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Multi-dimensional modeling and large-scale simulation of hydrogen absorption/desorption phenomena in metal hydride vessels (MHVs)

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ABSTRACT

In this paper, a three-dimensional (3-D) hydrogen absorption/desorption model is applied to two different real-scale metal hydride vessels (MHVs). The model is then validated against experimentally measured metal hydride temperature and H/M ratio evolution data from a hydrogen charge/discharge cycle. The two experimental vessels were designed to have identical dimensions and contain the same mass of ZrCo (125 g), but one is loaded with copper fins and the other with copper foams. Since the real-scale vessel geometries involve several million computational grid points, a parallel computational methodology has been employed to reduce the computational turnaround time. This comparison highlights this substantial improvement in agreement between simulation and experiment obtained by conducting full-scale simulations of the whole MHVs. In addition to model validation, detailed key contours are analyzed to elucidate hydrogen charge/discharge characteristics in whole-scale MHV geometries. This study demonstrates the validity of our 3-D hydrogen absorption/desorption model for optimization of practical MHV design and operating conditions.

1. Introduction

Obtaining the internal heat transfer capability required for fast hydrogen charging and discharging is a key factor for metal hydride vessel (MHV) optimization. Many researchers have presented heat transfer vessel designs with improved hydrogen charging and discharging performance [1–5]. Kang et al. [1] tested a thin double-layered annulus MHV and achieved hydrogen charging and discharging rates of 72.5 Pa m^3 s^{-1} and 15.6 Pa m^3 s^{-1}, respectively. They then compared the copper foam and copper fin based MHV designs during the hydrogen absorption/desorption processes [2]. Dhaou et al. [3] fabricated MHVs equipped with a finned spiral heat exchanger and tested hydrogen absorption and desorption performance. They clearly showed that the finned spiral heat exchanger substantially reduced charging time. Andreasen et al. [4] conducted hydrogen desorption tests using MHVs equipped with various aluminum fin configurations. Their experimental data showed that the thermal gradient inside the MHV was reduced as a result of the internal and external fins, successfully demonstrating improved heat transfer capability. Singh et al. [5] designed an MHV with a finned tube heat exchanger comprising annular copper fins and copper flakes, and then experimentally investigated the effects of inlet pressure and coolant temperature on the hydrogen charge performance. They attained the shortest charging time, 490 s at an inlet pressure of 15 bar and coolant temperature of 288 K.

Meanwhile, a parallel effort has been made by several MHV modeling groups to simulate the hydrogen charging and discharging processes in MHVs with various heat transfer enhancements [6–13]. Melnichuk et al. [6] developed a one-dimensional (1-D) MHV model and numerically compared the heat transfer performance between heat-fin and honeycomb typed MHV designs during hydrogen absorption. Their simulation results indicated that faster heat removal was achieved with the heat-fin design, owing to the shorter heat transfer path from the metal hydride powder to the outer wall when compared to the honeycomb design. Yoo et al. [7] developed a 3-D hydrogen absorption model and demonstrated that using a thin double-layered annulus ZrCo hydride bed design is essential to obtaining a more uniform temperature and hydrogen/metal (H/M) ratio profile. They also simulated the thin double-layered design during hydrogen desorption and showed that this results in superior discharge performance when compared to the simple cylindrical bed design, owing to more effective heat transfer [8]. Askri et al. [9] developed a two-dimensional (2-D) hydrogen absorption model and evaluated the dynamic behaviors of various MHV designs including a cylindrical tank with external heat-fins, a cylindrical tank with flowing coolant, and a cylindrical tank with a concentric tube equipped with heat-fins. They showed that the hydrogen charging time was considerably reduced when the concentric heat exchanger tube equipped with fins was used with flowing coolant. Laurencelle et al. [10] developed a 1-D hydrogen absorption/desorption model and

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investigated the effects of using aluminum foam in planar, cylindrical, and spherical MHV geometries. Much better hydrogen charge/discharge behaviors were predicted with aluminum foam. Mellouli et al. [11] numerically evaluated the MHV performance with and without a metal foam heat exchanger. Their 2-D calculation results indicate that the use of aluminum foam enhanced the rate of heat removal during hydrogen absorption and substantially shortened hydrogen charge time when compared to the case without metal foam. They also addressed the effects of various metal foam parameters such as the material, pore size, and density on the hydrogen charging performance.

In our previous studies, the 3-D metal hydride model was applied to simplified MHV geometries wherein the size of the computational domain was reduced via geometrically symmetric conditions [12,13]. Although the simulation results generally agree with experimental data, some deviations which cannot be overlooked occur between the metal hydride temperature evolution profiles. This indicates that real-scale simulations accounting for the whole experimental MHV geometry may be necessary to more accurately address hydrogen charge and discharge behaviors. The present study aims to conduct large-scale hydrogen absorption/desorption simulations based on the whole MHV. A parallel computational methodology has been employed to substantially reduce the computational turnaround time and relax the memory requirement. Such a multi-dimensional and real-scale computational tool is highly desirable for the design and engineering of commercial-size MHVs.

