Lithium ion Battery Parameter extraction using the Physics Based Mathematical model and Neural Network method

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ABSTRACT

Lithium-ion batteries, owing to their extensive usage, necessitate precise modeling for the accurate prediction of future performance and aging characteristics. This paper presents a physics-based mathematical model integrated with an optimized neural network-based artificial intelligence (AI) model to efficiently forecast the output voltage and other crucial battery parameters. Within the realm of battery management systems, the state of charge (SoC) emerges as one of the most pertinent parameters, making it an ideal input for the neural network to facilitate the quality estimation of battery parameters. Additionally, this paper investigates the prediction of discharge capacity based on the obtained output voltage, further enhancing the understanding of battery characteristics.

1. Introduction

In recent times, Lithium-ion batteries are being used in many industrial sectors as a major rechargeable energy resource such as in electric vehicles and consumer electronic devices. The advantages of lithium-ion batteries over other types of energy storage devices include high energy and power density with the least amounts of memory effect and resulting capacity loss. However, despite these advantages and applications, the lithium-ion battery suffers from problems due to side reactions.

The electrochemical lithium-ion battery model represents the internal states of a battery in a realistic way as it is derived from the microstructure of a lithium-ion battery. However, it is very challenging to accurately estimate the parameters because the electrochemical lithium-ion battery model is composed of complicated coupled partial differential equations, and the model involves a large number of parameters and boundary conditions.

Many studies have been conducted to accurately estimate the parameters of lithium-ion batteries. Some of these are based on physics-based modeling or Jacobian based algorithms such as the Levenberg-Marquardt method or neural network based ai modeling. However, such methods require many iterations for good results, thus considerable time is required to estimate the parameters of lithium-ion batteries.

Deep learning is lately being used to some extent in research to predict the parameters of Lithium-ion batteries. In this paper, a deep neural network-based solution is designed to estimate not only the capacity of the battery but also the additional parameters representing its electrochemical states. For this purpose, a neural network is used to consider the relation between voltage, current, temperature, C-rate, and state of charge on positive and negative electrodes of the battery.

In this paper, we have used the pybamm module which is based on python. Python Battery Mathematical Modelling (Pybamm) solves continuum models for batteries, using both numerical methods and asymptotic analysis. Several battery models are implemented and can easily be used or compared. Some of the useful models are Single Particle model (SPM), Single Particle Model with electrolyte (SPME), Doyle-Fuller-Newman Model (DFN), and Single Particle Model with Temperature variance (SPMT). We used this module to collect data by performing the simulation for SPMT Model [2]

2. Methodology

In the previous section, we gained information about the different cases that we are going to study in this paper. This section deals with the procedure that is essential to perform the simulation.

2.1 Fetching the Experimental Data

In order to obtain the experimental data required for the simulations, we considered the plot between open circuit voltage and the state of charge. Open circuit voltage (OCV) is an essential characteristic parameter of lithium-ion batteries as shown in Fig.1, which can be used to study the changes in electronic energy associated with electrode materials, and for the estimation of battery state of charge (SOC). SOC is also a required parameter as it conveys the data about available energy in a battery that assists in devising charging/discharging strategies. Therefore, the curve between OCV and SOC has great importance in the field of lithium-ion battery modeling.

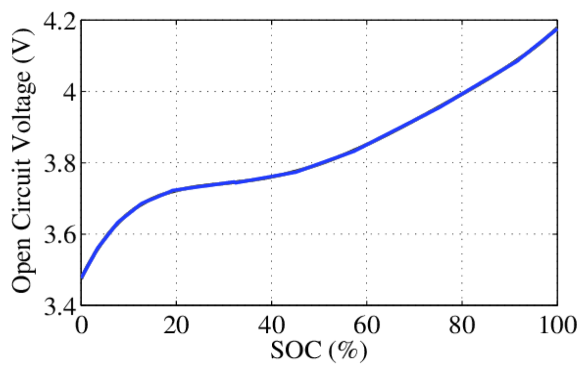

Fig.1 Experimental Data plot of OCV and SOC

2.2 Parameter setup and simulation

Here, we will review the different parameters which are utilized for the simulation. First of all, we are evaluating our cases based on the Single Particle Model with Electrolyte (SPMe) of a lithium-ion battery. We select the full thermal model, which helps in solving the spatially-dependent heat equation based on the battery geometry, and couples the temperature with the electrochemistry. The default parameter set that comes with the SPMe model is considered but some of the values of input parameters are altered and these parameters are [1]:

Table 1 Input parameters for the SPMe of a lithium ion battery

Cell cooling surface area	0.068 m^2
Negative Electrode conductivity	150 $S.m^{-1}$
Negative current collector conductivity	600000000 $S.m^{-1}$
Initial concentration in negative electrode	2000 $mol.m^{-3}$
Positive electrode conductivity	20 $S.m^{-1}$
Positive current collector conductivity	36000000 $S.m^{-1}$
Initial concentration in positive electrode	31000 $mol.m^{-3}$
Current function	5 A

We increased the current in order to amplify the thermal effects. After providing the input values, we execute the simulation for 1hr for different values of C-rates. Once the simulation is completed, the output values for Negative electrode SOC, Negative electrode temperature [K], Positive electrode SOC, Positive electrode temperature [K] and Terminal voltage [V] are stored in CSV files. The following expressions are used to evaluate the performance of the neural network:

Root Mean Square Error – It is used to evaluate the performance which is defined as –

$$RMSE = \sqrt{1/N \sum_{i=1}^{N} \left(V_{(i)} - V_{(model)}\right)^2}$$

Relative Reduction Error – It is used to denote the improvement of the current models over SPMT –

$$RER = \frac{RMSE_{spmt} - RMSE_{hybrid}}{RMSE_{spmt}}$$

2.3 Neural Network setup

The Artificial Neural Network is a system motivated by the functioning of biological neurons. It is a processing architecture based on the human brain focusing on information representation by its ability to learn and adapt. They are commonly used to solve problems of classification, prediction, categorization, and optimization. They are also used in function fitting, data clustering and pattern recognition.

In general, an artificial neural network consists of three main layers as shown in Fig.2; an input layer with nodes to symbolize the input variables, one or more hidden layers with nodes that assist to reproduce the nonlinearity between the input and output, and an output layer to represent the output variable. The processing operation takes place at each neuron of both the hidden layer and output layer through the activation function. The input layer takes the input and forwards it to the first hidden layer. A hidden layer makes a nonlinear transformation of its input. For instance, the first hidden layer will transform x into ϕ (Wx + b),

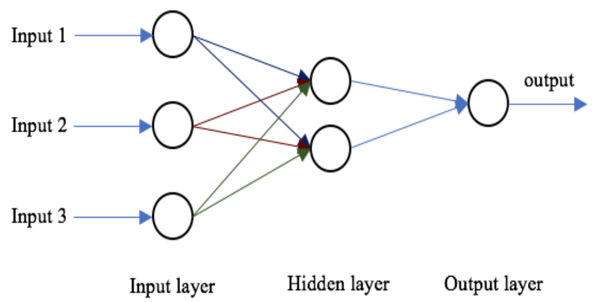

Fig:2 General Architecture of the Neural Network

where ϕ is a chosen nonlinear mapping often called an activation function, W is the weight matrix, and b is a correction term. The following hidden layers then run the same nonlinear transformation in sequential order. The model for training the data has been used as shown in Fig.3

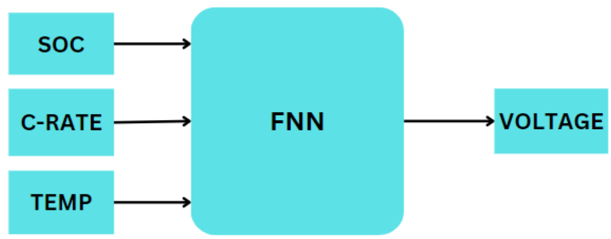

Fig.3 Block diagram of Neural Network Model shown output discharge capacity with the input parameters.

3. Results

Table.2: The RMSE and RER values at different C-rates

C_RATE	RMSE_SPMT	RMSE_HYBRID	RER
0.1	0.161677598	0.022796551	85.8
0.2	0.168122799	0.02868342	82.9
0.4	0.170615812	0.037925313	77.77
0.8	0.171122261	0.055680397	67.46
1	0.196030555	0.056294905	66.18
2	0.248116031	0.128522861	48.20
4	0.301769424	0.158051057	47.62
6	0.328343209	0.198475867	39.55
8	0.360787193	0.242935716	32.66
10	0.391214096	0.287422011	26.53

