Artificial Neural Network Simulation of Battery Performance

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Abstract

Although they appear deceptively simple, batteries embody a complex set of interacting physical and chemical processes. While the discrete engineering characteristics of a battery, such as the physical dimensions of the individual components, are relatively straightforward to define explicitly, their myriad chemical and physical processes, including interactions, are much more difficult to accurately represent. Within this category are the diffusive and solubility characteristics of individual species, reaction kinetics and mechanisms of primary chemical species as well as intermediates, and growth and morphology characteristics of reaction products as influenced by environmental and operational use profiles. For this reason, development of analytical models that can consistently predict the performance of a battery has only been partially successful, even though significant resources have been applied to this problem. As an alternative approach, we have begun development of a non-phenomenological model for battery systems based on artificial neural networks. Both recurrent and non-recurrent forms of these networks have been successfully used to develop accurate representations of battery behavior. The connectionist normalized linear spline (CNLS) network has been implemented with a self-organizing layer to model a battery system with the generalized radial basis function net. Concurrently, efforts are under way to use the feedforward back propagation network to map the "state" of a battery system. Because of the complexity of battery systems, accurate representation of the input and output parameters has proven to be very important. This paper describes these initial feasibility studies as well as the current models and makes comparisons between predicted and actual performance.

1. Introduction

We have initiated an effort to reduce design and manufacturing defects, as well as the time and cost for product realization through the use of advanced design and production technologies. Historically, battery development has relied heavily on a very pragmatic "build and test" approach to demonstrate that a particular design can meet the requirements of an application. Due to the time-intensive nature of the testing that is needed, this point design approach is expensive and typically has difficulty responding to changing or divergent sets of requirements. Power source performance and manufacturing models will alleviate these problems, and provide enhanced capability for evaluating product performance, reliability, and life. The availability of advanced design tools will also facilitate product improvements by linking specific design features with desirable performance attributes. In order to accomplish this, an infrastructure of proven models, tools, and processes will be necessary. Toward this end, we are implementing a model-based design approach for power sources, beginning with model development for some types of lithium ambient-temperature batteries.

A battery comprises a complex set of interacting physical and chemical processes, the purpose of which is the conversion of chemical energy into electrical energy. For this conversion process to occur, chemical species must be physically present at the electrode surface. The transport of species to the surface can occur in several ways, including diffusion, migration, or convection. Once at the surface, or at least in the near-surface region of the electrode, these species interact at the atomic and/or molecular level. These interactions, which are controlled by the thermodynamics and kinetics of the reactions of chemical species present in the near surface region of the electrode,

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ultimately result in the transfer of at least one electron at each electrode. Besides these two electron transfer reactions (the cell half reactions), the species can undergo other chemical reactions, or may precipitate from solution. After reaction, the products are often transported away from the electrode. There are also many other processes occurring that may affect battery behavior such as long-term decomposition or corrosion of the constituents and other non-Faradaic side reactions. The formation kinetics and morphology of the products are often strongly influenced by the battery environmental conditions and use profile. In fact, due to the shear number and complexity of the processes taking place, and our inability to accurately describe some of them, it was not clear that an accurate phenomenological battery model could be developed.

In spite of these difficulties, there are countless papers describing various attempts to model cell behavior using a variety of computational approaches, including closed form, finite element, and finite difference. In fact, in our effort to develop useful engineering tools, we are also sponsoring development of a comprehensive parametric model of electrical performance for the lithium/thionyl chloride battery. The strength of the parametric approach is in its ability to link calculations of performance with individual cell components or actual cell processes, and to be able to easily handle a variety of cell designs by simply changing the appropriate parameters.