2. Numerical model

2.1. Model assumptions

Our previous papers present the details of our 3-D metal hydride hydrogen absorption and desorption model [7,8,12–17]. The main assumptions invoked in the model are:

(1) The gas phase obeys the ideal gas law.
(2) The powdery metal hydride region is treated as an isotropic and homogeneous porous medium characterized by uniform porous properties, such as the porosity, permeability, and tortuosity.
(3) Hydrogen and adjacent metal are in thermal equilibrium.
(4) The porous properties of the metal hydride, such as the porosity and permeability, remain constant during the hydrogen absorption process.

2.2. Conservation equations and source terms

On the basis of the presented assumptions, our metal hydride hydrogen absorption/desorption model is governed by three principles of conservation: mass, momentum, and thermal energy.

Mass conservation:

Hydrogen:

$$\frac{\partial \varepsilon \rho^g}{\partial t} + \nabla \times (\rho^g \vec{u}) = -S_m \tag{1}$$

In Eq. (1), the hydrogen density ρ^g can be described by the ideal gas law as follows:

$$\rho^g = \frac{P^g M^g}{RT} \tag{2}$$

Metal hydride:

$$(1-\varepsilon)\frac{\partial \rho^s}{\partial t} = S_m \tag{3}$$

In Eqs. (1) and (3), ε and S_m denote the porosity of the metal hydride powder and the local hydrogen absorption/desorption rate per unit volume, respectively. The detailed expression of S_m is given by the following kinetic expressions.

Hydrogen absorption:

$$S_m = C_a \exp\left(\frac{-E_a}{RT}\right)\ln\left(\frac{P^g}{P_{eq,a}}\right)\left(\left(\frac{H}{M}\right)_{sat} - \left(\frac{H}{M}\right)\right)\rho^s \tag{4}$$

Hydrogen desorption:

$$S_m = C_d \exp\left(\frac{-E_d}{RT}\right)\left[\frac{P^g - P_{eq,d}}{P_{eq,d}}\right](\rho^s - \rho_{emp}) \tag{5}$$

Ci and Ei denote the rate constant and activation energy for reaction, i, respectively, and ρ_{emp} is the hydrogen free-density of the metal powder. The H/M ratio representing the absorbed hydrogen to metal atomic ratio can be written as

$$H/M = \frac{2\left(\rho^s - \rho^s_{emp}\right)\Big/ M_{H_2}}{\rho^s_{emp}/M_{ZrCo}} \tag{6}$$

The hydrogen equilibrium pressures, $P_{eq,\,i}$, with the metal hydride is expressed as a function of the temperature and H/M ratio as follows:

$$P_{eq,i} = \exp\left(\frac{\Delta H}{R^g}\left(\frac{1}{T} - \frac{1}{T_{ref,i}}\right)\right)\cdot f\left(\frac{H}{M}\right) = \exp\left(\frac{\Delta H}{R^g}\left(\frac{1}{T} - \frac{1}{T_{ref,i}}\right)\right) \cdot\left[a_0 + \sum_{n=1}^{9} a_n\left(\frac{H}{M}\right)^n\right] \tag{7}$$

Hydrogen absorption:

$a_0 = 1.057,\ a_1 = 7.128,\ a_2 = -26.195,\ a_3 = 53.5,\ a_4 = -62.183$
$a_5 = 40.54,\ a_6 = -13.185,\ a_7 = 0.927,\ a_8 = 0.55,\ a_9 = -0.106$

Hydrogen desorption:

$a_0 = 0.728,\ a_1 = 25.171,\ a_2 = -123.453,\ a_3 = 333.922,\ a_4 = -541.846$
$a_5 = 547.488,\ a_6 = -346.054,\ a_7 = 132.671,\ a_8 = -28.143,\ a_9 = 2.53$

In Eq. (7), $f(H/M)$represents the H/M ratio dependent term and was approximated as a ninth-order polynomial function for both hydrogen absorption and desorption. Fig. 1 shows a comparison of the equilibrium pressures experimentally measured by Konishi et al. [18] and calculated using Eq. (7). It should be noted that the equilibrium pressures, $P_{eq,\,i}$, for the hydrogen absorption reaction ($i = a$) and desorption reaction ($i = d$) are usually different, violating the phase rules. This phenomenon is referred to as hysteresis and the different expressions between the hydrogen absorption and desorption are obtained by combining the van't Hoff's relationship and interpolation of experimental pressure-composition isotherm data, which are addressed in the model.

Momentum conservation:

$$\frac{1}{\varepsilon}\left[\frac{\partial \rho^g \vec{u}}{\partial t} + \frac{1}{\varepsilon}\nabla\cdot(\rho^g \vec{u}\,\vec{u})\right] = -\nabla P + \nabla\cdot\tau + \rho^g \vec{g} + S_u \tag{8}$$

The momentum source term, S_u, in Eq. (8) physically accounts for viscous resistance arising due to the presence of porous media, representing momentum loss of the hydrogen gas flow in porous MHV components. Therefore, S_u is set to zero for nonporous regions such as the expansion volume, rendering the momentum equations above exactly equivalent to the Navier-Stokes equations. For porous MHV components, S_u is devised to recover Darcy's law and thus can be expressed as a function of the permeability, K, and dynamic viscosity, μ, as

$$S_u = -\left(\frac{\mu}{K}\right)\vec{u} \tag{9}$$

By considering the temperature field, the local thermal equilibrium between the solid metal hydride and the hydrogen gas was assumed as described above. Therefore, the energy equation can be expressed in terms of a single temperature variable, T.

Thermal energy conservation: