



Mechanistic approach developed to estimation of exchange current density and charge transfer coefficient in lead acid batteries

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Abstract

Understanding and accurate estimation of electrochemical parameters play a pivotal role in enhancing the performance and efficiency of electrochemical systems like batteries and fuel cells. The exchange current density and charge transfer coefficient are particularly critical factors as they are directly related to the shape and structure of the battery electrodes and influence the electrochemical processes occurring within electrodes of the battery. Considering a fixed value for these parameters for a type of battery is not accurate due to the varying shapes and structures of electrodes in different batteries. This paper presents a comprehensive mechanistic approach to determine these electrochemical coefficients based on a combination of experimental testing, one dimensional computational fluid dynamics simulation, and optimization. This study focuses on the investigation of a 4 ampere-hour lead-acid battery (IBIZA) with the determination of anodic and cathodic exchange current densities and charge transfer coefficients for both the lead and lead oxide electrodes, respectively. Mentioned parameters are derived for two scenarios (one-step constant current discharge and two-step constant current discharge). The values of α_a , α_c and i_0 for Pb and PbO₂ for scenario one with $0.2C_{\text{rate}}$ are found to be 1.95, 0.05, 9.99×10^{-3} , 0.05, 1.95 and 3.05×10^{-4} and with $0.2C_{\text{rate}}$ are 9.98×10^{-3} , 0.75, 1.25, 9.69×10^{-3} , 0.97 and 1.03, respectively. Mentioned parameters for scenario two are found to be 0.6, 1.4, 2.70×10^{-3} , 0.6, 1.4 and 2.40×10^{-4} , respectively.

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1 Introduction

The increasing share of the renewable energy sources in the grid, with the challenges posed by their intermittent nature, as well as the demand for the sustainable power solutions have necessitated the development of energy storage systems [1]. Batteries particularly play an important role in safeguarding the transition towards a low-carbon future by providing a reliable and efficient mean of energy storage [2, 3]. Consequently, the study of the battery behaviors and characteristics is essential for advancing the knowledge and developing more efficient batteries as the demand for efficient and sustainable energy solutions is increasing.

Simulation models such as the electrochemical models like general micro - macro modeling of battery dynamics, single particle (SP) models, system-level models like equivalent circuit models (ECM) and the data-driven models like black box modelling [4–8] as well as the methods like electrochemical impedance spectroscopy (EIS) [9] are valuable tools for studying the dynamic behavior of batteries under different working conditions and provide insight into several aspects of battery systems such as performance characteristics, thermal management, and capacity degradation. Some of these methods specially micro - macro modeling of battery dynamics used along with computational fluid dynamic techniques provide powerful solutions to investigate battery behavior, optimize battery designs, thermal management of the battery systems and study the effect of different operating conditions where experimental methods fall short or require costly financial and time resources.

Investigating battery behavior through modeling and simulation not only accelerates the research and development process but also contributes significantly to the enhancement of battery safety, reliability and performance. In order to utilize the electrochemical models, it is essential to understand the kinetics of electrochemical reactions which often involves the estimation of key parameters such as exchange current density (i_0) and charge transfer coefficient (α). The common methods used for estimation of these parameters include Tafel analysis, EIS, potentiostatic intermittent titration technique (PITT), galvanostatic intermittent titration technique (GITT), and combined techniques.

Tafel analysis is one of the fundamental methods for estimating α and i_0 which involves measuring the current-potential curves and fitting the data to mathematical equations. The other widely-used electrode kinetics model is the Butler-Volmer equation relating the current density to overpotential. Fitting the experimental data into this equation can give the estima-

tion for charge transfer coefficients and exchange current density [10]. Tafel analysis provides a straightforward and quick estimation of i_0 from the polarization curves. However, it has limited applicability to systems with complex reaction mechanisms [11, 12]. Khadke et al. [13] showed that using differential Tafel plots, the first order differential of the Tafel plots with respect to overpotential, can reduce the inaccuracy in estimation of i_0 and α . Becker et al. [14] carried out a mathematical modeling and experimental kinetics characterization of electrodes in Vanadium redox-flow batteries. They showed that using the Butler-Volmer equation can be used to describe the polarization curves within the states of charge between 25 and 75 percents. Liu et al. [15] investigated the role of exchange current density on the electrodeposition in Lithium metal batteries. They used the Tafel analysis to derive the exchange current density.

