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Short communication

Numerical simulation and optimization of nickel–hydrogen batteries

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Abstract

A three-dimensional, transient numerical model of an individual pressure vessel (IPV) nickel–hydrogen battery has been developed based on energy conservation law, mechanisms of heat and mass transfer, and electrochemical reactions in the battery. The model, containing all components of a battery including the battery shell, was utilized to simulate the transient temperature of the battery, using computational fluid dynamics (CFD) technology. The comparison of the model prediction and experimental data shows a good agreement, which means that the present model can be used for the engineering design and parameter optimization of nickel–hydrogen batteries in aerospace power systems. Two kinds of optimization schemes were provided and evaluated by the simulated temperature field. Based on the model, the temperature simulation during five successive periods in a designed space battery was conducted and the simulation results meet the requirement of safe operation.
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Keywords: Nickel–hydrogen battery; Computational fluid mechanics; Transient model; Numerical simulation; Temperature field

1. Introduction

Nickel–hydrogen technology is originally built up around individual pressure vessel (IPV) designs. Since 1983, there has been a gradual shift away from nickel–cadmium to nickel–hydrogen energy storage by many space programs [1]. The nickel–hydrogen battery is a desirable alternative for traditional batteries due to its higher energy density, high rate capability, long cycle life, and free of poisonous materials [2]. However, the nickel–hydrogen batteries retain huge heat and less uninformed temperature profiles under large loads or rapid charge/discharge, seriously leading to the performance fade [3]. Battery failure could also result from excessive temperature rise and steeper temperature gradient within a battery [4]. Therefore, it is of primary importance to study the temperature field of nickel–hydrogen batteries.

Traditionally, experimental testing is a main tool to test and design batteries. However, experiments are time consuming and costly, and experimentally it is difficult to determine the internal process during charge and discharge [2]. With the rapid development of computer technology, modeling and simulation have become an indispensable approach in the design and optimization of many engineering systems [5]. Modeling and simulation are powerful methods for identifying battery mechanisms, predicting the cell performance for design and optimization, and reducing the cost and time expended on the experiments. Gu et al. [6] constructed a three-phase electrochemical model for nickel–metal hydride cells using the micromacroscopic coupled approach. Shi et al. [3] developed a two-dimensional thermal model to predict the temperature distribution of cylindrical 8-Ah Ni/MH battery. However, there are few publications on three-dimensional thermal model of IPV batteries for analysis and design.

In the present work, a three-dimensional, transient thermal model of an IPV nickel–hydrogen battery was constructed for simulating and analyzing the temperature field of the battery with different design and operational conditions.

Abbreviations: IPV, individual pressure vessel; CFD, computational fluid dynamics.

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Nomenclature

c	specific heat ($J\,kg^{-1}\,K^{-1}$)
E	battery voltage (V)
E_H	heat value voltage of battery (1.508 V)
F	Faraday constant (96,487 $C\,mol^{-1}$)
ΔH_R	enthalpy of charging reactions (145.50kJ mol^{-1})
ΔH_{SR}	enthalpy of charging side reactions (285.83 kJ mol^{-1})
I	total current (A)
I_d	total discharge current (A)
n	amount of gain and loss electrons in electrochemical reactions
P	pressure of battery cavity (atm)
q_0	heat-generation rate by oxygen recombination (W)
Q	energy source item ($W\,cm^{-3}$)
t	time (s)
T	temperature (K)
V	volume of battery cavity (m^3)
V_d	operation voltage (V)
V_{Ni}	volume of nickel electrode (m^3)

Greek letters

η	charging current efficiency
λ	thermal conductivity ($W\,cm^{-1}\,K^{-1}$)
ρ	density ($kg\,cm^{-3}$)

2. Operational principle and geometric model of the IPV nickel–hydrogen battery

2.1. Operational principle of the IPV nickel–hydrogen battery

"Back to back" stacking arrangement was used in the IPV nickel–hydrogen battery [1]. The electrode stack was contained in a sealed pressure vessel that was filled with certain-pressure hydrogen gas. Fig. 1 shows the structure of an electrode stack.

Shown in Fig. 1, the electrode stack is surrounded by hydrogen gas. The positive nickel electrode is filled with electrolyte in its pore structure. The negative platinum electrode is filled with hydrogen gas in its spacing. The polypropylene separator filled with electrolyte is placed between the nickel and platinum electrodes.

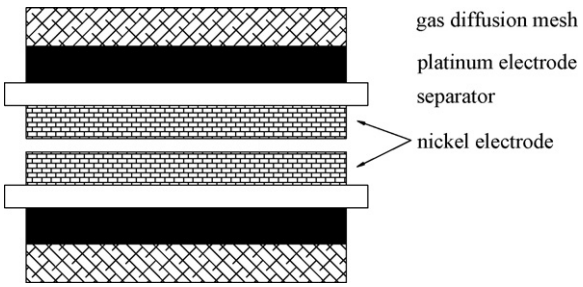

Fig. 1. Schematic diagram of an electrode stack.

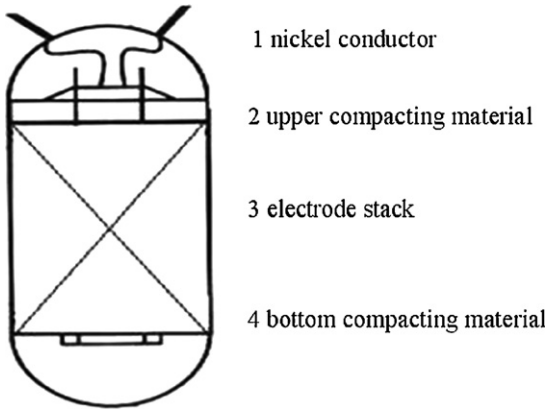

Fig. 2. Framework of an IPV battery.

Electrochemical reactions in the nickel–hydrogen battery are given below [1,5,7,8]:

At the nickel electrode $NiOOH + H_2O + e^- \underset{\text{charge}}{\overset{\text{discharge}}{\rightleftharpoons}} Ni(OH)_2 + OH^-$ (1)

with the side reaction $2OH^- \rightarrow \frac{1}{2}O_2 + H_2O + 2e^-$ (2)

At the platinum electrode $\frac{1}{2}H_2 + OH^- \underset{\text{charge}}{\overset{\text{discharge}}{\rightleftharpoons}} H_2O + e^-$ (3)

with the side reaction $\frac{1}{2}O_2 + H_2O + 2e^- \rightarrow 2OH^-$ (4)

Net reactions within the battery $NiOOH + \frac{1}{2}H_2 \underset{\text{charge}}{\overset{\text{discharge}}{\rightleftharpoons}} Ni(OH)_2$ (5)

2.2. Geometric model of the IPV nickel–hydrogen battery

Generally, the electrode stack of an IPV nickel–hydrogen battery is composed of back-to-back single chip cells that are in turn connected in parallel [1]. The electricity generated from the electrochemical reactions is conducted outside by its nickel conductor. Fig. 2 shows the framework of an IPV nickel–hydrogen battery. The components of an IPV nickel–hydrogen battery as shown include (from top to bottom) nickel conductor (pos. 1), upper compacting material (pos. 2), the electrode stack (pos. 3), bottom compacting material (pos. 4), with the rest areas full of hydrogen gas.

The electrode stack of a nickel–hydrogen battery consists of 26 single chip cells, with a gas diffusion mesh between every two single chip cells. The physical and thermal properties of electrode stack and shell is listed in Table 1. The materials and some physical aspects of a single chip cell are given in Table 2.

In fact, internal configuration of an actual IPV nickel–hydrogen battery is more complex. Polysulfone materials and internal nickel conductor both have irregular structures. Much spacing exists in the interior electrode stack

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