Palestine Journal of Mathematics

Vol 14 (Special Issue IV), (2025) , 78–86

MATHEMATICAL MODEL DEVELOPMENT OF CELL VOLTAGE OF A LI-ION CELL FOR EFFICIENT ELECTRIC MOBILITY APPLICATIONS.

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MSC 2010 Classifications: Primary 33E30

Keywords and phrases: Lithium-ion cell; cell voltage; mathematical model; equivalent circuit model; applied mathematics

The authors are very thankful for the guidance and support by the Center for Automotive Research and Tribology, IIT Delhi, for the work done under the Summer Faculty Research Fellow Program from 14th May-12th July 2024.

Abstract As the world demand for energy is now focused on sustainable energy sources, lithium-ion (Li-ion) cells have been increasingly adopted, particularly for electric vehicle applications. From a technical performance point of view, assessing and predicting various operating parameters and internal states of the cell are crucial in assessing the safety and reliability of electric vehicles. Among the various cell models developed for this purpose, mathematics-based empirical equivalent circuit models (ECMs) have gained practical acceptance because of their inherent properties of ease of model parameter identification and moderate model fidelity. In this paper, we discuss the role of applied mathematics in the field of battery design in electric mobility, the mathematical modelling process of cell voltage in various order equivalent circuit-based models for electric vehicle applications with the principal theorem on which the modelling is based, the mathematical description of various processes in the cell, governing equations, assumptions, limitations applied and the ability of the developed model to reproduce the observed cell voltage.

1 Introduction

Applied mathematics has a significant purpose in the development and sustainability of any technology. It helps to comprehend the characteristics, design, redesign, optimize and predict new system aspects. This paper explores the applications of applied mathematics in the promising field of energy storage technology. Among the various energy storage devices, batteries are utilized extensively for a variety of applications, ranging from small portable electronic devices to very high-power electric trucks. Currently, Li-ion battery technology is widely accepted and utilized because of its improved charge and power capability, cycle life, cost, operating temperature, size and superior safety. To ensure consistent design and performance improvement in any technology, understanding its working process, internal parameters and operating conditions is necessary. In Li-ion battery technology, for efficient design and performance optimization and for comprehending the influencing factors in the battery system, the internal electrochemical process, battery structure, temperature of the field and application requirements play vital roles. Research-oriented experimental methodologies adopted for this purpose have become challenging because of the numerous various controlling factors based on the location, temperature, power capacity, chemistry and parameters of the cell used. The overbearing complexity of battery systems and the rapid development of computer-based numerical simulation and data interpretation techniques have triggered the establishment of various cell models to maximize the performance analysis of cells. Specifically, an appropriate cell model is fundamental for estimating and predicting basic cell parameters such as the state of charge, cell voltage, run time, capacity fade, and life cycle and developing optimization strategies. [1, 2] For this purpose, the choice of the cell model varies, regardless of the design or thermal or mechanical analysis of the battery system to be performed. Table 1 classifies different cell models adopted based on their application, nature and type of data fed for analysis [3].

The key novelty of this paper lies in developing a validated, low complexity and high-fidelity ECM model tailored for real-time applications in electric mobility. Unlike conversational theoretical overviews, this study presents a structured modelling approach backed by real cell parameter data, enabling accurate voltage prediction in electric vehicles. Moreover, by systematically comparing ECM variants demonstrating practical implications for model-based design in battery systems. The paper also adds unique value to applied mathematical modelling in energy storage. This paper is organized as follows. Section II will investigate the role of mathematics in various battery models. Section III explains the modelling approach of the mathematically based equivalent circuit model (ECM) for electric mobility applications. The development of an ECM model and its validation in depicting the battery behaviour and conclusions are included in sections IV and V.

Table 1. Classification of Battery Models

Model Name	**Nature**	**Data Type**	**Purpose**
1. Electrochemical	Electrochemical	Physical, Semi-empirical	Cell Design
1. Peukert's model 2. Akhmetov and Vrudhula 3. State space	Analytical	Empirical and semi-empirical	Prediction
1. Simple R_{int} 2. RC 3. Thevenin model 4. PNGV 5. Impedance	Electrical	Semi-empirical	SoC estimation, Real-time control
1. ECM thermal	Thermal	Physical and semi-empirical	Real-time control
1. AI/ML based	Abstract	Empirical	SoC, SoH estimation
1. Electrothermal 2. Thermo-electrochemical 3. Thermo-mechanical	Combined	Physical and semi-empirical	Real-time control