As an alternative to this approach, we have completed initial studies of artificial neural networks (ANNs) to simulate battery system behavior. Modeling of power source behavior with ANNs has not been previously demonstrated, but this approach clearly has benefits, for example enhanced computational efficiency. An ANN learns about system behavior by being trained with a set of data that gives examples of measured output for different sets of input conditions. In the power source case, the inputs can include many factors, such as the chemistry, state-of-charge, load profile, size, temperature, and possibly the previous use and environmental history, while the outputs are voltage, current, and deliverable capacity. When modeling with ANNs, time consuming and difficult measurements of the fundamental cell parameters are not necessary since only electrical performance data under the conditions of interest are used for training. The connectionist normalized linear spline (CNLS) network has successfully modeled constant load discharges with a generalized radial basis function set and a feedforward back propagation network is being evaluated for simulation of battery voltages and capacity under variable load and temperature conditions. Although future battery performance is often highly dependent on past behavior and treatment, both recurrent and non-recurrent forms of these networks have been investigated in this study for representing the discharge behavior of primary lithium batteries.

2. Neural Networks Used to Simulate Electrochemical Systems

The ANN is an inductive, or data-based model for the simulation of input/output mappings. The ANN can be used in numerous frameworks to simulate many types of system behavior including physical, financial, and, as will be shown here, electrochemical systems. ANNs require training data to learn patterns of input/output behavior, and once trained, can be used to simulate system behavior within that training space. They do this by interpolating specified inputs among the training inputs to yield outputs that are interpolations of training outputs. The reason for using ANNs to simulate system behavior is that they provide accurate approximations of system behavior and are typically much more computationally efficient than phenomenological models. This efficiency is very important in situations where multiple response or prediction computations are required. Some examples of computationally intensive applications are: (1) optimization of system

performance, (2) system identification, (3) system design, and (4) Monte Carlo analysis of probabilistic system response.

Our ultimate objective is to simulate complex electrochemical systems for both optimization of system performance and system design. ANNs are able to efficiently accomplish this simulation without extensive identification of physical parameters such as cell impedance or diffusion characteristics that are required in parametric models. There are a number of ANN architectures available to facilitate our electrochemical simulation. The structure, rules of operation, and environment for general ANNs have been discussed in detail, for example, in Rumelhart and McClelland [1] and Vanluchene and Sun [2]. Though there are many types of ANNs to accomplish our task, the two used to model battery behavior are the feedforward back propagation network (BPN) and the connectionist normalized linear spline (CNLS) network. The BPN is the most widely used ANN and it is described in detail in many texts and papers, for example Freeman and Skapura [3], and Haykin [4]. The BPN is very general in the sense that it can approximate mappings over a wide range of input dimension. It has been shown that, given sufficient training data, a BPN with at least one hidden layer and sufficient neurons can approximate a mapping to arbitrary accuracy (Hornik, Stinchcombe, and White [5]). The CNLS network is an extension of the radial basis function neural network (Moody and Darken, [6]) and is described in detail in Jones, et. al., [7]. The CNLS net is designed to approximate a functional mapping by superimposing the effects of basis functions that approximate the mapping in local regions of the input space. Because the CNLS net is a local approximation network, it is inefficient for this network to be used in applications involving systems with high dimensional input spaces.

The objective of any mapping ANN can be expressed mathematically using the following input/output notation and terminology. Let $\{x\}$ represent a vector of inputs presented to a system. The system to be simulated operates on the data in $\{x\}$, yielding an output vector $\{z\}$. There is a functional relationship, $\{z\} = g(\{x\})$, for $\{z\}$ and $\{x\}$ where the function $g(.)$ is assumed to be deterministic but unknown. An ANN is constructed so that it can also be used to operate on the inputs $\{x\}$ to yield $\{y\}=h(\{x\})$. The function $h(.)$ is deterministic, has a pre-established framework, and parameters $\{p\}$. The function $h(.)$ will be an approximation to the system function $g(.)$. Given a sequence of input/output exemplars $\{x_j\}$ and $\{z_j\}$, j=1,...,R, we seek to adjust the parameters $\{p\}$ of the ANN to minimize the error between the actual system output $\{z\}$ and the ANN output $\{y\}$, when presented with the same input $\{x\}$. This is accomplished through a training process that involves error minimization through variation of the parameters $\{p\}$. The error minimization can be performed using a local search (for example, gradient search, least mean square, Newton's method) or global search (for example, simulated annealing, genetic algorithm). Once training is complete, it is hoped that, given an input $\{x\}$ different from those used during training, an ANN will yield outputs $\{y\}$, that are accurate approximations of the outputs $\{z\}$ produced by the system being modeled. The ANN serves as an interpolator of output vectors among the output exemplars as a function of the position of the input vector among the input exemplars. A diagram of this process is shown in Figure 1.

