

Physics-Based Models, Sensitivity Analysis, and Optimization of Automotive Batteries

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ABSTRACT

The analysis of nickel metal hydride (Ni-MH) battery performance is very important for automotive researchers and manufacturers. The performance of a battery can be described as a direct consequence of various chemical and physical phenomena taking place inside the container. In this paper, a physics-based model of a Ni-MH battery will be presented. To analyze its performance, the efficiency of the battery is chosen as the performance measure, which is defined as the ratio of the energy output from the battery and the energy input to the battery while charging.

Parametric sensitivity analysis will be used to generate sensitivity information for the state variables of the model. The generated information will be used to showcase how sensitivity information can be used to identify unique model behavior and how it can be used to optimize the capacity of the battery. The results will be validated using a finite difference formulation.

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INTRODUCTION

There are several different approaches that are used to model car batteries. Most of them can be separated in two main categories. The first approach, also known as the circuit-based approach, tries to model the behavior of the battery as an electric circuit, (Salameh et al. [1], Chen and Rincon-Mora [2] and Seaman and McPhee [3]). This results in a conceptually simple model. However in this approach, the actual physical parameters stay hidden and there is no explicit relationship between the model parameters and the battery parameters. This is precisely the point where the benefit of using a chemistry-based approach becomes apparent. In this second approach, the actual chemical reactions and other electrochemical processes inside the battery are captured (Newman et al. [4] - [6], Dao et al. [7], Wu et al. [8], and Banerjee et al. [9]). Due to its dominance in hybrid vehicles, a Ni-MH battery has been chosen for

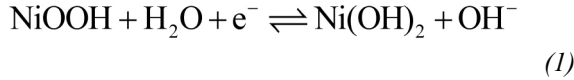
analysis in this paper. The main objective of this work is to perform analytical sensitivity analysis on a physics-based model of a nickel metal hydride battery. The Ni-MH battery model presented here is based on the battery model presented in Wu et al. [8] and Banerjee et al. [9]. This chemistry-based battery model allows users to access physical parameters of the battery directly, which makes this model suitable for design optimization.

Direct differentiation is used to generate the sensitivity equations from the governing equations, which are then solved to evaluate the sensitivities of the state variables with respect to the model parameters. In this paper, the feasibility of the use of sensitivity information for the optimization of NiMH battery model has been discussed.

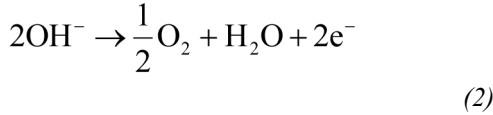
MODELLING OF NI-MH BATTERIES

To capture the electro-chemical phenomenon inside the battery, one needs to start from the basic chemical reactions taking place at the individual electrodes. For this model the following chemical reactions are considered.

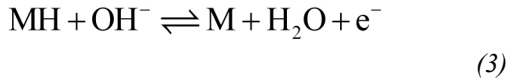
Main reaction on positive electrode:



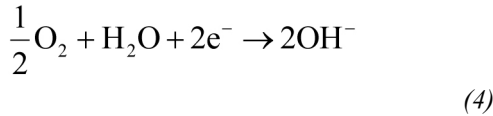
Side reaction on positive electrode:



Main reaction on negative electrode:



Side reaction on negative electrode:



The metal M in the negative electrode is an inter-metallic compound, usually a rare earth compound.

Governing Equations

To model these reactions the effects of two important quantities, that define the generation of the electromotive forces, must be captured properly. The first quantity is known as the open circuit potential difference and is given by the Nernst equation, Equations (5), (6), (7). The quantity ϕ denotes the thermodynamically predicted potential difference of the corresponding Red-ox reactions.

$$\phi_1 = U_1 + (T - T_{ref}) \frac{\partial U_1}{\partial T} + \frac{RT}{F} \ln \left(\frac{c_{\text{H}^+, \text{max}} - c_{\text{H}^+}}{c_e c_{\text{H}^+}} \right) \quad (5)$$

$$\phi_2 = U_2 + (T - T_{ref}) \frac{\partial U_2}{\partial T} + \frac{RT}{2F} \ln \left(\frac{p_{\text{O}_2}^{0.5}}{c_e^2} \right) \quad (6)$$

$$\begin{aligned} \phi_3 = U_3 + (T - T_{ref}) \frac{\partial U_3}{\partial T} - \frac{RT}{F} \ln c_e + 9.712 \times 10^{-4} \\ + 0.23724e^{-\left(\frac{28.057c_{\text{MH}}}{c_{\text{MH}, \text{max}}}\right)} - \frac{2.7302 \times 10^{-4}}{\left(\frac{c_{\text{MH}}}{c_{\text{MH}, \text{max}}}\right)^2} + 0.010768 \end{aligned} \quad (7)$$

The quantities used in the equations (5), (6), (7) are summarized in Table 1 and 2. Detailed description of the terms can be found in Banerjee et al. [9].

