses across the battery, the experimental setup shown in Fig. 6 is employed. This single-loop circuit is constructed from a DC power supply (Keysight E36312A) as a discharger of constant current, a relay to control when
TABLE 1. Tested Battery parameters.

| Parameter               | Energizer Li-Ion | Duncell NiMH |
|-------------------------|------------------|--------------|
| Chemical system         | LiFeS₂           | NiMH         |
| Form factor             | Cylindrical      | Cylindrical  |
| Nominal capacity (mAh)  | 3000             | 2500         |
| Nominal voltage (V)     | 1.5              | 1.2          |
| Cut-Off voltage (V)     | 0.9              | 1            |
| Dimensions (mm)         | 14.5Ø × 50.5     | 14.5Ø × 50.5 |
| Mass (g)                | 15               | 30           |
| Operating Temperature (°C) | -40 to 60          | -10 to 50     |
| Storage Temperature (°C) | -40 to 60          | 5 to 30       |

the current is applied to the battery in the circuit, and a waveform generator (Keysight 3360A) to produce square waves that trigger the relay at a set frequency. In addition to that, to measure the voltage and current response of the battery, two Digit Multi-meters (Keysight 34465A 6 1/2) are used, one connected in series with the battery to measure the current and the other connected in parallel across the battery to measure the voltage.

Both batteries are discharged at a C/2 rate; therefore, to capture the dynamics of the batteries, the lithium-ion is pulsed at 1.5 A, whereas the Nickel Metal Hydride is pulsed at 1.25 A regulated by the discharger. To produce the square-wave profile of the current, the waveform generator triggers the relay at a constant frequency of 2.8 mHz with a 50% duty cycle. Furthermore, the sampling rate of the multi-meters was set to 0.4 Sa/s and data acquisition readings were logged using the BenchVue software from Keysight. Fig. 7 displays the experimental test rig and instrumentation used. The experimental setup was similar to that used in [13].

In addition, two independent datasets developed by [24]– [25] for a Samsung INR18650-20R battery were utilized. Shown in Table 2 are the parameters of the battery tested [31]. The first dataset was an incremental current OCV test, where the battery was pulsed at a constant current at 25°C. The current load profile allowed the battery to rest until the relaxation period reached steady state; therefore, the OCV-SOC relationship was established. This dataset was used to tuned and optimize the modal parameters to fit the output system response, \( V_{out} \), to the measured terminal voltage. The second dataset was a low current OCV test at which the battery was discharged at a constant C/20 rate at 25°C to estimate that the terminal voltage corresponded to OCV. This dataset was used to validate the modal parameters tuned to the incremental current OCV test from the first dataset.

TABLE 2. CALCE Battery parameters.

| Parameter               | INR 18650-20R |
|-------------------------|---------------|
| Chemical system         | LiNiMnCo /Graphite |
| Form factor             | Cylindrical   |
| Nominal capacity (mAh)  | 2000          |
| Nominal voltage (V)     | 3.6           |
| Cut-Off voltage (V)     | 2.5           |
| Dimensions (mm)         | 18.33Ø × 64.85 |
| Mass (g)                | 45            |
| Operating Temperature (°C) | 0 to 50            |
| Storage Temperature (°C) | -30 to 60       |

The next section discusses the experimental results, the proposed model’s ability to match the measured terminal voltage and predict the mass transfer and boundary-layer effects, and the OCV of the batteries tested.

V. RESULTS & DISCUSSION

This section presents the experimental measurements and the results of the proposed model to match the terminal voltage of three different electrochemical cells. In addition, the effects due to the mass transfer and the double-layer were predicted by the model and displayed, along with the OCV estimation of the batteries. Lastly, the model was validated through a low-current OCV test for the INR 18650-20R battery. The parameters of the proposed modal battery model were numerically tuned for both lithium-ion cells and the nickel metal hydride battery. The parameters of the modal decomposed
battery model are listed in Table 3. As shown in the table, the parameters were tuned as a function of the SOC. The SOC was computed through (3) with the measured current and the capacity of each battery known. To improve the fitment of the simulation results, the parameters were optimized by employing the method of nonlinear least squares via the Trust-Region-Reflective algorithm. Each parameter was tuned as a lookup table in terms of the SOC as 20 discrete values from 0.05 to 1. This was accomplished using the parameter estimation toolbox in MATLAB Simulink.