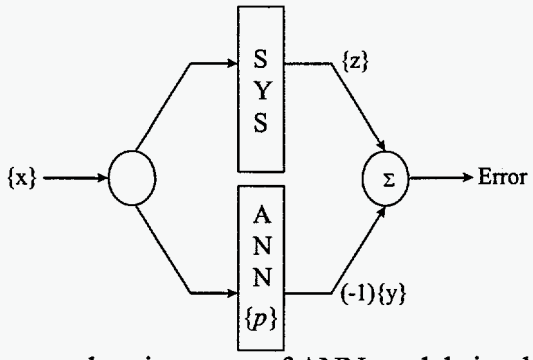

Figure 1. Diagram showing error of ANN model simulating system.

ANNs can be used simply to map inputs to outputs without reference to their temporal ordering, or they can be used to map system characteristics at time index t_j to the same characteristics at time index t_{j+1}. The latter form of ANN is called recurrent. We mention this framework for use of ANNs because we have briefly used them to model some aspects of battery behavior with the CNLS network. In addition, these recurrent nets may prove useful in the modeling of the temporal evolution of electrochemical system behavior under both constant and pulsed conditions.

3. Modeling of Electrochemical Systems with ANNs

As mentioned previously, many attempts have been made in different frameworks to model electrochemical systems. Because these systems are so complex, the ability to develop an accurate parametric model that can be used for both optimization of performance and system design has been limited; therefore, time-consuming build and test procedures remain the norm. Therefore, using ANNs to efficiently simulate and predict the behavior of these systems could prove to be extremely cost and time effective while improving system performance. The electrochemical system used for these studies of ANN modeling is the lithium/thionyl chloride battery. The challenge in this investigation is to use relatively simple but specialized experimental results to build a model that accurately and efficiently reflects real battery behavior under complex use profiles. Simulations of this battery system progressed from simple constant load discharges to more complex and practical simulations including temperature variation and load pulses. Recurrent and non-recurrent forms of neural networks were used in this study. Results of a sequence of model developments are presented in the following discussion.

Initial feasibility studies began by simply trying to replicate a discharge curve of the lithium/thionyl chloride battery with the CNLS network. Figure 2 shows a non-recurrent simulation of the battery voltage under a constant discharge load of 50 ohms at 25°C. As can be seen in the figure, the simulation approximates the experimental data very well. Because one of the major interests in this feasibility study is to determine if ANNs are able to predict the amount of capacity delivered by a battery, it is important that the nets be able to simulate the discharge curve near the "knee", i.e., where the voltage begins to drop. In this case, that is near 200 hours of discharge. Although the exemplars used to train the CNLS network are largely concentrated at about 3.5 volts (0 hours - 200 hours), the network was still able to capture the dynamics of the discharge at the knee. This is due to the local approximation capability of the radial basis functions used in the CNLS network.

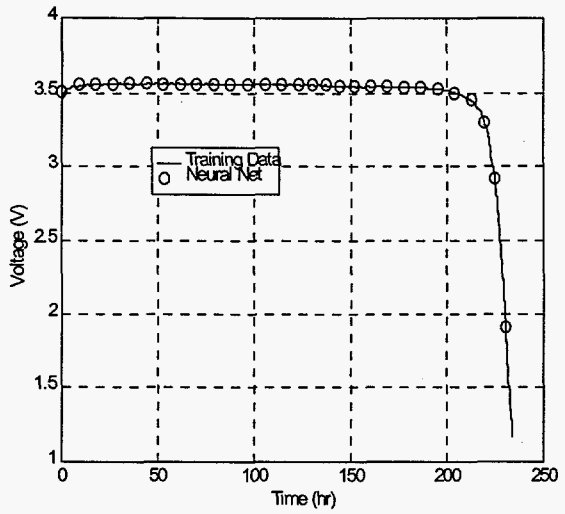

Figure 2. Non-recurrent CNLS simulation of battery voltage data (50 ohm discharge load, 25°C)

