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Application of artificial neural networks in design of lithium-ion batteries

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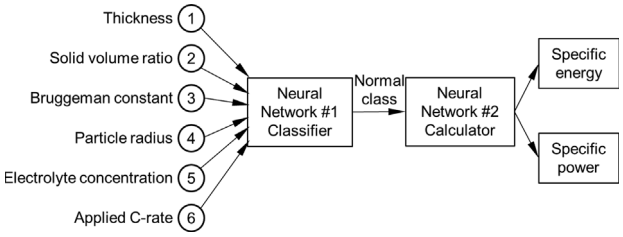
HIGHLIGHTS

- Neural networks are constructed using data from finite element simulations.
- Neural network classifies design variables based on specific energy capability.
- Neural network predicts battery performance with negligible computational cost.
- Global sensitivity analysis is performed to identify key impact variables.
- A design map is generated to satisfy both energy and power requirements.

GRAPHICAL ABSTRACT



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ABSTRACT

Simulation-based battery design encounters the difficulty of high computational cost. This paper presents a systematic approach based on the artificial neural network to reduce the computational burden of battery design by several orders-of-magnitude. Two neural networks are constructed using the finite element simulation results from a thermo-electrochemical model. The first neural network serves as a classifier to predict whether a set of input variables is physically feasible. The second neural network yields specific energy and specific power. Both neural networks are validated using extra finite element simulations out of the training data. With a global sensitivity analysis using the neural network, we quantify the effect of input variables on specific energy and specific power by evaluating large combinations of input variables, which is computationally prohibitive for finite element simulations. Among all parameters, the applied C-rate has the largest influence on specific power, while the electrode thickness and porosity are the dominant factors affecting specific energy. Based on this finding, we generate a design map that fulfills the requirements of both specific energy and specific power. Inparticular, we highlight the value of neural network in handling the non-linear, complex and computationally expensive problem of battery design and optimization.

1. Introduction

Lithium-ion batteries have been widely used in various applications, ranging from consumer electronics to electric vehicles. To satisfy the ever-growing demands for higher energy and power capability, durability and safety of batteries, the design of lithium-ion batteries has become essential to avoid any unexpected loss of performance. Battery design based on experiments is time-consuming and expensive. In contrast, simulation-based design is not only more efficient, but also provides deeper insights into the mechanisms governing the battery performance.

Serving as a crucial step for simulation-based design, battery modeling has attracted growing interests. The majority of current battery models are based on the pseudo two-dimensional (P2D) electrochemical

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model, which is based on the porous electrode theory [1]. The P2D model has been used to optimize the cathode and anode thickness, porosity, particle size and many other important electrode parameters [2–4].

The lithium-ion battery is inherently a multi-physical system. A representative example showing its multi-physical nature is the interplay between electrochemical and thermal behaviors. Heat generated by electrochemical reactions alters the temperature distribution of the electrode, which successively affects the electrochemical processes. Note that many properties of battery components, such as the electrolyte diffusivity and conductivity, are strongly related to temperature [5]. Thus, an accurate simulation often requires a thermal model to be coupled with the P2D model. In order to appropriately address the thermal effect, researchers have contributed in thermal property characterization [6], heat generation rate measurement [7] and thermo-electrochemical coupled modeling [8–10].

Despite the significant progress in the thermo-electrochemical coupled modeling of lithium-ion batteries, there remains a large gap between modeling and simulation-based design. The computational cost can be prohibitively high if a fully-coupled thermo-electrochemical model is directly applied for battery design. In simulation-based battery design, thousands of simulations are often required to determine the optimal design variables. Moreover, the complex non-linear nature of the battery model may result in convergence problems under some sets of design variables. Besides, sensitivity of the design variables is also difficult to analyze due to the very high computational cost. Without sensitivity analysis the possible reduction of design space through eliminating insensitive design variables becomes inapplicable.

Recently, artificial neural networks (ANNs, also termed simply as neural networks (NNs) when there is no ambiguity) has been shown to solve complex non-linear problems. A notable example is the application of deep neural networks in the state-of-the-art artificial intelligence of Go [11]. Loosely analogous to biological neuron systems, ANN is a computational model that consists of a large collection of connected artificial neurons. The neurons and their connections can be trained with data to represent the relations between inputs and outputs. Compared to the physical modeling, ANN has advantages in predicting the output without the knowledge of the exact information of the modeled system. Another benefit of ANN is its computational efficiency, which enables its deployment in real-time applications. ANN has been extensively used in computer science, finance, engineering and many other fields. In the field of battery the ANN approach has been explored for state-of-charge (SOC) estimation [12,13]. However, ANN has not received enough attention for battery design. Considering the potential of ANN for handling highly nonlinear complex problems with significant computational cost, we propose an approach combining the strengths of physical modeling and ANN.