The other established method used for battery characterization is the EIS. In this method, a current or potential perturbation is applied and the potential or current response is measured. Barsukov and Macdonald [16] have provided a comprehensive overview of EIS including its applications in battery modeling. There are also numerous studies using EIS to estimate the battery electrochemical parameters especially α and i_0 [17–19]. The direct measurement of the current and potential transients allows for simplified data interpretation, yet it may not be suitable for more complex systems and also the accuracy of the results is sensitive to the experimental conditions [20].

PITT and GITT are also used for determining the electrochemical parameters of the battery electrodes such as the exchange current density and diffusion coefficient by applying constant-potential steps and constant-current pulses and measuring the current and potential responses. These methods can provide detailed information about the reaction mechanisms and also can be used for more complex electrochemical systems. However, they are sensitive to electrode parameters such as porosity, particle size distribution, and specific surface area and the data interpretations could become challenging for complex systems [17, 21].

Each method presents its unique advantages and challenges, contributing to specific areas in electrochemical systems studies. Tafel analysis offers simplicity and direct measurements but may fall short in intricate scenarios. EIS, PITT, and GITT are suitable for more complex systems, providing abundant information but demanding sophisticated data analysis. Data-driven methods such as the black-box model based on methods like neural network, genetic algorithm, and deep learning provide fast estimation of the battery parameters without the need to physically model the

system. However, the accuracy of these methods depends on the number of data samples and they do not provide any insight into the internal mechanisms governing the battery behavior. These models are especially useful for the estimation of the battery parameters such as state of charge and state of health [7]. On the other hand, the physics-informed data driven models [22–27] add the insight into the microscopic phenomena inside the battery at the expense of accuracy and certainty [28].

In this study, simulation with the advanced numerical methods, based on the micro-macro model of the battery dynamics, is used as a powerful tool for overcoming the experimental constraints. Unlike the above-mentioned methods, the proposed approach in this paper can provide a deep understanding of the phenomena occurring inside the batteries and offer detailed spatial and temporal analyses. It is well-suited for systems with complex kinetics, where experimental approaches may be challenging. The methods based on simulation of micro-macro governing equations of battery are capable to capture the transient behavior of batteries. There are several methods for the simulation of lead-acid batteries such as the finite volume method [29], the Keller-Box method [30], engineering models [31], and reduced-order methods [32–35]. Here, the Butler-Volmer equation is the critical tool in explaining the kinetics of electrochemical reactions within batteries. Two crucial parameters, the exchange current density and charge transfer coefficient, are essential to the Butler-Volmer equation. Accurately estimating them is vital for a complete understanding of battery performance.

The exchange current density represents the equilibrium rate of electrochemical reactions at the interface of battery electrodes and electrolyte, providing insights into the inherent kinetics of charge transfer processes. Simultaneously, the charge transfer coefficient characterizes the efficiency of charge transfer through the electrode-electrolyte interface. The mentioned parameters are influenced by electrode material, electrolyte composition, temperature, surface area, and morphology.

In conclusion, the literature showcases a diverse array of methods for estimating i_0 and α , each with its strengths and applications. Researchers often choose methods based on the specific characteristics of the electrochemical system under investigation, emphasizing the need for a restricted approach in parameter estimation. In this research, the mechanistic approach is employed to integrate experimental techniques, theoretical models (micro-macro modeling of battery dynamics whose parameters are correlated by the Butler-Volmer equation), advanced numerical methods like

Computational Fluid Dynamics (CFD), and optimization techniques. This integration contributes to a comprehensive understanding of electrochemical kinetics, enabling the extraction of the relevant parameters. The mechanistic method presented in this study has the capability to be systematically utilized across a wide range of batteries for estimating exchange current density and charge transfer coefficient. The originalities of this study are as following:

