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Three-dimensional modeling and sensitivity analysis of multi-tubular metal hydride reactors

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HIGHLIGHTS

- A novel three-dimensional model of a metal hydride reactor was proposed.
- In the model the effects of the flow of heat transfer fluid were considered.
- N was defined to assess the effects of neglecting the fluid temperature variation.
- The effect of the contact conductance was discussed in detail.
- Sensitivity analysis for parameters influencing the reactor performance was given.

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ABSTRACT

In order to predict heat and mass transfer characteristics of metal hydride reactors accurately, a novel three-dimensional multiphysics model was presented. In the newly established model, the velocity field of the heat transfer fluid was obtained by solving the Navier–Stokes equations or the k-ε turbulence model. The model was numerically solved using the commercial software package COMSOL Multiphysics V3.5a. Two traditional models were also solved for the reactors under the same set of conditions. A dimensionless parameter N was defined to assess the effects of neglecting the variation of heat transfer fluid temperature on the hydrogen absorption rate. The results from numerical simulation indicated that when N is greater than 0.01, the variation of heat transfer fluid temperature cannot be neglected. In this case, the newly established model was valid while the other two models were not. Moreover, it was found that the effective thermal conductivity of the metal hydride, the flowrate of the heat transfer fluid and the contact resistance were crucial factors for improving the performance of the metal hydride reactors.

1. Introduction

Since some metal hydride materials, e.g. $LaNi_5$, TiFe and Mg_2Ni, were successfully developed, the applications of metal hydride have been immensely extended, such as hydrogen storage, heat pump, thermal energy storage, hydrogen thermal compression, isotope separation, etc [1,2]. The metal hydride reactors play an important role in the above systems, in which the metal hydride formation and decomposition occur. Identifying heat and mass transfer characteristics of the metal hydride reactors is the basis for the reactor design and optimization.

Many researchers have established mathematical models to analyse heat and mass transfer characteristics of metal hydride reactors. El Osery [3] and Lucas et al. [4] used one-dimensional mathematical model to describe the adsorption/desorption process in the metal hydride reactor. Jemni and Ben Nasrallah [5] formulated a mathematical model for the two-dimensional transient heat and mass transfer within a metal hydride reactor based on the volume averaging method. Their results indicated the local thermal equilibrium assumption was valid and the convective heat transfer could be neglected. Kuznetsov and Vafai [6] established an analytical criteria for the validity of local thermal equilibrium, steady state and frontal model approximation. Aldas et al. [7] extended the previous model to three-dimensional model and studied heat and mass transfer in a metal hydride bed. They found that hydrogen flow significantly influenced on the temperature profile, but the overall hydride formation was not affected by

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Nomenclature

A	cross-sectional area, m^2
A_h	heat transfer area, m^2
b	hydride bed thickness, mm
C_a	reaction rate constant, s^{-1}
c_p	specific heat, J kg^{-1} K^{-1}
d_H	diameter of the hydrogen injection tube, mm
d_i	internal diameter of the heat exchanger tube, mm
d_o	external diameter of the heat exchanger tube, mm
d_p	particle size, μm
E_a	activation energy, J mol^{-1}
h_{ex}	heat transfer coefficient between the hydride bed and the tube wall, W m^{-2} K^{-1}
K	permeability, m^2
k	turbulent kinetic energy, m^2 s^{-2}
l	length, mm
Mg	molecular weight, g mol^{-1}
$\dot{m}$	hydrogen mass absorbed per unit volume and unit time, kg m^{-3} s^{-1}
n	normal vector
Nu	Nusselt number
p	pressure, Pa
Pr	Prandtl number
Q_V	volumetric flowrate of heat transfer fluid, m^3 s^{-1}
q	thermal flux, W m^{-2}
r_h	heat transfer controlled reaction rate, mol m^{-3} s^{-1}
R_{ex}	thermal contact resistance, mm^2K W^{-1}
R_g	general gas constant, J mol^{-1} K^{-1}
Re	Reynolds number
T	temperature, K
t	time, s
U	overall heat transfer coefficient, W m^{-2} K^{-1}
u	X-axis velocity, m s^{-1}
V	volume, m^3
$\vec{V}$	velocity vector, m s^{-1}
v	Y-axis velocity, m s^{-1}
X	reacted fraction
w	Z-axis velocity, m s^{-1}
ΔH	reaction heat, J mol^{-1}
ΔX	typical heat diffusion length, mm

