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Modeling and Simulation of a Commercial Lithium-Ion Battery with Charge Cycle Predictions

Mónica Camas-Náfate [1], Alberto Coronado-Mendoza [1,*], Carlos Jesahel Vega-Gómez [1] and Francisco Espinosa-Moreno [2]

[1] Centro Universitario de Tonalá, Universidad de Guadalajara, Avenida Nuevo Periférico 555, Ejido San José Tatepozco, Tonalá 45425, Mexico
[2] Dirección de Investigación y Posgrado, Universidad Tecnológica de Tlaxcala, Carretera a El Carmen, Xalpatlahuaya, Huamantla 90500, Mexico
* Correspondence: alberto.coronado@cutonala.udg.mx; Tel.: +52-33-20-00-23-00 (ext. 64113)

Abstract: The analysis of the behavior of lithium-ion batteries has gained considerable interest in recent years. There are different alternatives for the analysis of this behavior; however, depending on the type of modeling, there are application and optimization restrictions. In this work, a hybrid model has been made that is capable of predicting the characteristics of a lithium-ion battery. As a novelty, the simplification, at the same time, facilitates the sampling of parameters for their prompt selection for optimization. A new model open to the user is proposed, which has proven to be efficient in simulation time. For example, one hour simulates it in 5 min, providing information detailing how these parameters, State of Health (SOH), Open Circuit Voltage (VOC), State of charge (SOC), and Number of charge and discharge cycles, in the face of temperature variations and charge and discharge cycles. Opening the possibility of optimizing the parameters with different techniques to estimate the performance and dynamics in the face of temperature change and charge and discharge cycles. A model based on linear regressions, manufacturer characteristics, and integrating equations in the electrical model of electrochemical phenomena is proposed.

Keywords: modeling; simulation; batteries; hybrid model

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1. Introduction

The battery is one of the main methods of energy storage, whose applications include renewable energy backup [1–5], applications in portable electronic devices [6], as well as electric and hybrid vehicles [7–10]. The lifetime of the batteries and the degradation process are areas of interest due to their application in commercial vehicles. However, having a reliable and durable battery system remains a big challenge [11]. Lithium-ion batteries (LiBs) stand out among the various battery technologies because they have no memory effect, show low self-discharge when not in operation, and exhibit good energy and power density [12–14], being the best option for electric vehicles (EVs), whose development depends on cycle performance, cost and battery safety [15].

A battery is made up of an anode, cathode, separator, electrolyte, and two current collectors (positive and negative). The anode and cathode store the lithium. The electrolyte carries positively charged lithium ions from the anode to the cathode and vice versa through the separator. The movement of the lithium ions creates free electrons in the anode, which creates a charge at the positive current collector. The electrical current then flows from the current collector through a device being powered (cell phone, computer, etc.) to the negative current collector. The separator blocks the flow of electrons inside the battery. It is necessary to know the electrochemical behavior of the electrolyte, together with the materials of the anode and cathode, to be able to carry out models that determine how the performance of the batteries is affected, optimization of parameters, and improvement in

the quality of the materials, for increased battery safety. Figure 1 shows the basic operating physical principle of a lithium-ion battery [1].

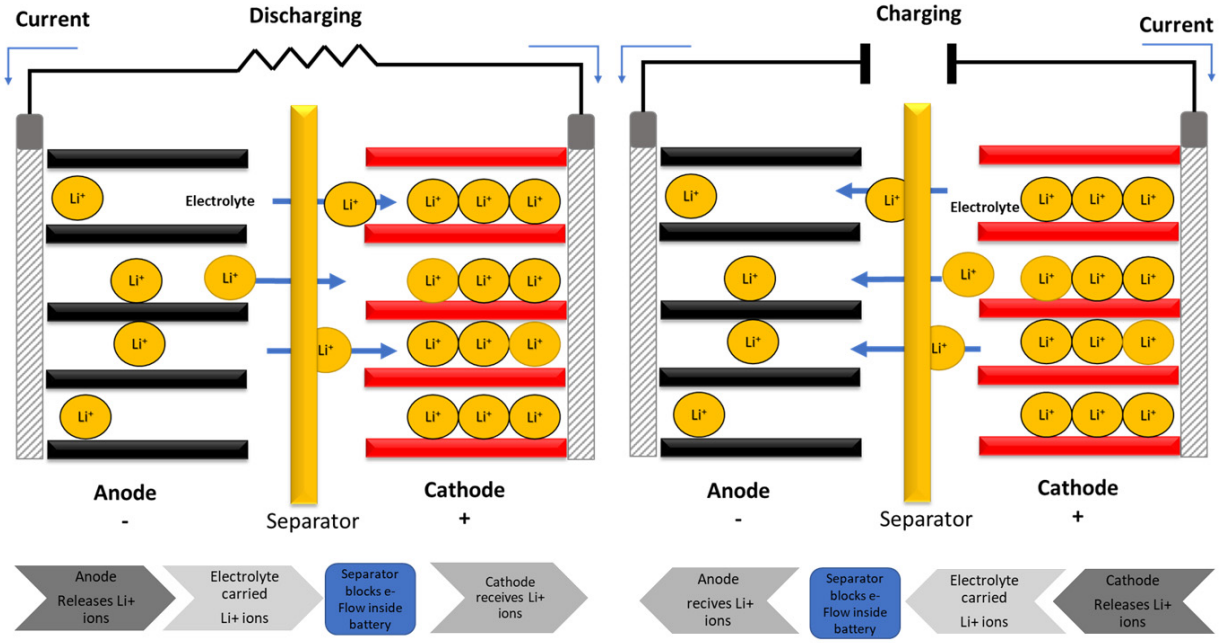


Figure 1. Basic operating physical principle of lithium−ion battery.

The degradation or aging of LiBs is quantified with the loss of capacity and the increase in internal resistance, characteristics of various parameters and conditions such as state of charge (SOC), state of health (SOH), depth of discharge (DoD), charge–discharge rate (C-rate) and the number of cycles (NCycles) [11,16,17]. These parameters can be monitored and optimized through a Battery Management System (BMS), whose main function is to ensure safe battery operation and behavior [18,19]. The prediction of the optimal operating parameters would allow knowing the remaining useful lifetime (RUL) of the batteries before replacing them, as well as overcoming range anxiety in EVs [15].

The investigation of the internal processes of batteries can be carried out through destructive experimental tests or life cycle tests [6]. However, reliable information can be obtained through electrochemical models, mathematical equations, and electrical circuits. [20]. In this work, hybrid modeling was presented to evaluate the electrochemical phenomenon and its sensitive parameters in a dynamic way.

It is possible to have a description of a robust and complex thermoelectrochemical modeling of its parameters and the behavior of the battery. This type of modeling is optimized through techniques such as the Dynamic Programming Technique since it occurs through multi-state simulation. This requires a high level of computation, and in addition to optimizing the battery from the point of view of its application, load management and even consumption habits with this model could not be performed [20,21].

The purpose of this model is the selection and simulation of parameters, an upcoming optimization by bio-inspired methods is carried out, showing us a prognosis of results comparable with previous experimentation, a simulation without optimizing, and the optimization carried out.