By using the expression for RMSE. we calculate the RMSE values

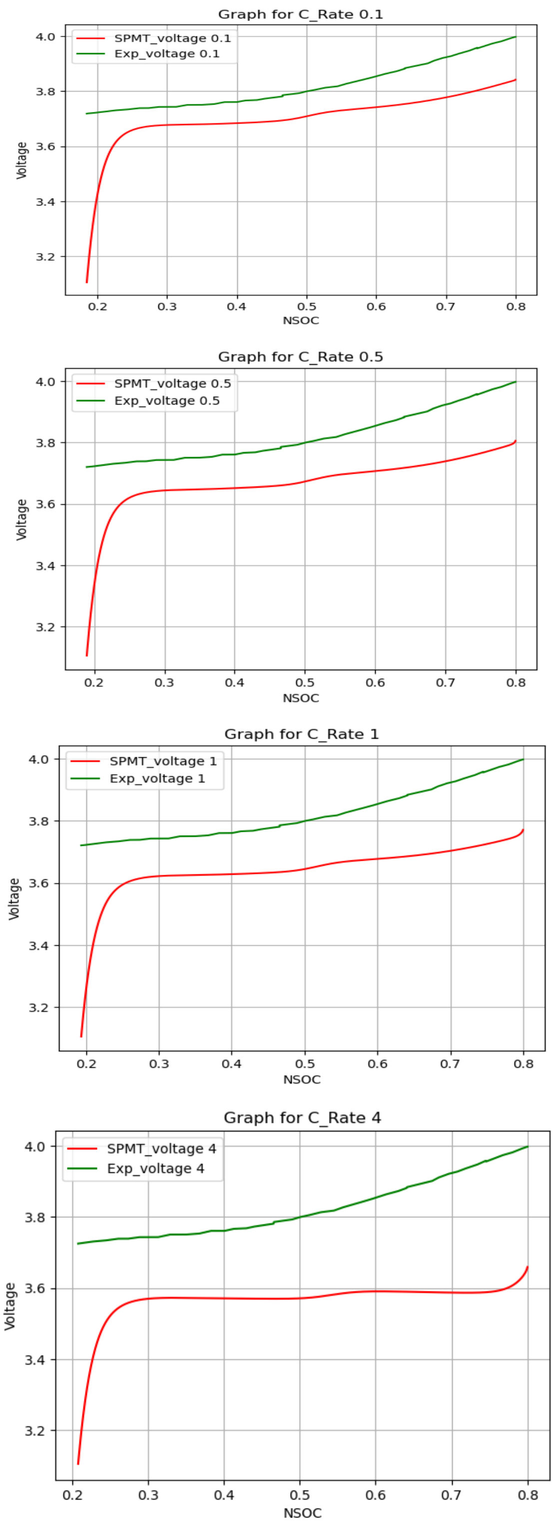

Fig.4 The graph shows the Experimental voltage and SPMT voltage over the SOC range of 0.2 to 0.8 for the C-rates of 0.1, 0.5, 1 and 4.

for the SPMT model and the FNN model for each C-rate value. The RMSE for the SPMT model is determined by using the SPMT_VOLTAGE and EXP_VOLTAGE values the values can be seen in Fig.4 for 0.1, 0.5, 1 and 4 C-rate. Similarly, other values at various c-rates are also considered and the RMSE for the FNN model is determined by utilizing the PREDICTED_VOLTAGE and EXP_VOLTAGE values. From the obtained values we can confirm that the RMSE_FNN values are better as compared to the RMSE_SPMT values. In order to get the margin by which the FNN values are better than SPMT, we calculate the RER values. From the RER values, it is confirmed that the FNN model consistently beats the SPMT model at different values of C-rates.

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4. Conclusion

The ever-increasing demand of Lithium-ion batteries is pressing the high demand for accurate and computationally efficient models. In this paper, we proposed the physics based mathematical model to predict the output voltage, state of charge and temperature of the Lithium-ion batteries. We conducted extensive simulations for the above-mentioned parameters using neural networks to get much higher accuracy compared to physics-based models. We estimated the output voltage for varying C-rates and for random current functions. We used the predicted voltage to estimate each battery parameter considering we don't know it for its analysis. We compared the predicted results with the original one and found significantly good accuracy. Our future work will include the estimation of the state of health of the battery for varying loads on the battery and for the aging of the battery.

5. References

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[2] Sulzer, Valentin & Marquis, Scott & Timms, Robert Robinson, Martin & Chapman, S. (2020). Python Battery Mathematical Modelling (Pybamm). 10.1149/osf.io/67ckj.