Apart from the thermodynamically predicted potential difference, the other important quantity in this context is the over potential, which can be directly related to the rate of chemical reactions using the Butler-Volmer equations.

$$j_i = i_{0,i} \left(e^{\frac{\alpha_i F}{RT} \eta_i} - e^{-\frac{\alpha_i F}{RT} \eta_i} \right) \quad (8)$$

where $i = 1, 2, 3$ are for the reactions given in equations (1), (2), (3). The quantities $i_{0,i}$ are the exchange current densities that are functions of the reactant concentrations and the operating temperature. The exchange current densities are defined at a reference concentration and temperature. But for the purpose of the model, it must be adjusted dynamically to reflect the effects of changing temperature and reactant concentration. The following equations are used for this purpose.

$$\begin{aligned} i_{0,1} = i_{0,1,\text{ref}} \left(\frac{c_{\text{H}^+}}{c_{\text{H}^+, \text{ref}}} \right)^{0.5} \\ \times \left(\frac{c_e}{c_{e,\text{ref}}} \right)^{0.5} \left(\frac{c_{\text{H}^+, \text{max}} - c_{\text{H}^+}}{c_{\text{H}^+, \text{max}} - c_{\text{H}^+, \text{ref}}} \right)^{0.5} e^{\left[\frac{E_{a,1}}{R} \left(\frac{1}{T} - \frac{1}{T_{ref}} \right) \right]} \end{aligned} \quad (9)$$

$$i_{0,2} = i_{0,2,\text{ref}} \left(\frac{c_e}{c_{e,\text{ref}}} \right)^{0.5} \left(\frac{p_{\text{O}_2}}{p_{\text{O}_2,\text{ref}}} \right)^{0.5} e^{\left[\frac{E_{a,2}}{R} \left(\frac{1}{T} - \frac{1}{T_{ref}} \right) \right]} \quad (10)$$

$$\begin{aligned} i_{0,3} = i_{0,3,\text{ref}} \left(\frac{c_{\text{MH}}}{c_{\text{MH}, \text{ref}}} \right)^{0.5} \\ \times \left(\frac{c_e}{c_{e,\text{ref}}} \right)^{0.5} \left(\frac{c_{\text{MH}, \text{max}} - c_{\text{MH}}}{c_{\text{MH}, \text{max}} - c_{\text{MH}, \text{ref}}} \right)^{0.5} e^{\left[\frac{E_{a,3}}{R} \left(\frac{1}{T} - \frac{1}{T_{ref}} \right) \right]} \end{aligned} \quad (11)$$

For the oxygen reduction reaction on the negative electrode, i.e. the reaction shown in equation (4), the expression shown in equation (12) is used for the current density. This acts as a limiting current equation. The model parameters used in these equations are summarized in Table 2.

$$j_4 = -\frac{p_{O_2}}{p_{O_2,ref}} (i_{0,4,ref}) e^{\left[\frac{E_{a,4}}{R} \left(\frac{1}{T} - \frac{1}{T_{ref}} \right) \right]} \quad (12)$$

The battery current can be calculated from the current densities of the reactions at the electrodes.

$$\begin{aligned} i_{cell} &= A_{pos} a_{pos} l_{pos} (j_1 + j_2) \\ i_{cell} &= -A_{neg} a_{neg} l_{neg} (j_3 + j_4) \end{aligned} \quad (13)$$

The mass balance equations for the cell are

$$\begin{aligned} j_1 &= F \frac{dc_{H^+}}{dt} \frac{L_{Ni(OH)_2}}{\rho_{Ni(OH)_2} l_{pos} a_{pos}} \\ j_3 &= F \frac{dc_{MH}}{dt} \frac{L_{MH}}{\rho_{MH} l_{neg} a_{neg}} \\ (A_{pos} a_{pos} l_{pos} j_2 + A_{neg} a_{neg} l_{neg} j_4) &= \\ &F \frac{dp_{O_2}}{dt} \frac{V_{gas}}{RT} \end{aligned} \quad (14)$$

The closed circuit voltage available from the cell can be calculated as

$$v_{cell} = v_{pos} - v_{neg} - i_{cell} R_{int} \quad (16)$$

Where v_{pos} and v_{neg} are the net potential difference between the electrode and the electrolyte solution for the positive and negative electrodes respectively and can be calculated from the open circuit potential differences, i.e. equations (5), (6), (7), and the over-potentials, i.e. equations (8), (12).

$$v_{pos} = \phi_1 + \eta_1 = \phi_2 + \eta_2 \text{ and } v_{neg} = \phi_3 + \eta_3 \quad (17)$$

The energy balance of the whole cell is described by the equation given below.

$$\begin{aligned} c_p m_{cell} \frac{dT}{dt} &= -\left(\frac{k}{e} \right) A_{cell} (T - T_a) \\ &+ |i_{cell} v_{cell}| - \sum_i j_i \left(\phi_i - T \frac{\partial U_i}{\partial T} \right) \end{aligned} \quad (18)$$

For the purpose of analysis it is also useful to define an additional state variable which would represent the state of charge (SOC) of the battery. Mathematically it can be expressed as a function of the concentration of $Ni(OH)_2$.

$$SOC(t) = \frac{c_{H^+,max} - c_{H^+}(t)}{c_{H^+,max}} \quad (19)$$

As mentioned before the current work is based on the model by Wu et al. [8] and Banerjee et al. [9]. The state variables used in the equations presented above are given in Table 1. The various model parameters used in the equations were measured from a 3.9 Amp-h VARTA Ni-MH battery at the Ford Motor Company Scientific Research Laboratory (Wu et al. [8]), and are summarized in Table 2. Further details can be found in Banerjee et al. [9].

Table 1. List of generalized states

States	Unit	Description
c_{H^+}	Mol/cm ³	Concentration of $Ni(OH)_2$
T	K	Temperature of the battery
c_{MH}	Mol/cm ³	Concentration of metal hydride
SOC	Unitless	State of charge
v_{cell}	Volts	Cell voltage
v_{pos}	Volts	Positive electrode potential
v_{neg}	Volts	Negative electrode potential
p_{O_2}	Atm	O ₂ pressure inside the battery
ϕ_1	V	Open circuit potentials
ϕ_2	V	
ϕ_3	V	
j_1	A/cm ²	Current densities for reactions
j_2	A/cm ²	
j_3	A/cm ²	
j_4	A/cm ²	
η_1	V	Over voltages
η_2	V	
η_3	V	
$i_{0,1}$	A/cm ²	Exchange current densities
$i_{0,2}$	A/cm ²	
$i_{0,3}$	A/cm ²	