The next practical test was to simulate this curve with a recurrent form of the CNLS net. The recurrent simulation is shown in Figure 3. This simulation predicts voltage (v_j) using time (t_j) and only one delayed network prediction of voltage (v_{j-1}) as inputs. The recurrent CNLS net simulated the experimental data very well with some minor degradation of predictions at the knee of the voltage-time curve compared to the non-recurrent case. The main source of error in this application arises from the iterated nature of the simulation. When the simulated voltage departs from the experimental curve, the error tends to persist because the predicted voltage at time t_j is based on a predicted voltage at time t_{j-1}. In order to diminish the chance of instability in response prediction, we added noise to the input exemplars to develop additional training sets, and used these in the training process. This provided robustness in the ANN predictions that diminished the potential for instability.

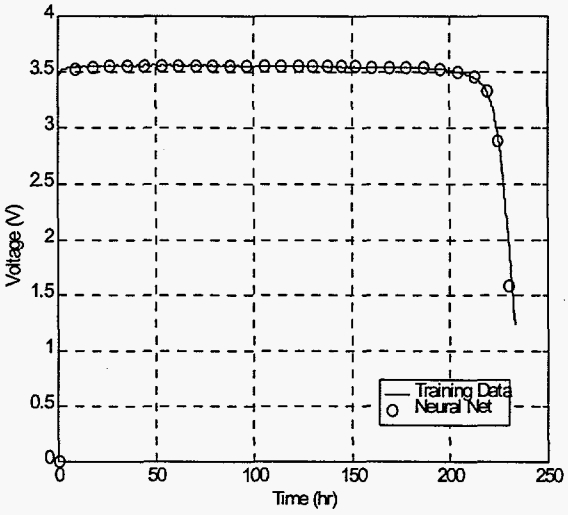

Figure 3. Recurrent CNLS simulation of battery voltage data (50 ohm discharge load, 25°C).

Both the non-recurrent and recurrent CNLS simulations of the battery data under constant load conditions were accurate. Our next step in increasing the complexity of ANN simulations was to

model a system with different loads. This was done, and the results are shown in Figure 4. The results indicate that the CNLS network can accurately simulate battery discharge curves with this additional dimension to the input space. Again, the accuracy with which this network predicts the discharge voltage is largely due to the local approximation capability of the CNLS network.

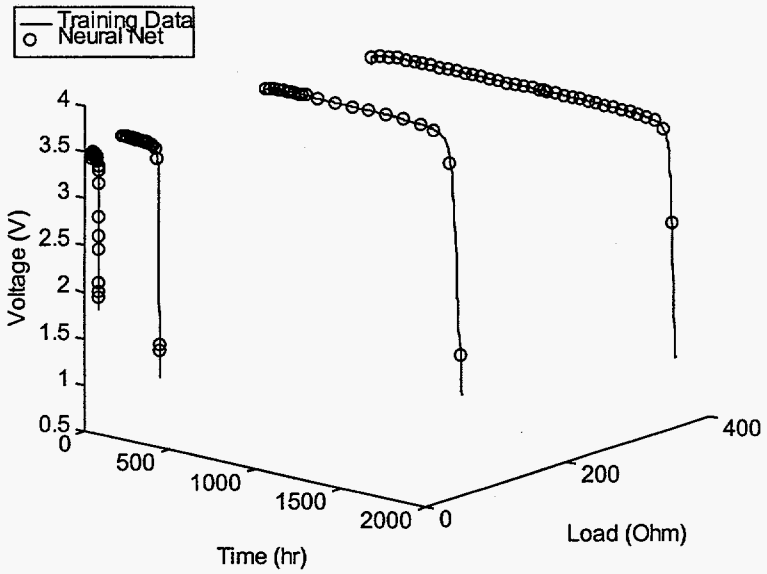

Figure 4. Non-recurrent CNLS simulation with load as an input (T=25°C).