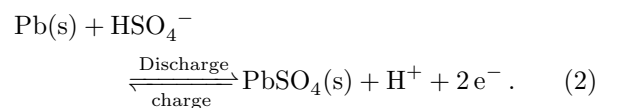
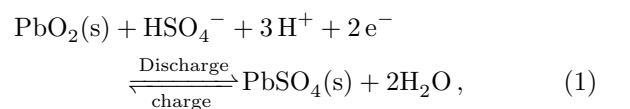
- Combination of CFD, optimization and experimental tests is the basis of the new mechanistic approach presented in this study.
- Using mathematical governing equation leads to more accurate results.
- The introduced method can be developed for a wide range of batteries.
- In this method, the procedure of determining exchange current density and charge transfer coefficient is more clear.

2 Method

In this study, the electrochemical parameters are extracted by coupling constant-current discharge experimental data, one-dimensional numerical modeling and simulation with Particle Swarm Optimization (PSO). The simulation of governing equations and optimization processes are developed in C++ and Python, respectively.

Mathematical model The governing equations for a battery consist of the solid potential, the electrolyte potential, and the electrolyte concentration equations which are coupled together using the Butler-Volmer equation. In this study, the conservation equations for electrochemical systems are solved in a one-dimensional manner through four regions: the positive electrode, electrolyte, separator, and negative electrode. It is important to note that all four regions, representing the positive electrode, separator, and negative electrode, are porous media. The schematic model of the battery is shown in [Figure 1](#). The positive electrode is PbO_2 , and the negative electrode is Pb .

The lead-acid battery electrochemical reactions occurring separately in the positive and negative electrodes are shown in equation (1) reaction and (2), respectively [32–34, 37].



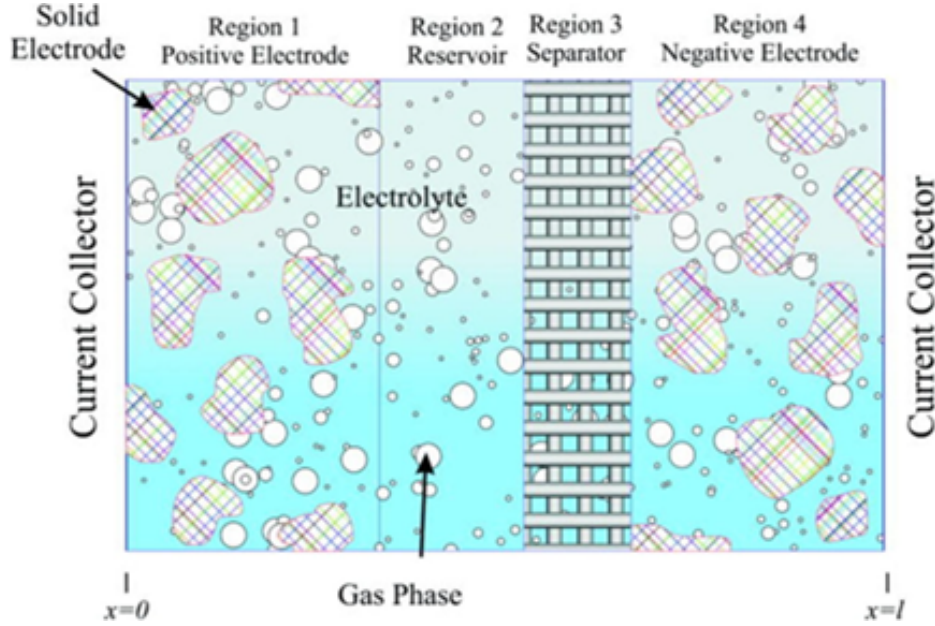


Fig. 1. Schematic representation of an electrochemical battery cell [36].

During the discharge process, oxidation reactions occur at the negative electrode, while reduction reactions take place at the positive electrode. In the battery discharge process modeling and simulation, the side reactions can be neglected because their rates are extremely low.