Greek symbols

α	modification coefficient
ε	volume fraction
ε_t	turbulence energy dissipation rate, m^2 s^{-3}
η	dynamic viscosity, kg m^{-1} s^{-1}
λ	thermal conductivity, W m^{-1} K^{-1}
ν	kinematic viscosity, m^2 s^{-1}
ρ	density, kg m^{-3}

Subscript

0	initial
e	effective value
eq	equilibrium
f	heat transfer fluid
g	hydrogen
in	inlet
m	mean
s	metal hydride bed
sat	saturation
t	turbulence
w	heat exchanger tube wall

hydrogen flow in the system. The effects of the radiative heat transfer were studied by Askri et al. [8]. They found that radiative effects on the sorption process were negligible in the case of the $LaNi_5$–hydrogen system, but very important for the Mg–H_2 system. Ha et al. [9] developed a two-dimensional model for unsteady heat and mass transfer in a metal hydride bed in the hydriding process. Their results showed that the higher thermal conductivity, smaller bed diameter and the presence of fins in the bed gave more enhanced heat transfer rate from the bed. Yang et al. [10,11] defined two key parameters, heat transfer controlled reaction rate and mass transfer controlled reaction rate, to analyse the performance of metal hydride reactors, which established a two-dimensional mathematical model to prove the validity of the parameter analysis. Chaise et al. [12] presented a criterion for quantifying the error which is made when the fluid flow is neglected. Mellouli et al. [13] developed a two-dimensional mathematical model to optimize the designs of the metal hydride storage tanks for fuel cell vehicles. Pourpoint et al. [14] investigated the thermal characteristics of the $Ti_{1.1}MnCr$ system using the experimental data and a basic numerical model. Veerraju et al. [15] presented a two-dimensional transient model of plate fin-and-elliptical tube type metal hydride reactors. Visaria et al. [16] formulated and solved one-dimensional and two-dimensional computational models for reactors packed with a high-pressure metal hydride ($Ti_{1.1}CrMn$). The one-dimensional model was used for calculating the maximum thickness of metal hydride layer in the initial design stage. The heat exchanger's thermal and kinetic response was obtained by the two-dimensional computational model in the final design stage. However, the models in the above literatures were formulated neglecting the variation of heat transfer fluid temperature [3–16]. MacDonald et al. [17] and Chung et al. [18] used one-dimensional energy equations to describe the temperature distribution of the air in the heat exchanger pipe. Freni et al. [19] presented a three-dimensional model to simulate the whole metal hydride-based hydrogen storage tank, and the computational domain included the heat transfer fluid. Krokos et al. [20] developed a detailed three-dimensional Cartesian model for a multi-tubular metal hydride tank, which included an energy balance equation for the cooling fluid. However, the above models are developed based on the assumption that the axial velocity for the heat transfer fluid is uniform and constant, but usually this assumption doesn't coincide with the practical conditions.

In this paper, a novel three-dimensional multiphysics model for metal hydride reactors was presented, in which the velocity field of the heat transfer fluid was obtained by solving the Navier–Stokes equations or the k-ε turbulence model. The computational domain was the whole reactor consisting of the metal hydride bed, the heat exchanger tube wall and the heat transfer fluid. The mathematical model was solved by the commercial software package COMSOL Multiphysics V3.5a. The validity of two assumptions was investigated, i.e. the variation of heat transfer fluid temperature is negligible, as well as that the axial velocity for the heat transfer fluid is uniform and constant. A dimensionless parameter N was defined to assess the effects of neglecting the variation of heat transfer fluid temperature on the hydrogen absorption processes. The three-dimensional distribution of the reacted fraction, temperature and gas velocity in the reactors was obtained, and the effects of some important parameters on the reactor performance were discussed.