A recurrent simulation using load as an ANN input variable was not possible using the experimental data shown in Figure 4 due to the variation in sample rate used for each individual load discharge.

The CNLS network uses a self-organizing layer on input exemplars to determine the center locations for its radial basis functions. This contributes to the accuracy for local approximations of the network. The advantages of the local approximation, however, were not conducive to the interpolation characteristics desired at this phase of our feasibility study. Therefore, the feedforward back propagation network (BPN) was used to further our investigation of ANN interpolation on battery data. Figure 5 shows the simulation of a constant load discharge at 300 ohms. The BPN was trained with 25°C constant load discharge data at 50, 250, and 400 ohms and an interpolated time series at 300 ohms is presented. The BPN provided very good interpolation characteristics for loads between 50 and 400 ohms.

At this point, we had generated some interpolation results for constant load discharge data (Figure 5). Our next objective was to extend our predictions to pulsed loads and variable temperature. Because little pulsed data were available at this point to use in our training sets, the isothermal, constant load discharge data were used to train the BPN in order to determine whether their use could be extended to pulsed load or pulsed temperature conditions. Specifically, the constant load discharge data available for training are outlined in Table I.

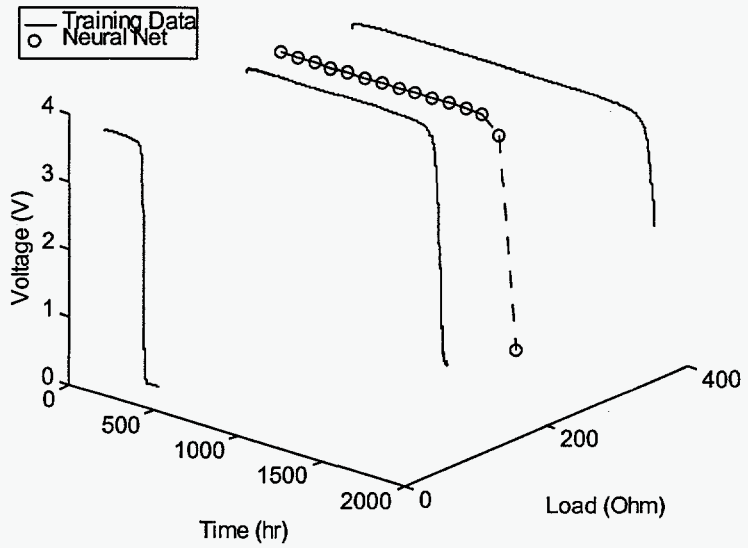

Figure 5. BPN interpolation of a constant load discharge at 300 ohms (T=25°C).

Table I. Constant load, constant temperature data available for ANN simulations.

Load (ohms)	Temperatures (°C)
50	-40, 25, 49
250	-40, 25, 49
400	-40, 25, 49

With these data, we would be able to simulate pulsed loads between 50 and 400 ohms, and temperature variation between -40°C and 49°C, or a combination of both. A load pulse could be simulated if we could determine the rule for an isothermal transition from one constant load discharge curve to another. Figure 6 shows a simulation developed by training the BPN with constant load discharge data at 50 and 250 ohms at 25°C. Once trained, the network was used to simulate a pulsed load condition between these two loads with 3-Amp hour capacity dwells at each load. Note that we have converted the independent temporal variable from time to current capacity used; this introduced a more convenient normalization of the temporal variable. With the pulsed load simulation, we were trying to identify how the deliverable capacity might vary depending on the pulsed load conditions. Because the measured capacity of these battery cells is known to change with load, a critical question is how to map the battery capacity "state" from one load to the other during a pulse. Specifically, the transition could be based on the "fraction of capacity delivered", the "absolute capacity used", or some other rule. One might expect the fraction of capacity delivered to give a better transition between the two loads, but it turned out that absolute capacity used seemed to perform a better mapping in this case. Therefore, this is the transition rule used in the sequel. Further investigation of this mapping rule needs to be done to determine the best forms of transition for all situations.