2 Role of applied mathematics in the field of battery modelling in electric mobility

Every battery model used in the design and performance assessment essentially makes use of mathematical expressions depending on model parameters for describing the electrochemical process and estimation of characteristic parameters. An accurate description of each microscopic aspect of a chemical reaction occurring within a cell is very complex and immensely time consuming. Hence, researchers have focused on the extraction of key factors of cell behaviour, such as the open circuit voltage (OCV), capacity fade, cycle life, and effects of temperature on aging, from models [4] in the form of mathematical relationships that are estimated based on accessible cell parameters. Electrochemical models are the most accurate and detailed. The complete model is defined primarily by numerous coupled partial differential equations with specific boundary conditions [5]. Solving these interdependent partial differential equations, together with rigorous knowledge of the chemical structure, composition, conductivity, and volume fractions and extraction of various thermodynamic and kinetic data of the cell, is very complicated, tedious and costly. Analytical models are simplified electrochemical models. They derived reduced-order partial differential equations with additional assumptions [6]. They are also sufficiently accurate yet incapable of representing dynamic characteristics in combined design with other systems and are complex. A balance between complexity, computation time and ease of interpretation determines the usefulness of a model. Thermal equivalent circuit models (TECMs) are preferred over other models because they are computationally efficient and accurate. They engage resistors and capacitors, which makes them simpler at representing cell characteristics with simpler mathematical exponential functions and heat generation [7]. Enhanced accuracy is traded off with increased computational time because of the large number of capacitors in the model. Abstract models have been developed and established based on machine learning (ML) and artificial intelligence (AI) algorithms, which are highly data driven. Thorough knowledge of statistical methodologies such as nonlinear regressions has been extensively applied for training datasets of cells [8]. Even though it is highly sensitive to nonlinear environments, accuracy is still easily influenced by training datasets and training methods. Combined models stand out because they can describe variables of different natures. Thermoelectric models are widely accepted in electric mobility studies [9]. Even though accurate, cost and complex circuitry and mathematical relationships between parameters make this approach challenging. Electric circuit models employ equivalent electric circuits and are hence named the equivalent circuit model (ECM). Equivalent electric circuits are simplified circuits comprising voltage/current sources, resistors and capacitors based on Thevenin's circuit theorem [10]. They described the cell characteristics via simple mathematical state space expressions, including charging and discharging phenomena of capacitors. The approach balances the aspects of simplicity, parameter extraction pace, implementation ease and cost efficiently. A higher-order ECM can explain nonlinear cell behaviours, culminating in reliable parameter predictions. This makes mathematically based ECM the predominantly preferred cell modelling approach for electric mobility applications.

3 ECM models and modelling approach for calculating the cell voltage

In the ECM approach, a circuit network representing a cell is formed via simple circuit components. An attempt to model the variation in the terminal voltage of a cell based on the internal resistance offered by various internal phenomena and the amount of charge stored or state of charge is performed via mathematical state space expressions. To ensure circuit intricateness, various ECMs applied for the application of electric mobility are described.

3.1 Ideal Model

A single lone constant voltage source constitutes the ideal model unaffected by any internal parameter contrary to the practical output of all the cells. It assumes that the variations in the load and SOC are constant or do not impact the cell output voltage until the cell is completely discharged [3]. The model is improved by a linear model consisting of instantaneous voltage variations.

3.2 Internal Resistance Model

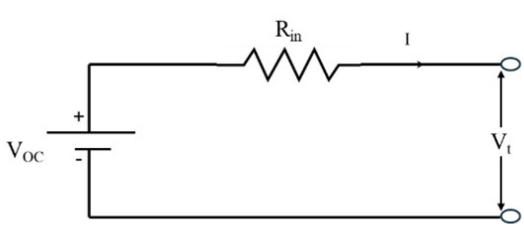

Figure 1. Internal resistance model

Figure 1 represents the internal resistance R_{in} or linear model composed of an internal resistance that simulates the internal mechanisms with an ideal voltage source V_{oc} [11]. The internal resistance simulates the voltage drop or energy loss due to heat from internal reactions. When the load is connected, the terminal voltage V_T is modeled as:

$$V_T = V_{\text{oc}} - R_{\text{in}} I \tag{3.1}$$

The modelled simple mathematical circuit expression as per Kirchhoff's law calculates the instantaneous voltage drop based on Ohm's law, which is attributed to the electrolyte concentration. This model is incapable of simulating dynamic characteristics. The different instantaneous drops are practically observed while charging and discharging process is simulated with a more accurate model [12], as shown in Figure 2.