Governing equation As the electrochemical reactions occur at the interface of the electrode and electrolyte, the maximum gradient of all unknown parameters is in the direction of the electrode thickness. Modeling a one-dimensional battery simulation aligns with this scenario. Additionally, in a tightly sealed battery pack, the mass and momentum conservation equations can be omitted in order to focus on solving the electrode and electrolyte charge conservation equations and electrolyte concentration. All of the governing equations are listed in Table 1 [29]. The values of input parameters for one dimensional simulation are shown in Table 2.

In electrochemical reactions, chemical species are produced or consumed at the interface of the electrode and electrolyte. The transfer current density for the actual main reactions in a lead-acid battery, derived from the Butler-Volmer equation, can be determined from equation (3):

$$j = i_0 \left(\frac{C}{C_{\text{ref}}} \right)^\gamma \left(\exp \left[\frac{\alpha_a F}{RT} \eta \right] - \exp \left[\frac{-\alpha_c F}{RT} \eta \right] \right) \quad (3)$$

The equations related to the solid potential, electrolyte potential, and acid concentration are coupled through the Butler-Volmer equation. By simultaneously solving these coupled equations through numerical simulation, assuming boundary and initial conditions as per Table 3 [29], the unknown parameters, solid potential, electrolyte potential, and electrolyte concentration, can be determined. A one-dimensional numerical solution of these equations provides high accuracy and efficient solving time.

The most accurate method for determining the battery voltage under specific operational conditions is through experimental testing with which the accuracy of other methods is evaluated.

Experimental method In this research, an experimental discharge test was carried out using the NEWARE battery tester BTS4000. The tester has features such as a response time of less than or equal to 20 milliseconds to meet rapidly changing power requirements, 0.1% full-scale accuracy for current and voltage, a data acquisition frequency of 10Hz (optional 100Hz), a minimum pulse width of 500 milliseconds, and the capability to process more than 1 million records. The experimental setup is shown in Figure 2.

The tests were carried out under Constant-Current (CC) discharge mode in the battery tester. This mode is particularly useful for analyzing the discharge behavior of various types of batteries.

Table 1. Governing equations [29].

Solid charge conservation	$\nabla \cdot (\sigma^{\text{eff}} \nabla \phi_s) - Aj = 0$
Electrolyte charge conservation	$\nabla \cdot (k^{\text{eff}} \nabla \phi_e) + \nabla \cdot (k_D^{\text{eff}} \nabla \ln C) + Aj = 0$
Electrolyte concentration	$\frac{\partial(\varepsilon C)}{\partial t} = \nabla \cdot (D^{\text{eff}} \frac{\partial C}{\partial x}) + a_2 \frac{Aj}{2F}$
Specific active surface area	$A = A_{\text{max}} \text{SOC}^\zeta$
State of charge	Positive electrode: $\frac{\partial \text{SOC}}{\partial t} = + \frac{\nabla \cdot i_e}{Q_{\text{max}}}$ Negative electrode: $\frac{\partial \text{SOC}}{\partial t} = - \frac{\nabla \cdot i_e}{Q_{\text{max}}}$ $\nabla \cdot i_e = Aj$
Effective properties	$\sigma^{\text{eff}} = \sigma \varepsilon_s \zeta$ $k^{\text{eff}} = k(1 - \varepsilon_s)^\zeta$ $k_D^{\text{eff}} = k_D(1 - \varepsilon_s)^\zeta$
Porosity	$\varepsilon_s + \varepsilon_e = 1$ $\frac{\partial \varepsilon_e}{\partial t} = - \frac{\partial \varepsilon_s}{\partial t} = a_1 \frac{Aj}{2F}$ Positive electrode: $a_1 = \left(\frac{MW_{\text{PbSO}_4}}{\rho_{\text{PbSO}_4}} - \frac{MW_{\text{PbO}_2}}{\rho_{\text{PbO}_2}} \right)$ Negative electrode: $a_1 = - \left(\frac{MW_{\text{PbSO}_4}}{\rho_{\text{PbSO}_4}} - \frac{MW_{\text{Pb}}}{\rho_{\text{Pb}}} \right)$
Butler-Volmer	$j = i_0 \left(\frac{C}{C_{\text{ref}}} \right)^\gamma \{ \exp(\frac{\alpha_a F}{RT} \eta) - \exp(-\frac{\alpha_c F}{RT} \eta) \}$ $\eta = \phi_s - \phi_e - U_{\text{ref}}$ $\alpha_a + \alpha_c = n$

Table 2. Input parameters value.