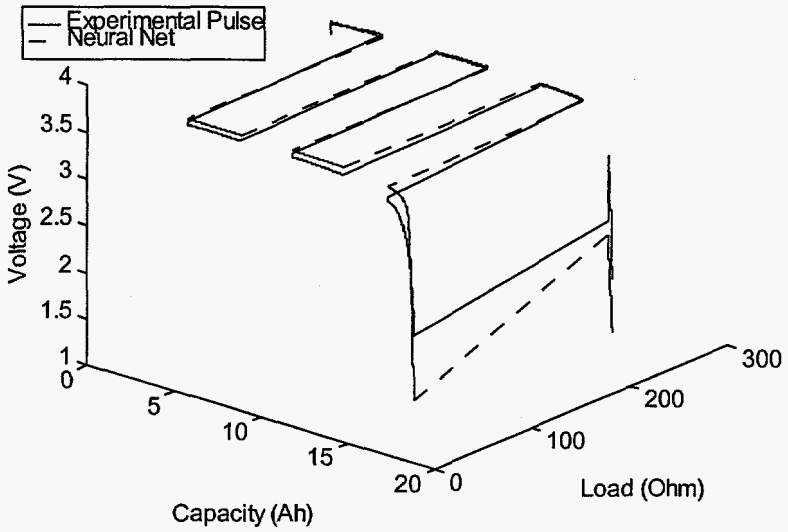

Figure 6. Isothermal pulsed load simulation between 50 and 250 ohms at 25°C.

As mentioned above, the simulation shown in Figure 6 is based on the network being trained with constant load discharge data. The experimental pulse displayed in Figure 6 is based on data that were gathered later. A slight difference is noticeable between the experimental voltage curve and the simulated curve at 50 ohms. The constant load discharge data at 50 ohms that were used to train the BPN had a slightly higher voltage level than the actual pulsed data at that load, which is reflected in this simulation. The simulated pulse also seems to approach failure (voltage < 2V) slightly before the experimental pulse, causing a more rapid drop-off at the knee. Currently, we are testing other batteries with varied load pulse profiles in attempts to fully understand the transition between load curves during pulse discharge and to determine if observed differences between actual and predicted behavior are a result of cell-to-cell variability. Likewise, tests are being run on batteries in which only the temperature is varied so we can identify a rule for the transition from one temperature to another under constant load. In this case, it may be more likely that the "fraction of capacity delivered" rule will be followed for transition as there are greater fluctuations in measured capacity when moving from one temperature to another (especially to low temperatures) than occur over this range of loads. Once further tests are performed and the rules for moving between loads and temperatures are more completely understood, we intend to simulate a profile in which both the load and temperature are pulsed. We currently have experimental data taken under this type of condition. Specifically, the temperature cycle consisted of a cold, an ambient, and a hot level while the load was pulsed between a very low current background and a moderate on-pulse level. Constant load discharge curves are still being developed for the load range that corresponds to this test. Because our constant load discharge data were available at three different temperatures, an arbitrary simulation was done to predict the battery voltage using a BPN network trained with capacity, load, and temperature inputs. Figure 7 shows this arbitrary simulation of a load and temperature pulse (the three solid lines at each load represent the three temperatures used in training).