**TABLE 3. Modal battery parameters.**

| Symbol       | Description                  | Units  |
|--------------|------------------------------|--------|
| $c_{OCV}$(SOC) | Rigid body mode damper       | rad/s  |
| $\omega_{MT}$(SOC) | Mass transfer natural frequency | rad/s  |
| $\omega_{DL}$(SOC) | Double layer natural frequency | rad/s  |
| $\zeta_{MT}$(SOC) | Mass transfer damping ratio  | -      |
| $\zeta_{DL}$(SOC) | Double layer damping ratio   | -      |
| $b_{OCV}$(SOC)  | Rigid body mode input gain   | rad/Ns² |
| $b_{MT}$(SOC)   | Mass transfer input gain     | rad/Ns² |
| $b_{DL}$(SOC)   | Double layer input gain      | rad/Ns² |

To tune the parameters accurately and obtain a model that represents the physical dynamics of the battery, the natural frequency values were limited to the maximum and minimum values according to the angular frequency values typically observed in electrochemical cells, as reported in the literature. Table 4 shows the angular frequency values obtained experimentally via the electrochemical impedance method for batteries [32].

The damping ratios were constrained to be greater than unity because all the transient behaviors were observed to be overdamped. In addition to that, the modal input gains were allowed to take any positive value. However, the initial $C_{OCV}$ range was not known; it was found by iterating that an upper bound is required to achieve the optimizer convergence. The optimized and tuned parameters of the model for all three batteries can be referred to in the Appendix.

**TABLE 4. Typical Angular frequency values for a battery cell.**

| Parameter | Effect               | Range (rad/s) |
|-----------|----------------------|---------------|
| $\omega_{LM}$ | Electric & Magnetic | $10^5 \cdot 6.3 \times 10^6$ |
| $\omega_{DL}$  | Double layer         | $0.1 \cdot 10000$ |
| $\omega_{MT}$  | Mass transfer        | $0.09 \times 10^7 \cdot 12.5$ |
| $\omega_{SOC}$ | Cycling, SOC        | $4 \times 10^6 \cdot 7 \times 10^4$ |
| $\omega_{RE}$  | Reversible           | $2 \times 10^7 \cdot 3 \times 10^6$ |
| $\omega_{AE}$  | Aging                | $6.2 \times 10^8 \cdot 2 \times 10^6$ |

Future developments of the proposed model can lead to frequency effects due to cycling, reversibility, and aging effects being considered, for instance, a higher-order model with a higher degree of freedom. The timeline for these dynamic effects to impact the voltage response and the battery has to be cycled from hours to years; therefore, they were not considered in this study.

**A. ENERGIZER ULTIMATE LITHIUM BATTERY**

Fig. 8 displays the current measured experimental through the battery.

**FIGURE 8. Energizer ultimate lithium measured current.**

As can be seen from the Fig. 8, the current increases from 0 A when the relay is open to the target C/2 discharge rate when the relay is triggered by the waveform generator. This load profile causes a transient output voltage, which reveals the battery dynamics. Using the current data from Fig. 8, the SOC of the battery was calculated using (3) and is presented in Fig. 9.

**FIGURE 9. Energizer ultimate lithium computed SOC.**

The SOC of the battery began at 100% and decreased with each current pulse. The battery is almost fully discharged; therefore, the modal parameters can be optimized for nearly the entire discharge period. From the computed SOC, the modal parameters were then tuned as a function of SOC. Once the parameters have been optimized, the system was then simulated using the experimental current draw as the input. Shown in Fig. 10 is the predicted terminal voltage as a function of time compared to the measure voltage experimentally.

With each current pulse, the voltage drops primarily due to the mass transfer and double-layer modes, and when the
current load is removed, most of the voltage is recovered from the vibration of these modes. However, a small portion of the voltage is permanently lost owing to the zero-hertz mode.