The objective of this paper is to present a method of applying the neural network in simulation-based battery design. Using the simulation results from the electrochemical-thermal model as training data, we obtained two neural networks with satisfactory accuracy. The first neural network, acted as a classifier, is used to predict whether a set of input variables is physically feasible. The second neural network is used to calculate the specific energy and specific power for any given set of input variables. These two trained neural networks are used to perform very large-scale Monte Carlo simulations, which are computationally too expensive to be achievable using the finite element method (FEM). The analysis of Monte Carlo simulation results provides many important insights in the battery design. In this paper, we first demonstrate that this neural network can be used to generate the Ragone plot, which is an important characteristic curve for electrochemical devices. Second, a global sensitivity analysis based on the Monte Carlo simulation results provides a sensitivity ranking of the input variables on specific energy and specific power. This ranking helps identify the limiting process inside the battery, thus reducing the design space. The sensitivity analysis can also help understand the influence of input inaccuracy on the outputs, thus determining the acceptable inaccuracy range for each input parameter. Finally, we characterize the battery performance with respect to most sensitive parameters, and generate a design map to satisfy the requirements of both specific energy and specific power.

2. Methodology

The first step in constructing a neural network is to determine the inputs and outputs. We are particularly interested in design variables that can be controlled in battery manufacturing. As the two most important battery performance indicators, specific energy and specific power are selected as outputs. Once the input variables are determined, we sample representative sets of variables using the design of experiments (DOE) algorithms. Using the sampled variables as inputs, a thermo-electrochemical finite element model is run to yield specific energy and specific power. The inputs and associated outputs are utilized to train the neural network. In order to validate the neural network, we compare predictions from the finite element simulation and the neural network. Once the artificial neural network is constructed with satisfactory accuracy, Monte Carlo simulations are performed for further analysis, such as the global sensitivity analysis and optimization.

2.1. Electrochemical and thermal modeling

We use the P2D model, as listed in Table 1, to resolve the solid concentration in the particle domain (the coordinate along particle radius is denoted as r), and the electrolyte concentration, electrolyte potential and solid potential in the electrode domain (the coordinate along electrode thickness is denoted as x). We denote the thickness of the negative electrode as L_n, the thickness of the separator as L_s, and the thickness of the positive electrode as L. The negative electrode, the separator and the positive electrode occupy the regions of $0 \le x \le L_n$, $L_n \le x \le L_n + L_s$, and $L_n + L_s \le x \le L_n + L_s + L$, respectively.

Table 1
Governing equations and boundary conditions of the electrochemical model.

Domain	Governing Equations	Boundary and Initial Conditions
Particle	$\frac{\partial c_s}{\partial t} = \frac{D_s}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c_s}{\partial r}\right)$	$r = 0$: $\frac{\partial c_s}{\partial r} = 0$; $r = r_p$: $D_s\frac{\partial c_s}{\partial r} = -\frac{i}{F}$; $t = 0$: $c_s = c_{s0}$.
Electrode	$\frac{\partial}{\partial x}\left(\sigma_s^{eff}\frac{\partial \Phi_s}{\partial x}\right) - a_s i = 0$	$x = 0$: $\Phi_s = 0$; $x = L_n$: $\frac{\partial \Phi_s}{\partial x} = 0$; $x = L_n + L_s$: $\frac{\partial \Phi_s}{\partial x} = 0$; $x = L_n + L_s + L$: $\sigma_s^{eff}\frac{\partial \Phi_s}{\partial x} = -i_{app}$.
	$\frac{\partial}{\partial x}\left(\kappa_e^{eff}\frac{\partial \Phi_e}{\partial x} + \kappa_D^{eff}\frac{\partial \ln c_e}{\partial x}\right) + a_s i = 0$	$x = 0$: $\frac{\partial \Phi_e}{\partial x} = 0$; $x = L_n + L_s + L$: $\frac{\partial \Phi_e}{\partial x} = 0$.
	where $\kappa_D^{eff} = -\frac{2RT\kappa_e^{eff}}{F}\left(1 + \frac{d\ln f_{\pm}}{d\ln c_e}\right)(1 - t_+)$	
	$\varepsilon_e\frac{\partial c_e}{\partial t} = \frac{\partial}{\partial x}\left(D_e^{eff}\frac{\partial c_e}{\partial x}\right) + \frac{(1-t_+)}{F}a_s i$	$x = 0$: $\frac{\partial c_e}{\partial x} = 0$; $x = L_n + L_s + L$: $\frac{\partial c_e}{\partial x} = 0$; $t = 0$: $c_e = c_0$.