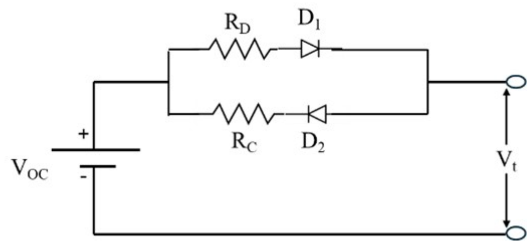

Figure 2. Internal resistance modeled for charging and discharging

$$V_T = V_{\text{oc}} + R_{\text{c}} I \qquad \text{during charging} \tag{3.2}$$

$$V_T = V_{\text{oc}} - R_{\text{d}} I \qquad \text{during discharging} \tag{3.3}$$

Even with enhanced accuracy, dynamic internal changes are not simulated.

3.3 Voltage Source-Based Model

The model circuit is shown in Figure 3. Various internal phenomena are simulated as different

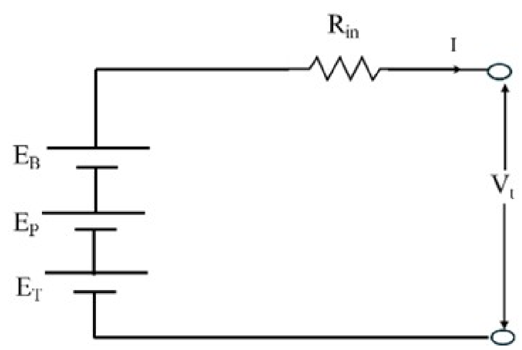

Figure 3. Model with various voltage sources

voltage sources in the model [12]. The terminal voltage is a simple mathematical expression modelled on the basis of Kirchhoff's law as

$$V_T = E_B + E_P + E_T - R_{\text{in}} I \tag{3.4}$$

where E_B, E_P, and E_T are internal, polarization and temperature effect-based voltage sources, respectively. The decoupled consideration of voltage sources limits its scope.

3.4 Resistance–Capacitance (RC) Model

The model shown in Figure 4 consists of capacitor C_B and C_P with series resistances R_B and R_P, which describe the stored charge capacity, polarization effect, termination resistance and

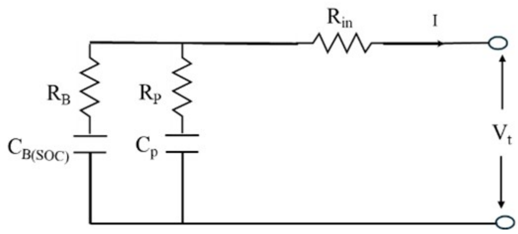

Figure 4. RC model

surface capacitive resistance, respectively [13]. C_B takes a larger value than C_P does. The modelled circuit expressions based on Kirchhoff's law are as follows.

$$\frac{dV_B}{dt} = -\frac{V_B}{(R_B + R_P)C_B} + \frac{V_P}{(R_B + R_P)C_B} - \frac{R_P I}{(R_B + R_P)C_B} \tag{3.5}$$

$$\frac{dV_P}{dt} = \frac{V_B}{(R_B + R_P)C_B} - \frac{V_P}{(R_B + R_P)C_B} - \frac{R_B I}{(R_B + R_P)C_B} \tag{3.6}$$

$$V_T = \frac{R_P}{R_B + R_P} V_B + \frac{R_P}{R_B + R_P} V_P - R_{\text{in}} I - \frac{R_B R_P}{R_B + R_P} I \tag{3.7}$$

The RC model is adopted in Li-ion cell simulations in the automotive sector.

3.5 Thevenin Model

The model based on Thevenin's equivalent circuit is the most accepted model among all the ECMs. The model consists of an ideal voltage source V_{oc} in series with internal resistance R_{in} and an RC parallel loop [14]. The instantaneous and the polarization voltage drops are perfectly simulated by R_{in} and the parallel loops of R_1 and C_1. The number of RC loops determines the order and accuracy of the model trading off with complexity, for simulating the terminal voltage, which completely follows the cell charging and discharging profile voltage according to its chemistry. The first-order Thevenin model is shown in Figure 5.