Density , g cm ⁻³	
PbO ₂ electrode	9.7
Pb electrode	6.3
PbSO ₄	11.34
Conductivity , S cm ⁻¹	
PbO ₂ electrode	500
Pb electrode	4800
Maximum electroactive area , cm ² /cm ³	
PbO ₂ electrode	148
Pbelectrode	200
Maximum capacity , C/cm ³	
PbO ₂ electrode	1400
Pb electrode	1800
Operating temperature , °C	25

Table 3. Boundary conditions.

Boundary condition	$\frac{\partial \phi_e}{\partial x} \Big _{x=0} = 0$
	$\frac{\partial \phi_e}{\partial x} \Big _{x=l} = 0$
	$-\sigma^{\text{eff}} \frac{\partial \phi_s}{\partial x} \Big _{x=0} = I(t)$
	$-\sigma^{\text{eff}} \frac{\partial \phi_s}{\partial x} \Big _{x=l} = I(t)$
	$\frac{\partial c_e}{\partial x} \Big _{x=0} = 0$
	$\frac{\partial c_e}{\partial x} \Big _{x=l} = 0$

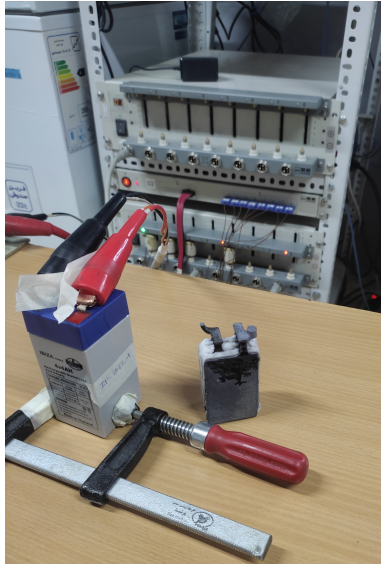


Fig. 2. Test setup.

In the CC discharge mode, the tester applies a constant-current load to the battery being tested. This load is maintained at a steady level throughout the entire discharge process. By doing so, the tester can simulate the real-world scenarios where a device draws a constant current from the battery until its voltage drops to a predetermined cutoff point.

As mentioned in introduction and literature review, there is no sufficiently accurate method to obtain the exchange current density, as well as the anodic and cathodic charge transfer coefficients. If these parameters are properly selected, the simulation should be able to closely follow and estimate the experimental voltage-time curve. Therefore, accurate values for these parameters are crucial for the simulation to predict the experimental test with high precision and lead to obtaining an accurate distribution of concentration and potential across the electrode and electrolyte. The proposed method provides valuable information to researchers about the phenomena occurring inside the battery by combining the experimental constant-current discharge data and the one-dimensional simulation of the fundamental mathematical governing equations of the battery.

Optimization Optimization is a mathematical and computational approach used to find the best possible solution to a problem among a set of feasible alternatives. In this study, the goal is to minimize the objective function based on root-mean-square deviation (Eq. (4)).

$$\text{OF} = \sqrt{\sum_{\text{time}} (\phi_{\text{sim}} - V_{\text{Exp}})^2} \quad (4)$$

In Python, a library called `pymoo` is developed which extends the Particle Swarm Optimization (PSO) method. Particle Swarm Optimization is a population-based optimization algorithm inspired by the social behavior of birds and fish. The PSO method is effective for continuous optimization problems and its simplicity and efficiency make it widely used in various fields such as engineering, finance, and machine learning.

The PSO method incorporates the following parameters: w , the inertia weight that controls the impact of the previous velocity, c_1 and c_2 , acceleration constants, and r_1 and r_2 random values between 0 and 1. A higher w gives more influence to the current velocity, promoting exploration, while a lower w favors exploitation. Common values for w range between 0.4 and 0.9. Commonly, it starts with a higher value and gradually reduces over iterations. The acceleration constants control the influence of personal best (p_{best}) and global best (g_{best}) on the particle's movement, respectively. Common values for c_1 and c_2 are typically between 1.5 and 2.0. Higher values increase the influence of p_{best} and g_{best} , promoting exploitation. In this study we use default values which are 0.5 and 1.5 for w and c_1 and c_2 , respectively. The number of generation was used for termination condition.