The simulated response was able to fit onto the measured terminal voltage with a 4.84% standard deviation error.

To further elaborate on how the simulated results were fitted to the experimental voltage and predict the nonlinear dynamics of the battery, Fig. 11 is illustrated. Subplot 11 (a) shows a rescaled plot of the current pulses, specifically, the current pulses that occurred at the time interval of $6000 \leq t \leq 7000$. Furthermore, subplot 11 (b) displays the displacement signals $r_{\text{MT}}$ and $r_{\text{DL}}$, which correspond to the mass transfer and double-layer effects, respectively. As expected, the higher natural frequency mode, which corresponds to the double-layer effect, dominates the instantaneous drop and recovery periods in the battery voltage. This effect is caused by the charge layer formed between the electrode and electrolyte, which resembles the behavior of a capacitor [32]. Moreover, the lower-frequency mode, which is designated by mass transfer effects, dominates the transient period of the voltage response. This is due to the transport of ions as a consequence of diffusion, which is caused by the gradient in the concentration and migration caused by the forces of the electric field [32]. Additionally, subplot 11 (c) illustrates the details of the corresponding experimental and simulated responses on a scale apt to observe the dynamics of the mass transfer and double-layer modes decoupled.

Moreover, Fig. 12 presents the OCV predicted by the quasi-static component of the experimental data and the modal signal $V_{\text{OCV}}$. The experimentally based OCV was determined by taking the voltage value at the top of each relaxation period peak relative to the SOC.

This neglects any minor remaining transient to steady state due to the frequency and duty cycle that generated the current load. In contrast, the simulation-based OCV is obtained directly from the internal model signal $V_{\text{OCV}}$ and compared to the calculated SOC for every simulated time step. In general, good agreement is found, indicating that the modal representation may be useful as an OCV estimator.

**B. DURACELL NICKEL METAL HYDRIDE BATTERY**

Shown in Fig. 13 is the current measured experimental through the battery.
Similarly, the current increases from 0 A to the designated C/2 discharge rate current when the relay is triggered at the set frequency. From the current load, the SOC was computed and is displayed in Fig 14.

Initially the battery was fully charged and was discharged to almost 15%; therefore, the modal parameters were tuned relative to SOC in that range only. Fig 15 shows the measured terminal voltage and the simulated system response of the modally decoupled coordinates corresponding to the current load shown in Fig 13. The proposed model response was capable of matching the experimentally measured terminal voltage of the battery with a 0.82% standard deviation error. The behavior of the Energizer ultimate lithium and the Duracell nickel metal hydrides was qualitatively similar. In general, the Energizer ultimate lithium is better able to maintain its voltage as it is discharged to near-zero SOC.

Fig. 16 demonstrates the rescaled plots of the output modal displacement signals of the cell for the current load that occurred at 6000s ≤ t ≤ 7000s.

The current pulses that occurred at that time interval are displayed in Fig. 16 (a). Moreover, analogous to the Energizer ultimate lithium cell and in agreement with literature, the mass transfer effects dominated the transient response at low frequencies whereas the double-layer effects caused the instantaneous drop in the voltage response at higher frequencies. The mass transfer and boundary-layer output signals are shown in Fig 16 (b). Furthermore, the rescaled measured terminal voltage in contrast to the simulated system response is displayed in Fig 16 (c).
Fig. 17 displays the OCV estimated by the modal signal \( V_{OCV} \), relative to the voltage measured experimentally at the peaks of the relaxation period.

As shown in the figure, the proposed model estimated the OCV of the battery within high level of accuracy, therefore, the model can be utilized to estimate the OCV of a battery. Furthermore, additional validation of the model is required, and the following subsection presents the data developed by [23], [24].

**C. SAMSUNG INR 18650-20R BATTERY**

This section presents the data obtained from the CALCE battery research team [23]. The datasets were used to compare the results obtained by Zhang et al. [24] to the proposed model’s simulated response. As mentioned, two datasets were utilized. The first dataset was used to estimate and identify the modal parameters and the second dataset was used to validate the identified parameters. Fig. 18 displays the current load at which the battery was discharged at for the incremental current OCV test.