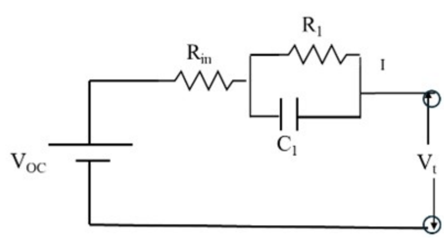

Figure 5. First-order Thevenin equivalent circuit model (1RC)

The equation for the first-order ECM in discrete form [15] for simulation model construction and calculation is as follows.
The mathematical exponential function in the expressions considers the charging and discharging aspects in the voltage profile.

$$V_T(k) = V_{\text{oc(soc,k)}} - R_0 I_k - V_{OCT,k} \tag{3.8}$$

$$V_{\text{OTC},k+1} = V_{\text{OTC},k}\, e^{\frac{-T_s}{\tau_{\text{OTC}}}} + R_{\text{OTC}} \left[1 - e^{\frac{-T_s}{\tau_{\text{OTC}}}}\right] I_k \tag{3.9}$$

where V_T is the cell terminal voltage, I is the cell current, V_{oc} is the cell open circuit voltage, R_o is the internal ohmic resistance, and τ OTC $= R_1 C_1$ is the time constant of the one-time constant (OTC) or 1RC network.

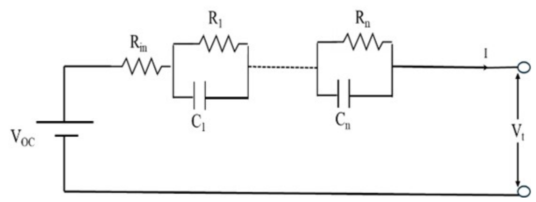

Figure 6. nth-order Thevenin equivalent circuit model

A first-order model, particularly for NMC Li-ion cell chemistry, serves the purpose of a robust simulation model for two- and three-wheeler mobility applications. A second-order model, which is also known as the dual polarization (DP) model, compensates for and efficiently simulates the static and all dynamic characteristics of a cell for high-power automotive applications [16, 17]. The nth-order Thevenin model circuit is shown in Figure 6 for understanding. An order above 2 increases the computation time, implementation complexity and cost, which is not justified against the requirement.

3.6 PNGV Model

A partnership for a new generation of vehicles (PNGV) model proposed as a part of cooperative research work between the U.S. government, Daimler Chrysler, Ford and General Motors, as shown in Figure 7, is an addition of a series capacitance C_0 to the Thevenin model [16]. The terminal voltage is modelled as follows:

$$V_T = V_{OC} - IR_{\text{in}} - V_{C_o} - V_{C_1} \tag{3.9}$$

$$\dot{V}_{C_0} = \frac{1}{C_0} I \tag{3.10}$$

$$\dot{V}_{C_1} = -\frac{1}{R_1 C_1} V_{C_1} + \frac{1}{C_1} I \tag{3.11}$$

Unexpectedly, the bulk capacitance caused errors in the model output.

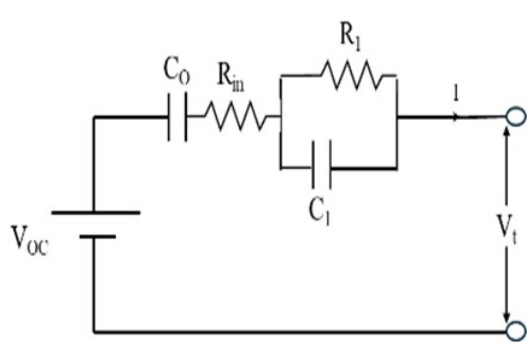

Figure 7. PNGV model

3.7 General Nonlinear (GNL) Model

An improvement in the PNGV model with separate loops for ohmic, concentration and electrochemical polarization and accommodating cell self-discharge culminated in the general nonlinear (GNL) model shown in Figure 8. The model is very accurate yet highly complex, with many parameters.