Model hybridization is an important process for battery modeling. By combining the advantages of one and minimizing the disadvantages of the other, it allows the modeling to be adapted according to the subsequent application.

One of the novelties to come from this work is the optimization of the model through optimization techniques, such as PSO and GA. This is due to the fact that the selection of the parameters and application of the use of the battery if the batteries are charging through renewable energies, adaptation to micro-grid systems, energy demand the same, and the

use of electric vehicles as part of a Smart grid, even economic office can be optimized using this basic model.

With optimization, as the second part of the research carried out, it is expected to reduce errors and improve the trend in terms of simulated behavior with what was presented in the experimental phase.

A new model open to the user is proposed, which has proven to be efficient in simulation time. For example, one hour simulates it in 5 min, providing information detailing how these parameters (SOH VOC SOC, Number of charge and discharge cycles) in the face of temperature variations and charge and discharge cycles.

2. Types of Battery Modelling

According to the application, battery models vary in complexity [22–25]. Battery models also depend on the environment and specific parameters to analyze. Some of the studied models for LiBs are equivalent circuit models (ECM) and physics-based models (PBM) [15].

Several electrochemical models study interactions between electrochemical and thermodynamic reactions to analyze battery aging.

To describe and analyze the behavior of a battery for electromobility purposes, Sheperd's model is one of the most widely used and well-known models. It consists of using voltage and current terms, which depend on the Peukert equation. This model is mainly for lead acid batteries, so for lithium batteries, it is necessary to change the model, but the definitions of certain parameters and phenomena that describe the behavior of the battery as an electrochemical energy storage system are preserved [19].

Battery capacity is expressed in ampere-hours (Ah) and indicates the amount of current a battery can provide over time. The rate at which the battery discharges is expressed as the C-rate. This indicates how many hours a battery with a given capacity will last. The battery capacity depends on the discharge rate, and it is inversely proportional; the higher the discharge rate, the smaller the capacity. As it is presented by [19], the relationship between fast and slow discharge can be calculated with Peukert's law and is expressed by the Peukert exponent. Some battery chemistries are more affected by this phenomenon than others.

The energy balance of the batteries allows to establish their thermal behavior, which allows establishing of the corresponding equations for the prediction of characteristics such as heat generation, cell temperature, and its relationship with respect to time, allowing us to find voltages and battery capacities. These theoretical voltages and also the capacity of the theoretical batteries (see Equation (1)) allow us to calculate the amount of energy delivered by the cell, and according to the weight or volume, they give us two parameters commonly used in the characterization of batteries: specific energy and energy density, respectively [20,21].

$$E_{teo} = Vbat_{teo} \times Cap_{bat} \quad (1)$$

where $Vbat_{teo}$ is the theoretical battery voltage, while Cap_{bat} the battery capacity.

It is necessary to include electrochemical parameters such as overload behavior, gas generation, internal temperature changes, and internal resistance. These last two parameters can be analyzed from another perspective through the use of other types of models [23].

2.1. Electrochemical Models

This type of models allows the experimental and analytical analysis of the redox processes taking place inside the cell. As these electrochemical phenomena are analyzed in greater depth, they become more complex to model. For instance, the temperature is determined by the output heat and cooling processes under different conditions. The temperature modeling combines phases of heat generation, energy balance, and surface distribution in the different sections of the battery in order to model and design the necessary conditions for its packaging and distribution, as well as for its treatment in the management, control, and optimization of batteries through Battery Management Systems [22–24]. The heat transfer process in a battery is normally unstable, varies with

time, and is determined by an internal heat source. It is necessary to establish the operating conditions as well as the technical limits of the batteries to determine the modeling of heat generation, which depends on the state of the battery and the entropy process of the cell. Authors report that the total heat transfer and the cell phase heat are relatively small, which allows an equivalence between the entropy and Joule heating. Assuming there is no heat exchange with the surroundings, the basic form of the battery heat capacity is given by Equation (2) [25,26].

$$q = I\left[(Vbat - VOC) + T\frac{\partial U_o}{\partial T}\right] \quad (2)$$

where q is the battery heat generation rate, I is battery current, $Vbat$ is measured voltage, VOC is open circuit voltage, T is cell temperature, and $\frac{\partial U_o}{\partial T}$ is the entropy heat coefficient. This behavior dynamic has allowed deeper analysis in the thermal modeling of batteries since the first models developed by Pals and Newman, where they carried out different tests and conditioning of thermal modeling for lithium polymer batteries [27]. Some electrochemical models with thermodynamic approaches use the experimental characterization of commercial cells to analyze the three-dimensional behavior of heat transfer and how it affects the battery, including its components, charge, and discharge [28].

One of the approaches for thermal modeling is to use analogies to electrical models [29,30]. This can be achieved by doing an equivalence between heat and current flow so that a change in current can be analyzed as a temperature change. In electrical terms, the temperature is analyzed by voltage, while thermal change resistance is represented by electrical resistance, and they can be converted into equivalent electrical parameters through the use of the battery material's thermodynamic properties.

The heat balance equation was proposed as part of the model to predict the temperature of the battery core and surface according to the law of electricity. The convection phenomenon between the battery surface and the surroundings was also considered [31].

In this paper, they make an extensive review of the methodologies and parameters for modeling batteries from a thermal point of view. This, in turn, allows batteries to be analyzed through the electrochemical phenomena that interact or cause heat, as well as their consequences. In addition to establishing certain operating ranges and the authors who "abuse" these parameters to study how this affects the battery, it is overexposed.

It is a necessary review to know the operating ranges and to see how situations in which these parameters change can be modeled, in addition to opening the door to the optimization of materials and prevention conditions to avoid damage to the batteries.

The same work reviews different battery modeling techniques for behavior prediction, the advantages and disadvantages of these, the most outstanding results, simulation times, and detection of parameters that determine future failures. They highlight the use of neural networks and the use of density-based spatial clustering (DBSCAN) of applications with noise in the increase in voltage thanks to the determination of long-term damage and the use of a thermal model in an equivalent circuit model that was previously found and parameters thanks to the use of electrochemical impedance spectroscopy [32].

2.2. Hybrid Models

They are characterized by their simplicity in elaboration since they facilitate understanding and analyze and open the possibility of optimization with lower computational cost. Electrical models respond to macroscopic stimuli and electrical responses in equal magnitudes. These parameters are useful for microscopic behavior characterization without experimental investigation.

Taking into account electrochemical parameters and transforming them into electrical models give guidelines to know the reaction within the battery, and help to establish relations between macroscopic and microscopic parameters such as current and voltage and electrolyte potential or electrodes current density, respectively. In addition to being able to predict the general behavior of the battery, materials, as well as other parameters, can be optimized using mathematical techniques by adding experimental analyses. Hybrid models

use arrangements of electrical components equivalent to electrochemical parameters to analyze what occurs on the battery bulk and surface [33–35].