The physical and electrochemical parameters such as exchange current density and charge transfer coefficient are extracted using constant-current discharge process experimental data, simulation, and optimization. Using the correct values for α and i_0 , a precise understanding of the physical and electrochemical concepts of a battery can be achieved through CFD simulation based on the fundamental equations governing the battery. The introduced method is shown in the the flow chart of [Figure 3](#).

3 Result and discussion

The Butler-Volmer equation plays a central role in the realm of electrochemical kinetics, offering essential insights into the mechanisms governing charge transfer at electrode-electrolyte interfaces. This equation is a cornerstone for understanding the complex kinetics of electrochemical reactions in diverse applications such as batteries, fuel cells, etc..

As previously mentioned, two key parameters within the Butler-Volmer equation are critical in describing the rate of electrochemical reactions: exchange current density and charge transfer coefficient. Exchange current density represents the hypothetical current at equilibrium when oxidation and reduction rates are equal, revealing the inherent activity of the electrochemical system in the absence of applied potential.

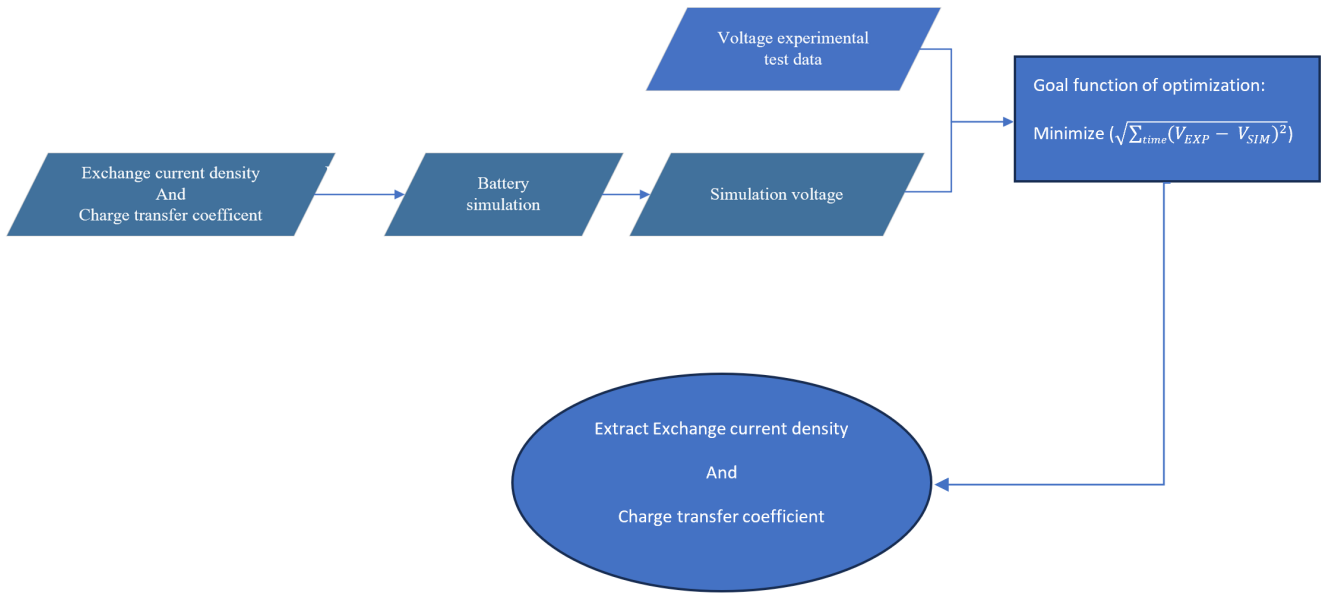


Fig. 3. Flow chart of the method used to extract i_0 , α_a and α_c .