The battery was pulsed with 1 A for 12 minutes and allowed to recover for 2 hours to reach steady state. With the SOC computed through (3) and the current load utilized as the input force to the system, the modal parameters were tuned and optimized to fit the measured terminal voltage obtained experimentally. Fig. 19 (a) displays the simulated model system response in contrast to the measured terminal voltage for the overall discharge period. Fig. 19 (b) displays a rescaled plot for the pulses that occurred during the time interval of \( 20000s \leq t \leq 50000s \). Additionally, Fig 19 (c) illustrates the double-layer and mass transfer effects predicted by the model.

As displayed in the figures, the system response of the proposed model had the capability to match the measured terminal voltage with a 1.03% standard deviation error, which indicates the high level of precision of the model.
Moreover, to validate the tuned parameters, the low current OCV test was utilized. The primary goal of the low current OCV test was to validate that the OCV of the battery corresponded to the measure terminal voltage. Fig. 20 demonstrates the current load of the low current OCV test. The battery was discharged at 0.1 A.

![FIGURE 20. Low current OCV test current load.](image)

FIGURE 20. Low current OCV test current load.

Fig. 21 displays the OCV estimated by the proposed model in contrast to the measure terminal voltage of the battery.

![FIGURE 21. Low current OCV test experimental voltage & simulated response.](image)

FIGURE 21. Low current OCV test experimental voltage & simulated response.

The simulated response of the model and the measured terminal voltage fit with a 0.26% standard deviation error; therefore, it can be deemed appropriate to validate the optimized parameters from the incremental current OCV test. In addition, shown in Fig. 22 are the OCV estimations by the proposed model for the incremental and low current OCV tests.

![FIGURE 22. OCV estimation for the low and incremental current OCV tests.](image)

FIGURE 22. OCV estimation for the low and incremental current OCV tests.

The OCV predicted by the proposed model for both current profiles are in perfect agreement. Additionally, the OCV predicted by the model is in close agreement with that reported by Zhang et al. [24], which used the equivalent circuit model.

**VI. CONCLUSION**

The study conducted in this paper proposed a novel mechanical analog to predict the nonlinear behavior of a battery in modal coordinates. The dynamics of the battery were predicted utilizing a three-degree-of-freedom, 6th order spring-mass-damper system. The system was then decomposed into modal representation and considered as three independent single-degree-of-freedom modes to account for the discharge, mass transfer, and double-layer effects induced in the battery. The model parameters were tuned and optimized relative to the SOC to fit the response of the system to the experimental voltage measurements using a nonlinear least-squares method through the Trust-Region-Reflective algorithm. Consequently, the model successfully predicted the overall discharge of the batteries and matched the dynamic behavior of the voltage response with a 4.83% standard deviation error owing to the pulsed current load. The tuned parameters were validated utilizing an independent dataset with a different load profile and matched the terminal measured voltage within 0.26% standard deviation error. Furthermore, the double-layer and mass transfer effects on the battery were simulated and presented. Finally, the open-circuit voltage was projected and validated using quasi-static data.

The use of electrochemical cells, especially lithium-ion batteries, has increased significantly over the last decade. As engineers, it is critical to enhance the power and energy that can be delivered by a battery; therefore, the proposed model is useful for predicting the quasi-static voltage in a dynamic setting.

A typical battery cell exhibits various dynamic effects with respect to time. Only the effects of the discharge, double layer, and mass transport were considered in this study. However, the potential of a higher-order and degree-of-freedom spring-mass-damper system in modal representation is valid for enhancing the dynamic prediction of the model and accounting for cycling and the overall runtime of the battery. Furthermore, the dynamics of charging a battery cell can also be predicted by the proposed model by analogously changing the direction of the input force. In addition, for higher-capacity cells that are discharged at high rates, the parameters can be tuned as two-dimensional lookup tables, relative to the state of charge and temperature change.
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