This type of model uses a capacitor to represent the battery charge capacity and several resistances to symbolize voltage drops caused by electrochemical phenomena such as temperature variation or battery internal resistance associated with materials [23,36], while free software (Cantera) and its subsequent implementation in Matlab for a model of thermodynamics and kinetics is utilized through the use of a work scheme to insert electrochemical parameters. Traditionally, this modeling is conducted by means of the single-step equilibrium potential of the Butler–Volmer kinetics and mass-action kinetics; however, these authors use modeling based on molar thermodynamic data. This process gives way to greater flexibility and adapts physical phenomena for the intercalation of materials. An interesting contribution of these researchers is that they provide a practical guide in addition to an important bibliography for the selection of parameters. The required theoretical background was derived and discussed, and implementation details were given [37].

A Thévenin equivalent circuit allows mathematical modeling of phenomena and systems of different kinds, with data previously obtained through data synthesis or experimentation [23,33]. Using different charge/discharge profiles allows for to study of the interaction with the systems to be fed [33]. Electrochemical devices such as batteries and fuel cells share operating principles, and from an electrical approach, this leads to a model adaptation to the devices [38–40]. A basic battery equivalent circuit is shown in Figure 2, which includes a capacitor, a resistance, and a power supply as its main components.

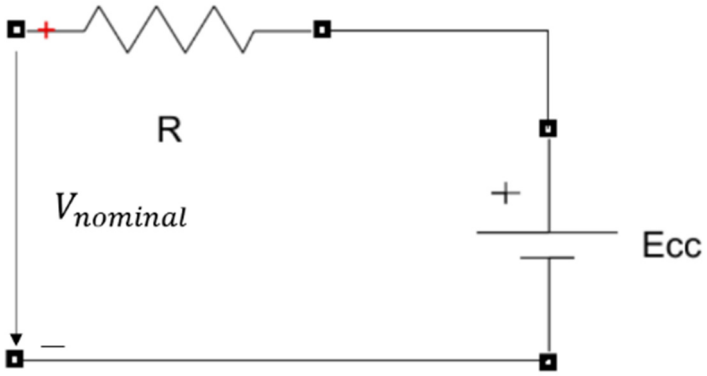


Figure 2. A linear model of a battery.

An electrical model feature combined with an electrochemical model is known as hybrid modeling. It assigns and determines conditions sensitive to dynamic changes, allowing the phenomenon to be analyzed in real time. The main difference between hybrid and electrochemical is that the latter involves high computing capacity during simulation, whilst hybrid models require less capacity by selecting which parameters can be part of an objective function, thus making an optimization feasible, leading to an error reduction existing in experimental methodology. Predicting upcoming results and comparing them with previous results to perform decision-making in processes in which the battery is part of an energy system, such as electric mobility.

2.3. Lithium-Ion Battery Models

For lithium batteries, current models do not present a correlation between charge and discharge cycles and the effect of temperature on it, which makes the analysis of battery life affected. The lithium-ion concept uses two materials that allow the reversible exchange of lithium ions. The anode is a thin layer of graphite in which lithium atoms have been inserted (LiC_6), while the cathode can be made of a transition metal lithium oxide such as $LiCoO_2$. A liquid electrolyte is usually a lithium hexafluorophosphate ($LiPF_6$) mixed with a carbonate solution. Lithium-ion polymer batteries have an electrolyte that is made of gelled polymer. Its energy density is higher than the other lithium-ion cell, but its monitoring and

balancing circuitry is more complex. The maximum cell voltage (more than 4 V) and also the minimum cell voltage (around 2.7 V) must be carefully monitored, and they exhibit high energy density and have a typical voltage of 3.7 V.

There are authors who point out the importance of seeking an improvement in terms of speed for the parameterization of battery characteristics, and this is of vital importance due to the growing battery manufacturing industry for the electricity market. Therefore, they used the accelerated model parameterization procedure (AMPP) technique and compared it with the galvanostatic intermittent titration technique (GITT), improving the speed by 90%. The selection of the parameters can be thanks to experimental methodologies that provide an extensive database, and it is necessary to develop a "filling" process that culminates in an ECM. Another characteristic pointed out in this work is the difference between the experimental techniques; the AMPP must have highly sophisticated equipment, while the GITT does not require certified equipment for use in laboratories only. The methodology is to establish a certain pulse, which generates heat, to then "rest" and resume the process while the process rests and is reactivated; there will be sensors monitoring the behavior that will help improve the modeling. The purpose of this parameterization is to contribute to accurate modeling, and with the probability of optimizing with the Matlab optimization toolbox, while for our work, it is sought that the model can be optimized by different simple techniques and by the most recent ones, which are not yet part of the aforementioned toolbox. Being an experimental technique, it must have several controls, such as humidity and temperature; these parameters are also taken into account for parameterization [41].

Other authors carry out an exhaustive analysis using test equipment, as well as with equivalent circuits. This behavior is designed and simulated with the intention of controlling it through IGBTs, since, according to these authors, this application has not been studied in depth, mainly its characteristic of being used as switches in optimization processes.

To analyze this phenomenon, they used long and short time periods to see the change in impedance, specifically using the HMPO method; this method is a multiple particle optimization method, which would mean great computational power, in addition to a detailed process. of optimization.

These authors handle high voltage ranges for their target (which would be the reason for using the HPSO method, in addition to specialized experimental equipment.) These authors still reduced simulation times due to the use of an equivalent circuit plus the support of an optimization model and selection of parameters.

The modification of the pulse frequency (pulse ripple charging) allows the acceptance of capacitances in the battery to be evaluated in different evaluation currents [42].

3. Proposed Model

One of the most used methodologies is charging at constant voltages and discharging at constant currents; thus, recommendations given by the manufacturers were taken into account [43,44].

In this case, two model validation methods were developed, changes in the C-Ratio (CASEA) and changes in temperature (CASEB).

3.1. Nomenclature and Definitions

C-rate: discharge current is often expressed as a C-rate to normalize against battery capacity, which is often very different between batteries. It is a measure of the rate at which a battery is discharged relative to its maximum capacity.

Input current: This parameter varies depending on the case of analysis; for CASEA, there is a pulse generator that allows us to evaluate the conditions of $\pm$1A load at standard temperature conditions, while for CASEB, it has a fixed current of 4.7142 A, maximum limit for this model recommended by the manufacturer.

SOC: State of charge. Defined as the ratio of battery capacity vs. maximum capacity, expressed as a percentage. It is typically calculated using current integration to determine the change in battery capacity over time.

VOC: Open circuit voltage. It is the voltage between the battery terminals with no load applied. The open circuit voltage depends on the state of charge of the battery and increases with the state of charge.

The source voltage and a tabulation of battery states of charge, provided by the manufacturer, represent the non-linear dependence between the state of charge and the open circuit voltage [45].

DOD: Depth of discharge. Battery capacity that has been discharged is expressed as a percentage of maximum capacity. A discharge of 80% is referred to as a deep discharge.

Terminal voltage (V): This is the voltage between the battery terminals with the load applied. The terminal voltage varies with SOC and discharge/charge current.