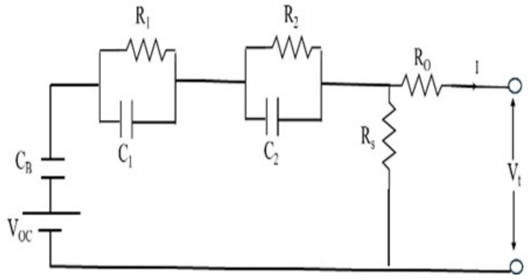

Figure 8. GNL model

4 Development of the First-Order Thevenin ECM Model and Validation Results

Various characterization tests are performed on the cells for extraction of parameters that are beyond the scope of this paper. An incremental open circuit voltage (IOCV) test is performed [18] on a sample cell 18650 and a LiNiMnCoO2/graphite lithium-ion cell with a nominal voltage and capacity of 3.6 V and 2 Ah [19], respectively. In this study, values ranging from 20 to 80% of the SOC bracket is employed for model validation, as they have a stable and linear relationship with the SOC, which indirectly leads to a better voltage following model, as shown in the validation results. The results are given in Table 2. Figure 9 displays the validation results. The parameters are then utilized in the first-order ECM to estimate the voltage in the DST cycle [20, 21] at various SOCs.

Table 2. Parameters derived for NMC cell at 25°C

SL No	R_{in} (Ω)	R_1 (Ω)	C_1 (F)	SOC
1	0.1037	0.0049	232.0458	0.9
2	0.1035	0.0067	155.1410	0.8
3	0.1033	0.0107	110.4553	0.7
4	0.1029	0.0109	289.0098	0.6
5	0.1027	0.0058	258.9568	0.5
6	0.1032	0.0061	230.4790	0.4
7	0.1037	0.0083	191.9090	0.3
8	0.1053	0.0092	209.5871	0.2

Root mean square errors as low as 32 mV and 40 mV are achieved with the DST profile at 25°C, which indicates good model performance by the first-order ECM of the NMC Li-ion cell for electric mobility applications.

5 Conclusion remarks

This paper focuses on the role of applied mathematics in Li-ion cell modelling for vehicular applications. Various modelling approaches are summarized by analysing their strengths and limitations. The application of mathematical-based Li-ion models, with an emphasis on equivalent circuit models (ECMs), in modelling the cell voltage is investigated along with the analytical descriptions of the charge discharge process. The development and validation of a first-order equivalent circuit model for an NMC chemistry Li-ion cell are illustrated. The study reveals that the first- and second-order Thevenin's equivalent circuit models exhibit robust convergence between the simulated and experimental cell voltages with acceptable error levels. The accuracy, computational time, ease of implementation in the battery management system environ-

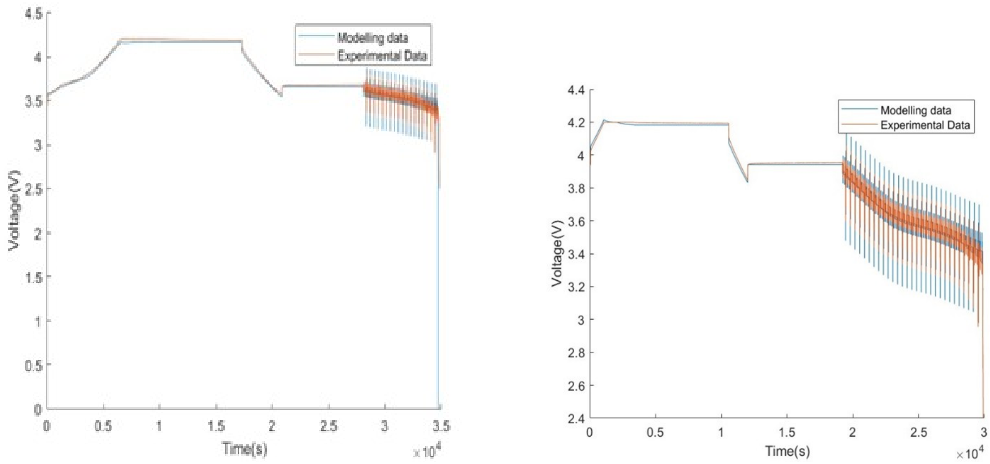

Figure 9. Validation results from the NMC cell using 1 RC model at (a) 25°C and 0.5 SOC and (b) 25°C and 0.8 SOC

ment, economic concerns, output error level, and acceptable complexity in mathematical modelling make Thevenin's model a universally accepted and preferred model for electric mobility cell/battery pack design and performance analysis.
The key contribution of this paper includes the integration of mathematical state space modelling techniques and validation with open source NMC battery data that ensures accurate simulation of charge discharge cycles at various SOC levels. This paper also provides a comparative understanding of various ECMs with quantitative simulation details. This enhances modern selection strategy in the battery management system.

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