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Three-dimensional modeling and simulation of hydrogen desorption in metal hydride hydrogen storage vessels

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ABSTRACT

A three-dimensional hydrogen desorption model is developed and validated against the temperature evolution data measured on a cylindrical LaNi₅ metal hydride vessel. The equilibrium pressure for hydrogen desorption in LaNi₅ is derived as a function of the H/M atomic ratio and temperature based on the experimental data reported in the literature. In general, the numerical simulations are in good agreement with the experimental data, which confirms the validity and accuracy of the proposed desorption model. Both the calculated and measured temperature profiles exhibit an initial sharp drop, which is indicative of a relatively rapid hydrogen desorption rate compared to the heat supply rate from the vessel external walls at the early stages. On the other hand, the effect of heat supply becomes influential at the latter stages, leading to a smooth increase in vessel temperature. This numerical study suggests that the efficient design of a storage vessel and heating system is essential for achieving rapid hydrogen discharging performance.

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Introduction

Hydrogen has been considered a good, carbon-free alternative to hydrocarbon fuels but problems, such as efficient environmentally friendly production, safety and proper storage, has hindered its development. Of the issues regarding storage, a range of hydrogen storage techniques have been evaluated in recent years. These can be categorized into three main areas: 1) high pressure gaseous hydrogen storage, 2) liquefaction of hydrogen gas and liquid-phase hydrogen storage, and 3) solid state reversible hydrogen storage with carbon materials or metallic hydrides. Among these technologies,

solid-state hydrogen storage methods using metal hydrides have attracted considerable attention owing to their relatively higher volumetric storage density, security and lower cost. One key issue for metal hydride hydrogen storage systems is to achieve rapid hydrogen charging/discharging rates under the appropriate operating conditions. As shown in Eq. (1), hydrogen absorption and desorption with metals are generally exothermic and endothermic processes, respectively, and the reaction enthalpy for hydrogen absorption/desorption, ΔH , differs according to the metal materials used.



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Therefore, choosing the appropriate metal material and optimizing the vessel design/operating conditions are of paramount importance to obtaining favorable hydrogen absorption/desorption behavior. A theoretical study of metal hydride vessels is ever-increasing, because it will enable a complete understanding of hydrogen absorption/desorption reactions and the resulting heat and mass transport phenomena in metal hydride vessels, as well as the development of computer-aided tools for design and optimization.

Many numerical models have been developed for metal hydride hydrogen storage systems [1–12]. Although most of these studies focused on hydrogen absorption reactions [1–12], numerical studies of hydrogen desorption process are relatively rare [9–12]. Wang et al. [10] developed a hydrogen desorption model and applied it to a LaNi₅ hydrogen storage vessel. Unfortunately, their desorption model was not evaluated by a comparison with experimental data. Chung et al. [11] developed a two-dimensional hydrogen absorption/desorption model and analyzed the effects of the expansion volume and heat convection on the hydrogen charging/discharging performance. Mellouli et al. [12] proposed three different heat exchanger designs for a LaNi₅ based hydrogen storage vessel. Using their two-dimensional hydrogen absorption/desorption model, they examined numerically the influences of the heat exchanger design on the hydrogen charging/discharging behavior. They reported that a properly designed heat exchanger can reduce the hydrogen charging/discharging times considerably. Unfortunately, neither Chung et al. [11] nor Mellouli et al. [12] provided a comparison of the hydrogen desorption simulations with experiments.

Although considerable efforts have been made to model the hydrogen desorption process in metal hydride hydrogen storage vessels, these models have not been validated against experimental data. Furthermore, a detailed numerical study of complicated transport mechanisms, involving coupled heat and mass transfer through a porous metal hydride vessel, is extremely important for enhancing our fundamental understanding of the hydrogen desorption processes. In this study, a three-dimensional metal hydride model is developed by rigorously accounting for the reaction kinetics and heat and mass transfer mechanisms during the hydrogen desorption process. Three-dimensional modeling is believed to be necessary for the design of an industrial metal hydride hydrogen storage vessel. The model was first validated against the experimental data reported by Jemni et al. [13] and used to present detailed contours for key parameters, such as the temperature, H/M atomic ratio, and hydrogen velocity.

Numerical model

Model assumptions

A three-dimensional metal hydride hydrogen desorption model was developed to investigate the key physical phenomena during the hydrogen desorption process. The assumptions made in the present model are as follows: (1) the gas phase (hydrogen) obeys the ideal gas law; (2) the powdery metal hydride vessel is treated as an isotropic and homogeneous porous medium characterized by uniform porous

properties, such as the porosity, permeability and tortuosity; (3) local thermal equilibrium is assumed between the solid metal and hydrogen gas; (4) the volumetric change of the metal hydride during hydrogen desorption is negligible; (5) the properties of the metal hydride, such as the porosity, permeability and thermal conductivity, remain constant during the hydrogen desorption process.

Conservation equations and source terms

Under the above assumptions, the metal hydride hydrogen storage model is governed by the conservation of mass, momentum and thermal energy.

Mass conservation:

Hydrogen:

$$\frac{\partial \epsilon \rho^g}{\partial t} + \nabla \cdot (\rho^g \vec{u}) = -S_m \quad (2)$$

where the gas density, ρ^g , can be described by the ideal gas law as follows:

$$\rho^g = \frac{P^g M^g}{RT} \quad (3)$$

Metal hydride:

$$(1 - \epsilon) \frac{\partial \rho^s}{\partial t} = S_m \quad (4)$$

In Eqs. (2) and (4), ϵ denotes the porosity of the metal hydride vessel and S_m is the local hydrogen desorption rate per unit volume. Therefore, the volumetric mass source term, S_m , is zero in the expansion volume subregion but nonzero in the metal hydride subregion. S_m can be expressed as follows:

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

In Eq. (5), C_d and E_d are the rate constant and activation energy for hydrogen desorption, respectively. ρ_{emp}^s is the hydrogen free-density of the metal powder, and P_{eq} is the equilibrium pressure for hydrogen desorption, which is strongly dependent on the temperature and H/M atomic ratio. The correlation of the equilibrium pressure with the temperature and H/M ratio can be derived best using the Van't Hoff relationship as follows [8]:

$$P_{eq} = \exp\left(\frac{\Delta H}{R_g T} - \frac{\Delta S}{R_g}\right) = f\left(\frac{H}{M}\right) \cdot \exp\left(\frac{\Delta H}{R_g} \left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right) \quad (6)$$

In Eq. (6), the dependence on the H/M ratio of the equilibrium pressure, $f(H/M)$, is normally obtained by a polynomial interpolation.

Momentum conservation:

$$\frac{1}{\epsilon} \left[\frac{\partial \rho^g \vec{u}}{\partial t} + \frac{1}{\epsilon} \nabla \cdot (\rho^g \vec{u} \vec{u}) \right] = -\nabla P + \nabla \cdot \tau + S_u + \rho^g \vec{g} \quad (7)$$

For the expansion volume, the momentum source term, S_u , in Eq. (7) is zero, and the momentum equations above are exactly the Navier–Stokes equations. On the other hand, S_u for the porous metal hydride vessel region is used to recover Darcy's law and can be expressed as a function of the permeability, K , and the dynamic viscosity, μ , as follows:

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