Internal resistance: Resistance within the battery, generally different for charging and discharging, is also dependent on the battery's state of charge. As internal resistance increases, the battery efficiency decreases, and thermal stability is reduced as more of the charging energy is converted into heat.

3.2. Data of Proposed Model

The Panasonic model NCR18650B battery has been selected, which is designed to be part of the pack of an electric vehicle, in addition to being used for other applications of electric mobility, such as that of an airplane [46]. Table 1 summarizes the main characteristics of this battery commercial model. The open circuit voltage and SOC of this battery are presented in Table 2. The parameter interaction of the proposed model is shown in Figure 3.

Table 1. Panasonic battery model NCR18650B characteristics.

Parameter	Value
Nominal voltage [V]	3.6
Nominal capacity [mAh]	3350
Nominal energy [Wh]	11.7855
Specific energy [Wh/kg]	243
Weight [g]	48.5
Room temperature [°C]	25
Used charge rates [C]	[0.5, 1, 2, 3, 4, 5]
Simulation time [s]	3600
Internal resistance [Ω]	0.234

Table 2. Battery open circuit voltage and SOC.

SOC	VOC
0.01	2.5
0.1	3.06
0.2	3.1875
0.3	3.2125
0.4	3.375
0.5	3.4375
0.6	3.5625
0.7	3.6875
0.8	3.71875
0.9	3.875
1.0	4.0626

Guidelines used to develop equations for this model are presented in Figure 4. In the case of a lithium-ion battery, this model considers that some parameters change over time, and therefore, characteristics such as the state of charge vary, making the *VOC* dynamic. Equations of this model that describe the equivalent circuit are presented in Figure 5.

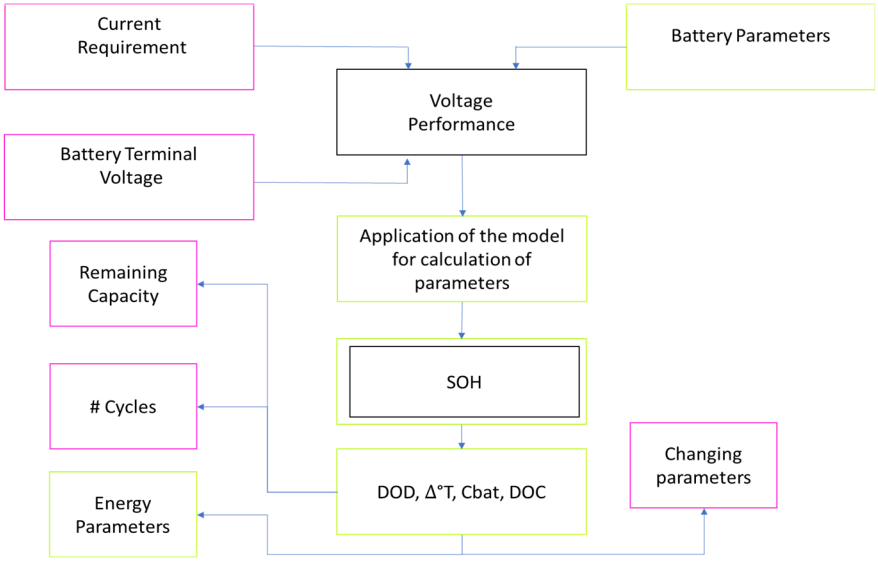


Figure 3. Proposed battery model block diagram.

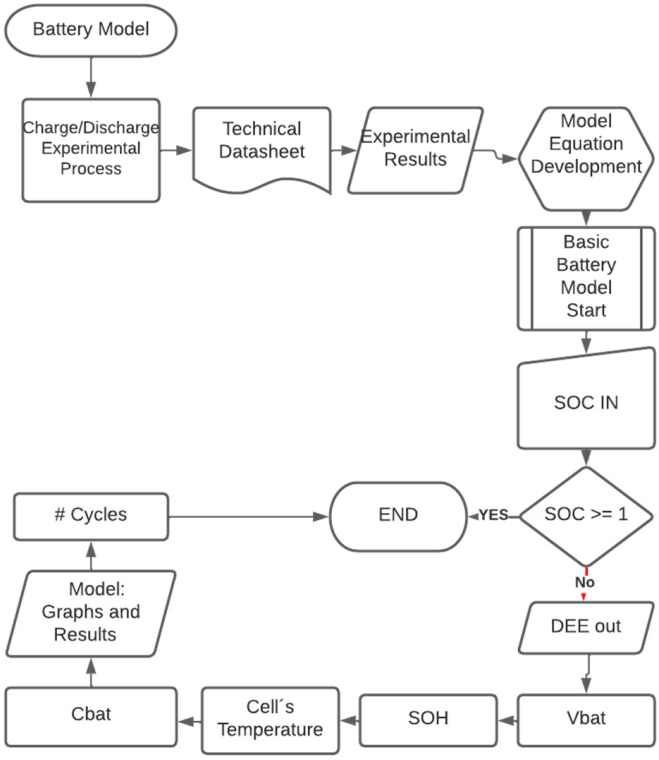


Figure 4. Proposed battery model flow diagram.

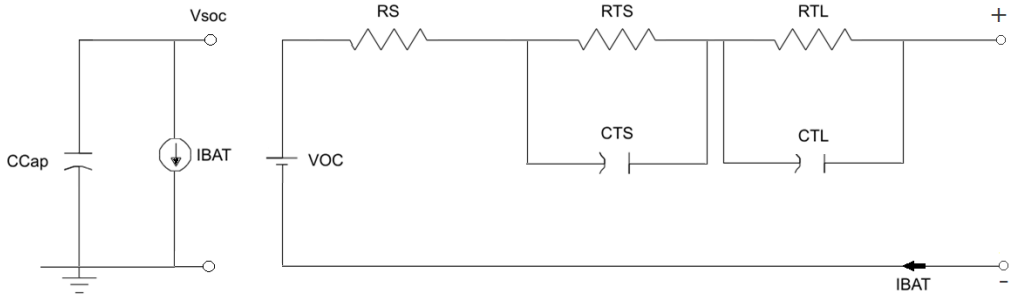


Figure 5. Proposed model.

3.3. Development of Proposed Model

Many authors have carried out experimental methodologies for the determination of the basic characteristic curves of the battery, and this allows the analysis and elaboration of a model that approximates its experimental data in order to be able to establish critical points of its behavior. Battery manufacturers provide us with useful parameters to model an approximation of the battery's behavior in real time, and knowing certain critical points of the battery allows us to open doors for treatment and improvements in the model through optimization techniques.

A characterization curve of the SOC and VOC relationship was obtained from the battery technical data sheet. This allows performing a linearization to obtain Equation (3) as part of the basic model proposed by [47]. With this equation, it is possible to relate phenomena in the battery, including its behavior regarding its temperature. The resulting relation provided two coefficients, α, and β, with values of 0.012 and 1.09, respectively.

$$Q_{bat} = \alpha + \beta SOC, \tag{3}$$

This basic model contemplates the behavior of the open circuit voltage, and it also shows the stages of long and short transients, expressed in Equations (4)–(6), respectively, and the general behavior of the voltage is the relationship of the three functions in Equation (7):

$$VOC = ((-1)/CCAP \times I_{profile}) + SOC, \tag{4}$$

$$-1/(RTS \times CTS \times VCTS) + 1/(CTS \times I_p), \tag{5}$$

$$-\frac{1}{RTLA \times CTLA \times VCTLA} + \frac{1}{CTLA \times I_{profile}}, \tag{6}$$

$$V_{bat} = VOC \times VTS - VTA - I_p \times R_{int}, \tag{7}$$

where CCAP is the ratio of the capacity C with respect to a determined experimental time, and I_p refers to the amount of current used to carry out the charge/discharge. There are components as an RC array (RTS, CTS: resistance, capacitance corresponding to the short transient; RTLA, CTLA: parameters for the long transient), and their interaction with the current as the output voltages in the short and long transient, VCTS and VCTLA, respectively.

Battery behavior can be described in a better way due to its interaction with SOC, VOC, and transient components, allowing the establishment of a function of cell bulk temperature, considering the experiment room temperature as a reference. This function is described in Equation (8):

$$T_{cell} = T_{amb} + [T_{amb} + (0.012 + 1.09 \times SOC)/(VOC - (1.05 \times SOC) - V_{nom})], \tag{8}$$

These data interact with SOC, and if it exhibits a value bigger than 1, it is considered an overload, being an indication of a possible battery failure. When graphed, it also shows the point where the battery begins to be damaged due to the stress provided by each charge and discharge cycle. This relationship is given based on the open circuit voltage, in addition to the fact that the terminal voltage (Vbat) is also affected as a consequence. The relationship of both gives the state of health of the battery (SOH), and it is shown in Equation (9):

$$SOH = \frac{Qm}{Qnominal}, \tag{9}$$

Another option to find SOH is the relationship between maximum battery capacity, capacity differential, and depth of dispatch. In order to reach this equation, it is necessary to solve polynomials for its treatment and to be able to find the capacity of the battery in a dynamic way, with coefficients δ (-0.025) y φ (1.05). This is expressed in Equation (10):

$$Cabat = [\delta + SOH^2 + (\varphi \times SOH) + V_{nom}]dt, \tag{10}$$

Using SOC behavior change versus time and battery charge-discharge stages through experimental time, it can be established an equation to predict the battery number of cycles, presented as follows:

$$N_{cycles} = |I_{profile}/((SOC - 1) \times V_{nom})|, \quad (11)$$

Using Faraday's Electrochemical Law, a relationship between Gibbs Free Energy and system-obtained energy can be established. Therefore, a "damage" spot can be found in every transient stage. This is due to materials aging and the number of cycles and leading to a variation in output battery capacity.

Equations (4) and (7) describe overall battery behavior in relation to voltage and time. Using a mathematical treatment based on Faraday's Electrochemical Law, thermodynamic changes inside the battery related to Gibbs Free Energy and Nernst Law, and parameters obtained in Equation (2), the following equations can be modeled. These equations describe cell temperature changes related to battery SOC changes.

The simulation in this work was carried out in Matlab software, using the Simulink tool, because of its ease of use in electrical parameters. The model is based on two separate circuits, related to each other by a controlled voltage source and a current source. The first circuit describes the charge and discharge of the batteries (Equations (7)–(9)), and the second circuit describes transient behavior (Equations (5) and (6)).

Dynamic cell behavior must be analyzed using a high-end device through experiments. Experimental methodologies allow us to study materials' electrochemical behavior and their interaction with the environment. Nevertheless, these methods are expensive and poorly able to make forecasts from the data [14,15,31].

4. Results

Validation of this modeling was made through experimental data and methodologies proposed by other authors. This model simulation was established with the following parameters and conditions:

1. Condition E1 occurs when there is a C-rate change (1C to 5C, using increments of 0.5C), with a constant current of 1A, at a constant temperature (25 °C).
2. Condition E2 occurs when the operating temperature varies (using 20 °C increments) at a constant charge rate of 3.2C, with a current of 4.7142 A, using a simulation time of 3600 s.

Experimental results and parameters determined by the manufacturer are presented in Table 3.

Table 3. Proposed model parameters and experimental data.

Parameter	Experimental Values	Proposed Values
RTS	0.0245	0.01
CTS	3384	1
RTL	0.261	0.02
CTL	20,249	5400

Figures 6–8 show the dynamic of terminal voltage, state of health, and battery capacity under condition 1 (E1). The mean square error is calculated (Table 4), which shows the differences between the established model and the proposed one for each condition.

Figure 6 shows the terminal voltage for different C-Rates as a function of time. When the C-Rate of the load increases, the discrepancy between the experimental model and the proposed model also increases with respect to the voltage at the terminals. However, the tendency is the same, allowing us to analyze the changes produced in each charge and discharge cycle.

Figure 7 presents the SOH changes. It can be useful to predict at which moment the battery efficiency will drop.

Output battery charge behavior and how it could be affected due to C-Rate change are presented in Figure 8.

The simulation results for condition 1 show a very good performance of the proposed model to predict the experimental behavior with an acceptable error.

Analysis and validation of the model through temperature changes (Condition 2) allow material design and physical composition of batteries. Additionally, it shows the behavior in the battery thermal stress states, which is the behavior through time and how the ambient temperature affects internal cell temperature. This leads to a parameter values variation, such as terminal voltage, as shown in Figure 9.

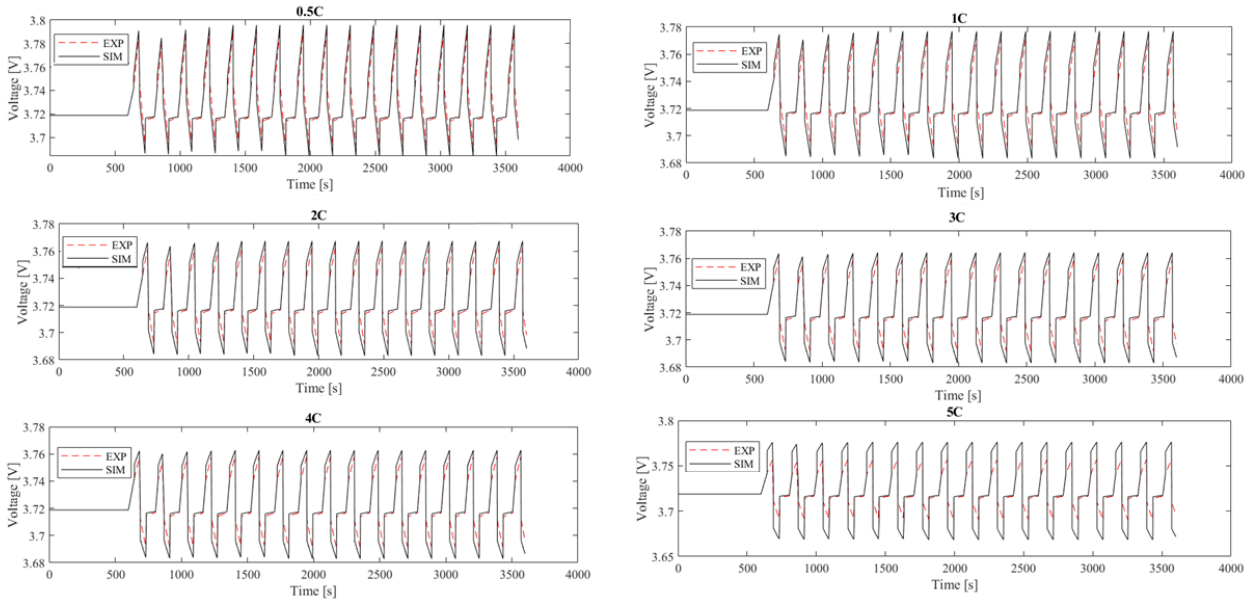


Figure 6. Terminal voltage for different C-Rates.

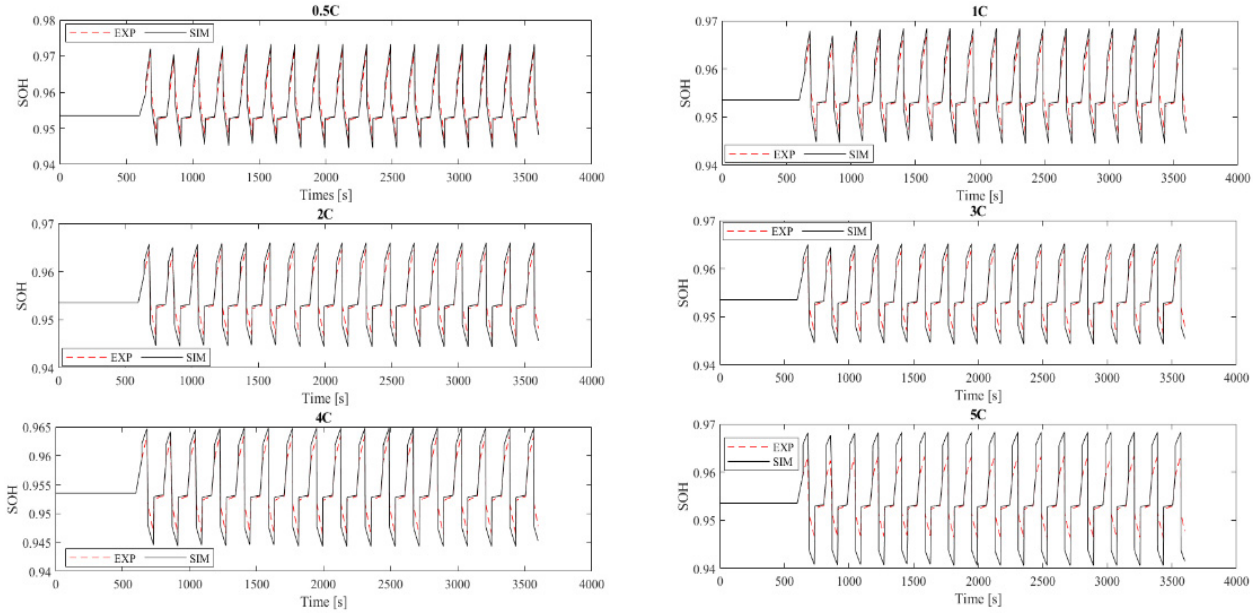


Figure 7. SOH for different C-Rates.

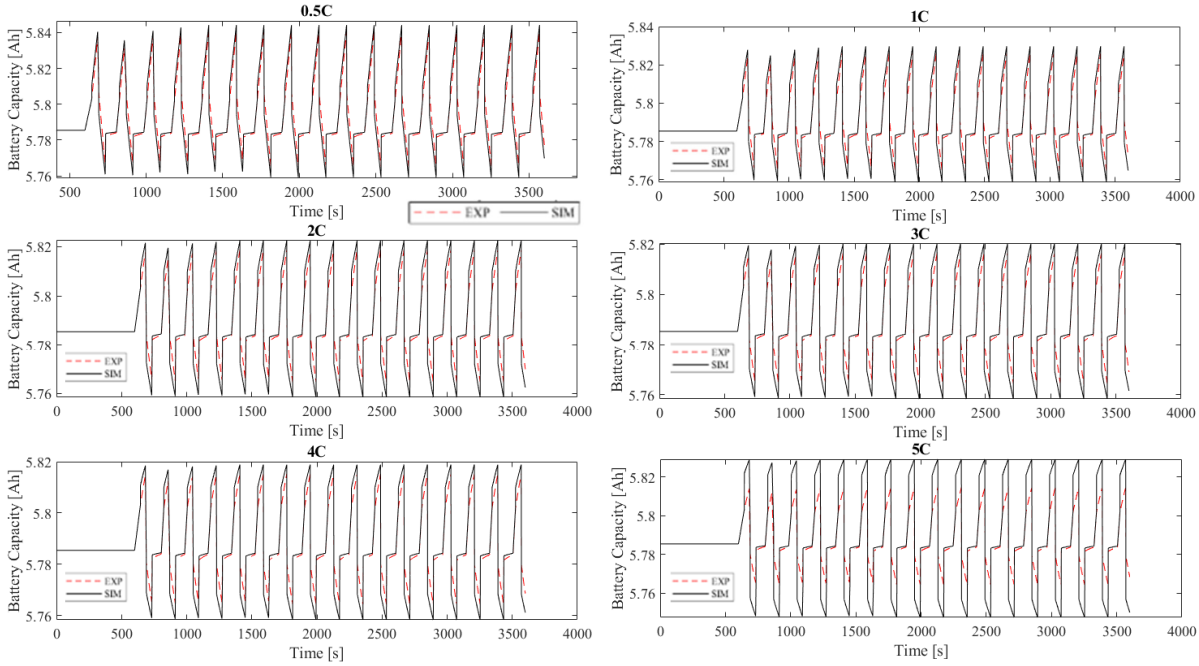


Figure 8. Battery capacity for different C-Rates.

Table 4. RMSE values obtained for E1, C-Rate.