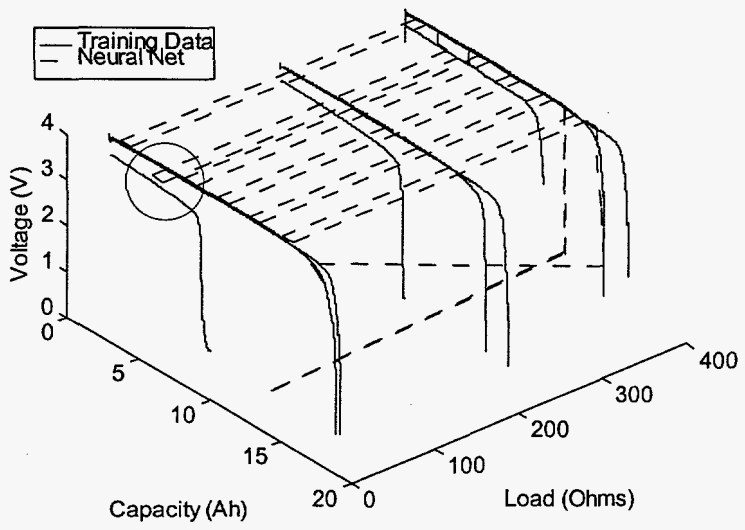

Figure 7. ANN simulation of arbitrary load and temperature pulse.

The important characteristics to note in this pulse profile are the ability of the network to predict the change in voltage from one temperature to another and that more capacity can be delivered when moving from a low temperature to a high temperature. An example of the network predicting a reduction in voltage moving from a higher to a lower temperature is shown above near 4 Amp hours of capacity removed (circled in the figure). Here, the network predicts a reduction of about 0.5 volts as the temperature is changed from 25°C to -40°C. Near 12 Amp hours removed, the simulation suggests no voltage output from the cell as the temperature is lowered from 25°C to -40°C, but shows capacity still exists when the temperature is returned to ambient. These types of responses shown in the simulation are clearly representative of the battery behavior seen in laboratory experiments and further analysis with ANNs will increase our understanding of discharge behavior under both constant and pulsed conditions.

4. Conclusions

Initial modeling efforts of electrochemical battery systems with artificial neural networks has proven to be very successful. Our feasibility study for this form of non-phenomenological modeling began by looking at single load constant discharge data. Both recurrent and non-recurrent forms of the CNLS network were utilized in simulating these curves. The CNLS network was able to accurately simulate these discharge curves and the local approximation capability of this network allowed excellent representation of the area surrounding the "knee" of the discharge curve. Although the CNLS network performed very well in the input space where training exemplars were located, the interpolation characteristics between load values were not expected to be as good. Efforts to improve the interpolation capabilities of the CNLS net are currently under way. At some point, the CNLS net may be combined with the BPN for battery simulation.

The parameters of the BPN do not explicitly depend on the training exemplars like the centers of the radial basis functions do in our CNLS network. Therefore, the BPN was used to investigate interpolation characteristics of battery data. Specifically, a 300 ohm constant load discharge simulation was performed with the BPN and the results compared very well to what is expected in

the laboratory. The BPN has also been used to simulate pulsed load conditions at constant temperature. The BPN was trained with constant load discharge data as no pulsed data were available. A pulsed load experiment matching the profile of the simulation has now been completed and the ANN prediction compares well to these experimental results (Figure 6). The ability of the BPN network to simulate battery pulsed discharge data when trained with the constant load exemplars is a significant finding of our work.

Our current efforts involve completing a similar experiment with variable temperature under constant load conditions. Once this information is available, we will be able to simulate a battery discharge in which both the temperature and load are arbitrarily changed. With additional experimental pulse data being generated, ANN architecture and training can be optimized to further increase the accuracy of our battery simulations. This will involve ANN training using experimental battery data where temperature and load are varied simultaneously. It is not clear that any simple rule or combination of rules will suffice to generate accurate ANN simulations of real battery behavior. Additional tools like genetic algorithms and/or genetic programming may be used to establish more accurate transition rules.

These initial efforts on battery modeling have proven to be very effective, and more complex simulations of battery behavior can likely be performed. With advanced study of ANN modeling, and the parametric model being developed, it is our hope that an advanced hybrid model can soon be constructed that will help design, optimize, and produce more efficient and robust battery systems.

5. Acknowledgment

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