Charge transfer coefficient, on the other hand, is a vital parameter reflecting the movement of charge carriers across the electrode-electrolyte interface during electrochemical reactions. This parameter is crucial for understanding the efficiency and speed of charge transfer, directly influencing the overall performance of electrochemical devices.

Therefore, the precise extraction and understanding of these two crucial parameters are vital for enhancing and optimizing the designs of electrochemical systems.

In this study, a commercial lead acid battery, manufactured by IBIZA, with the voltage of 4V and capacity of 4Ah is investigated. The details and specifications of the battery are listed in Table 4.

Table 4. IBIZA battery (4 V, 4 Ah) specification

Battery configuration	2S3P
PbO ₂ thickness (mm)	2.06
Pb thickness (mm)	1.52
separator thickness (mm)	1.30
Electrode surface dimension (mm × mm)	58.80 × 39.12

The sample battery discharge tests were carried out with two scenarios at the room temperature. The first scenario was a one-step constant-current discharge from full-charge voltage to the cut-off voltage at $0.1C_{rate}$ and $0.2C_{rate}$. The second scenario was a one-step constant-current discharge from full-charge voltage to the cut-off voltage at $0.2C_{rate}$.

The first scenario optimization results for i_0 , α_a and α_c of the Pb and PbO₂ electrode for $0.1C_{rate}$ were 9.99×10^{-3} , 1.95, 0.05 , 3.05×10^{-4} , 0.05 and 1.95, re-

spectively. The above mentioned parameters for $0.2C_{rate}$ were 9.98×10^{-3} , 0.75, 1.25, 9.69×10^{-3} , 0.97 and 1.03, respectively. The experimental test and the result of the simulation which are conducted with the mentioned parameter values for $0.1ans0.2C_{rate}$ are shown in Figures 4 and 5. The error value, which is calculated based on equation (4), for $0.1C_{rate}$ and $0.2C_{rate}$ is 0.35 and 0.10, respectively.

In order to check the accuracy of the obtained results for i_0 , α_a and α_c of the Pb and PbO₂ electrode, similar values with the first scenario ($0.1C_{rate}$) were used for the second scenario. The experimental and simulation results of the cell voltage versus time are presented in Figure 6.

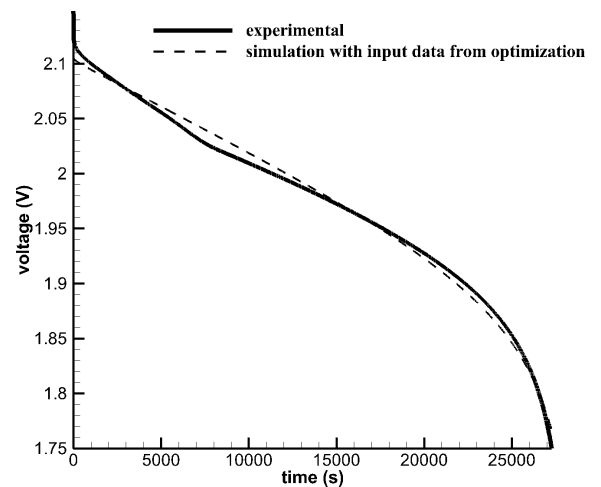


Fig. 4. Voltage of the cell during discharge ($0.1 C_{rate}$).

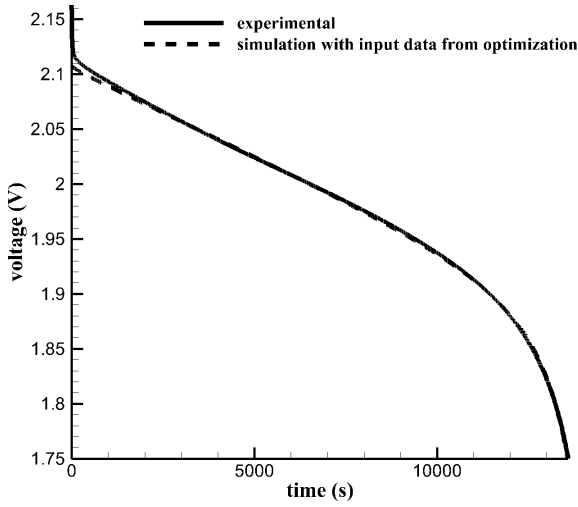


Fig. 5. Voltage of the cell during discharge(0.2 C-rate).

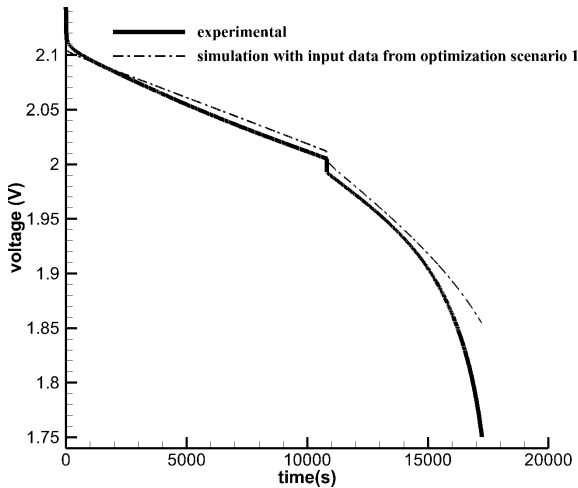


Fig. 6. Voltage of the cell during discharge (scenario 2 simulation with the input data of scenario 1 optimization).

The optimization was carried out again by using the second scenario simulation. The results for i_0 , α_a and α_c of Pb and PbO₂ were 2.70×10^{-3} , 0.6, 1.4, 2.40×10^{-4} , 0.6 and 1.4. The error value is 0.31 (Figure 7).

4 Conclusion

The different discharge profiles in each scenario created different electrochemical kinetic reactions. Hence, different values were obtained for the investigated parameters of the first and second scenarios. The exchange constant current and charge transfer were affected by concentration, temperature, and the electrode surface reactions which led to change in the kinetics of the lead-acid battery reactions with different discharge profiles.

Based on our research, the proposed method stands out as a robust and reliable approach for predicting the battery behavior and kinetic parameters across various operational conditions. As the results show, this study has demonstrated the effectiveness and versatility of the proposed method in providing accurate insights into intricate electrochemical processes governing battery performance.

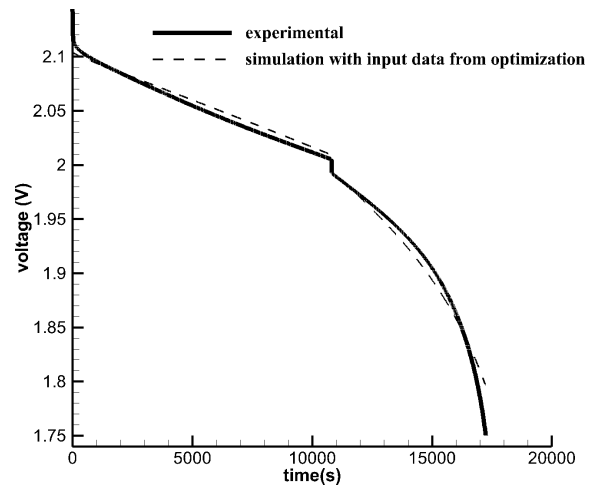


Fig. 7. Voltage of the cell during discharge (scenario 2).

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Nomenclature

A	Specific active surface area
A_{\max}	Maximum active surface area available at SOC = 1
C	Electrolyte concentration
C_{ref}	The reference concentration at which battery parameters are provided
D^{eff}	Diffusion conductivity
F	Faraday constant
i_0	Exchange current density
j	Current density transferred from electrode to electrolyte
k^{eff}	Effective electrolyte conductivity
k_D^{eff}	Electrolyte effective diffusion conductivity
U_{ref}	Open-circuit equilibrium voltage (In the negative electrode, its value is zero, while in the positive electrode, it is a function of the electrolyte concentration)

Greek symbols

ϕ_s	Solid potential
ϕ_e	Electrolyte potential
α_a	Anodic charge transfer coefficients
α_c	Cathodic charge transfer coefficients
σ^{eff}	Effective conductivity in the solid zone
η	Overpotential

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