Values	Output Capacity	SOH	$V_{terminal}$
0.5C	0.0072562	0.0024453	0.0072562
1C	0.0072396	0.0024453	0.0072396
2C	0.0072313	0.0024453	0.0072313
3C	0.0072285	0.0024453	0.0072285
4C	0.0072271	0.0024453	0.0072271
5C	0.013774	0.004655848	0.013774

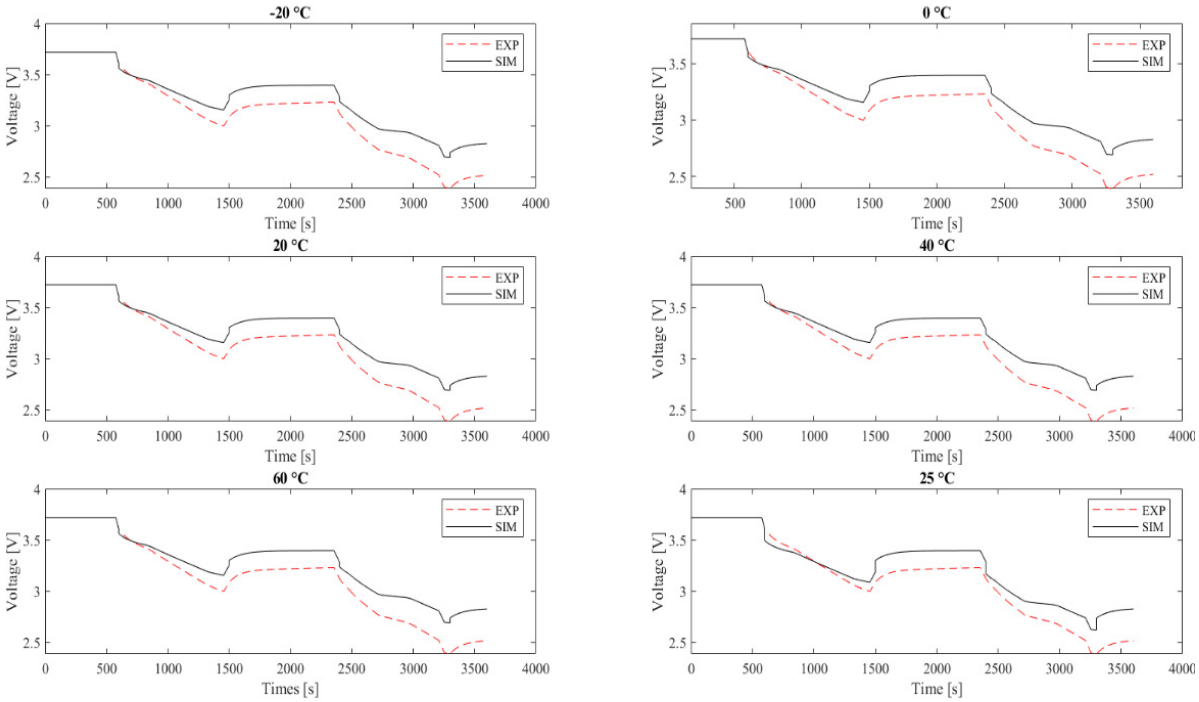


Figure 9. Model representation for terminal voltage.

Battery SOH and its behavior regarding the temperature are shown in Figure 10. Using this information, it can be seen how the battery deteriorates. This relationship enables a prediction and output capacity analysis, as shown in Figure 11.

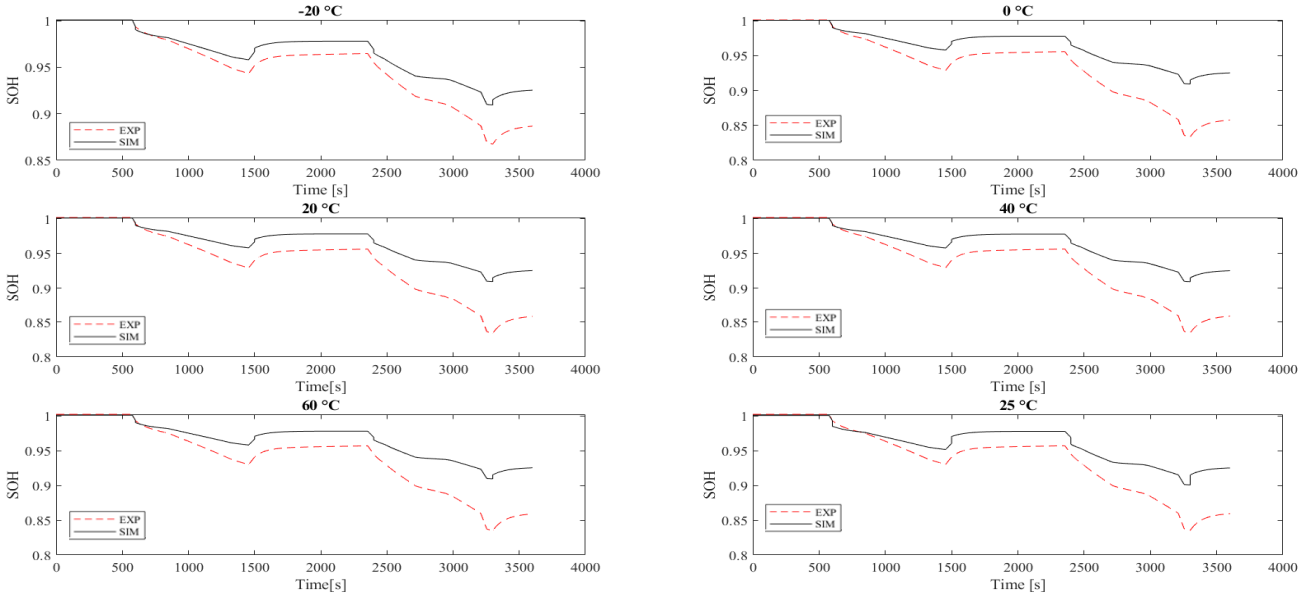


Figure 10. Battery SOH for comparing between experimental stage and proposed model.

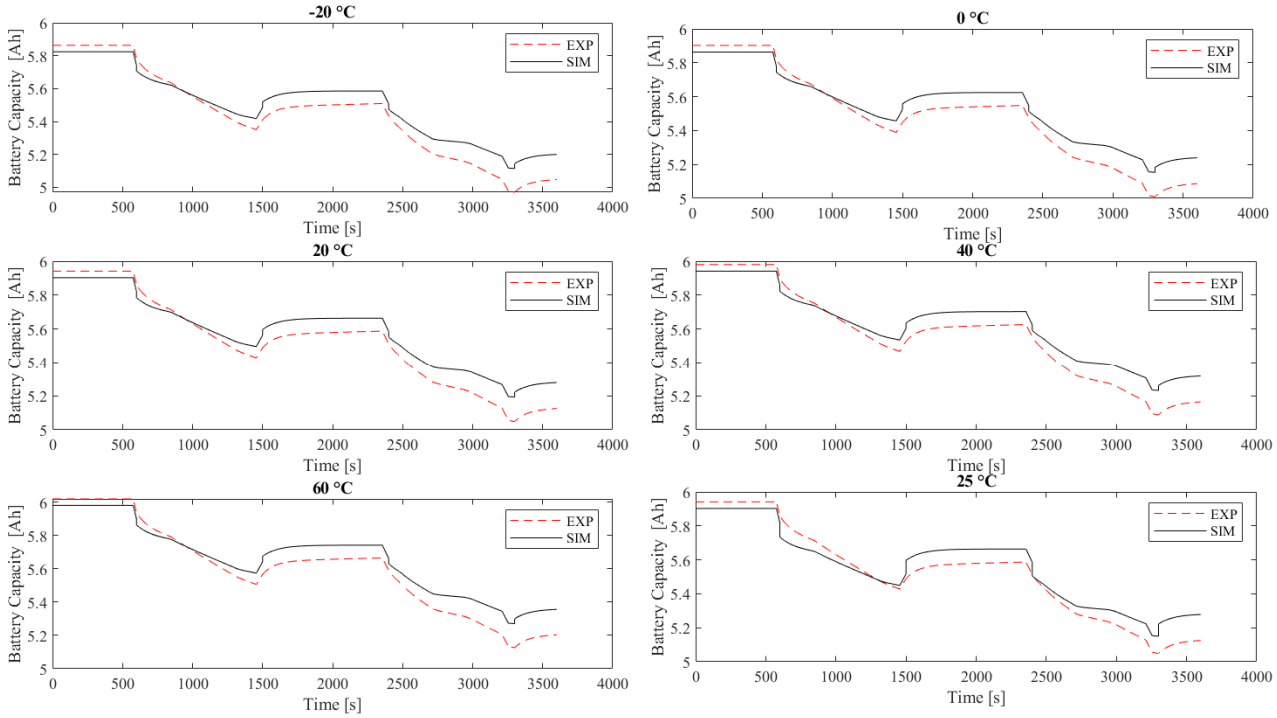


Figure 11. Output battery capacity changes regarding temperature.

Under condition 2, the error estimation of the proposed model with respect to the manufacturer data is greater than condition 1, but it still predicts the behavior for the three analyzed variables. This evaluation allows us to know the behavior of the battery through the elaboration of this model, analyzing in which temperatures the working range will be, as well as the temperature at which the greatest deterioration will be seen.

The changes in the parameters between each temperature are minimal, so in addition to the graph, we attach Table 5 with the differentials of the parameters.

Table 5. Rate of change in parameters.

Values	Simulation			Experimental		
	ΔVbat [V]	Cabat [Ah]	ΔSOH	ΔVbat [V]	Cabat [Ah]	ΔSOH
−20 °C	0.08	0.6270	0.083184	0.1133	0.82	0.1216
0 °C	0.07	0.6600	0.0749	0.1442145	0.82	0.14044
20 °C	0.0747	0.6270	0.0747	0.1448	0.78	0.1501
40 °C	0.0747	0.6280	0.0746	0.1413	0.83	0.1497
60 °C	0.0752	0.6300	0.0757	0.142	0.81	0.0826
25 °C	0.075	0.6300	0.075	0.1413	0.79	0.1583

The presented parameters are useful for making a forecast of the loading and unloading stages. Thus, through the analysis of the temperature parameters, some systems can be adapted that allow the correct estimation of its behavior; this is due to the fact that when certain peaks of changes in behavior are determined, the phenomenon or some consequences that the battery would suffer. The mean square error for E2 is shown in Table 6. Where the parameter with the most changes is the output capacity, with the temperature with the smallest error range being 25 °C.

Table 6. RMSE values obtained for E2, T-Rate.

Values	Output Capacity	SOH	$V_{terminal}$
−20 °C	0.12255096	0.044973	0.15813554
0 °C	0.12255096	0.044973	0.15813554
20 °C	0.12255096	0.044973	0.15813554
40 °C	0.12255096	0.044973	0.15813554
60 °C	0.12255096	0.044973	0.15813554
25 °C	0.11262698	0.034916	0.13617239

Number of Cycles

This parameter allows the analysis of the battery and takes it to real situations, how many charge and discharge cycles it will give under certain conditions. In this case, the factor to be analyzed is the temperature and how its operation is affected (at constant load); determining the number of cycles granted by the battery will allow for proposing better parameters for its work or even suggesting favorable environments for the battery.

In this case, it can be shown in Table 7 below how the number of cycles of this battery is predicted. These data are obtained experimentally, but since they are patented data, they are even considered an industrial secret [48] with respect to the established conditions, changes in temperature, and changes in c rate.

Table 7. Forecast of number of charge-discharge cycles in the established stages of simulation.

Stage	Number of Cycles		Time
E1	0.5C	377.16	3600 s
	1C	382	
	2C	385	
	3C	387	
	4C	388.2	
	5C	388.46	
E2	2178.48		3300 s

The main difference between the simulation times is due to the fact that the following cycle cannot be completed completely.

5. Conclusions

In this work, a model was developed that includes electrochemical parameters and integrates them into an electrical circuit in such a way that estimates of its behavior in different scenarios (temperature changes and changes in charge and discharge cycles) were obtained. Including a comparison with a mean square error between the simulation and experimental data allows the optimization of technical parameters for various applications.

This developed model has different applications; for example, it can be used to characterize new lithium-ion batteries. Being an open model, initial conditions and specific parameters that the providers grant can be modified. Predicting the behavior of the battery and comparing it with its experimental results.

Additionally, by showing the behavior and being adaptable to load and unload characteristics in addition to temperature, different scenarios can be suggested in which a demand profile can be integrated, and by analyzing that new behavior, a decision-making protocol could be initiated.

An application in the economic energy sector is that this model has the ability to adapt to microgeneration systems and intelligent energy systems in order to carry out an economic dispatch for energy management, indicating optimal moments for its connection or disconnection from a power distribution system.

Carrying out the comparison of the data obtained with the experimental proposal, given by several authors, and simulating it using Matlab validated the proposed model. Since the data obtained and the ability of the model to obtain other data on the behavior of the battery make simulation using software attractive, it opens the possibility of optimization and analysis of other characteristics in real time. Being a model with an electrical circuit, it can be analyzed from different platforms, which want to detail a feature in more depth.

For this study, the validation of the model was carried out first, comparing it with an experimental model. For this, loading and unloading parameters were established, as well as environmental temperature parameters. These features provide a more complete picture of battery behavior under certain stress conditions. The expected results for this work were that they behave in similar ways and that the technical details that differentiate an experimental model from the simulated one are the ones that give us the parameters that allow us to optimize the operation of the battery, improving the behavior as well as its app.

These used parameters are necessary for the optimization and application of different purposes. These purposes can be their use in microgrids, battery maintenance in electric vehicles, use as storage systems in smart homes, and even determining the optimal time for their removal and residual treatment, such as SOH and battery capacity.

This model takes into account aging processes as well as the dependence of certain parameters on temperature.

The joint analysis of these conditions allows us to establish the usefulness of this proposed model, which is to determine the characteristics and parameters that could be improved through optimization (using different metaheuristic techniques).

This proposed model has as its main functionality the opening of analysis for the user since he can have access to information that both the provider, corroborate said behavior with a special battery charge and discharge analysis equipment such as a BMS. Thanks to the simplicity of the model, and as it is expressed in an equivalent circuit, it can be simulated in software that allows the interpretation of the behavior of its parameters; knowing this, it will be possible to define if it is necessary to remove the battery from the user, or if the user can still use it as an energy storage device for his home, and that considering the parameters dependent on the user, it could be seen how it interacts with the network and how the user affects the behavior of a battery integrated into a micro network, which could be part of a Smart City system.

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draft preparation, M.C.-N.; writing—review and editing, F.E.-M. and C.J.V.-G.; visualization, F.E.-M.; supervision, A.C.-M.; project administration, A.C.-M.; funding acquisition, A.C.-M. All authors have read and agreed to the published version of the manuscript.

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