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An improved model for metal-hydrogen storage tanks – Part 2: Model results

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ABSTRACT

An enhanced 3-D numerical model, described in Part 1 [1] of this two part work, has been employed to study a metal-hydrogen storage system. In this manuscript we investigate the effect of varying the hydrogen in-flow rate and total amount of hydrogen inserted on the time taken to absorb/store the hydrogen and the temperature excursions. In addition, the ability to vary the temperature of the thermal management fluid has been used to examine the relative effect of a fixed fluid temperature and one which is hotter for desorption and colder for absorption.

It was found that a shorter time and a greater amount of hydrogen injection to the tank leads to a higher driving pressure and, as a result, higher rate of absorption. This must be moderated by constraints such as the pressure rating of the tank. Furthermore, compared to using the same constant temperature thermal fluid for absorption and desorption, switching the fluid temperature between 283 K for absorption and 343 K for desorption leads to faster hydrogen cycling and more complete hydrogen desorption in the tank. However, a constant fluid temperature of 313 K gives a reasonable performance over the same time duration, without the additional energy expenditure associated with switching the fluid temperature.

Introduction

Hydrogen storage devices must balance a number of competing factors and limitations for optimal performance. Good design will aim to optimise factors like storage yield and energy cost under standard operating conditions. Ideally the optimisation of these parameters can be carried out on a computer, saving time and money in the design process. However, this optimisation is only useful if the mathematical models are sufficiently accurate.

Improvement of mathematical models of metal-hydride storage systems enables the emulation of experimental variables of real systems more accurately and reliably. In this study, an enhanced three-dimensional multiphysics model of a metal-hydride tank, described in Part 1 [1], was used to explore the effects of hydrogen injection time and temperature cycling on system performance. This corresponds to the practical realities that hydrogen supply and withdrawal cannot be instantaneous, and thermal management may be unpractical at high supply or withdrawal rates.

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Nomenclature

T	temperature, *K*
P	pressure, *bar*
ρ	density, *kg/m^3*
ρ_{gT}	the total hydrogen density added to the tank, *kg/m^3*
$\vec{v}$	velocity vector, *m/s*
ΔH	enthalpy of formation, *J/kg*
ΔS	entropy change, *J/kg K*
E	activation energy, *J/kg*
λ	thermal conductivity, W/m K
R_g	universal gas constant, *J/mol$_{H2}$ K*
C_p	specific heat capacity, *J/kg K*
H_{gs}	convection coefficient between solid and gas, W/m^2 K
m	hydrogen mass absorbed or desorbed, *kg/m^3* s
μ	viscosity, *kg/m* K
d_p	mean particle diameter, *m*
V	volume, *m^3*
t_{Inj}	time of injection, s
t	time, *s*
ε	porosity
k	permeability, *m^2*
$\dot{\phi}_m$	hydrogen mass flow rate, (*kg/m^{3}s*)
$\dot{\phi}_\rho$	hydrogen flow rate, (*mol/m^{3}s*)
$\left(\frac{H}{M}\right)_{max}$	maximum hyrogen to metal ratio per formula unit at a certain temperature
$\left(\frac{H}{M}\right)$	hydrogen to metal ratio per formula unit
$\left(\frac{H}{M}\right)_{sat}$	maximum hydrogen to metal ratio per formula unit at room temperature
P_D	downstream pressure, *pa*
η'	maximum reacted fraction
η	reacted fraction
E_p	expansion coefficient
$\vec{n}$	outward surface normal vector
r_0	radius of cooling tube, *m*
R	reactor internal radius, *m*
h	convective heat transfer coefficient, W/m^{2}K
$H(x)$	Heaviside step function
t_{sm}	time for smoothing the Heaviside function
l	tank length, *m*
Cv	discharge coefficient
A	cross sectional area, *m^2*

Subscripts

a	absorption
d	desorption
eff	effective
s	solid phase
g	gas phase
r	radial
z	axial
ref	reference
eq	equilibrium
i	initial
f	final
fl	heat exchange fluid

Most of the recent studies [2–8] of metal-hydride systems have been devoted to the optimum designs of heat transfer systems in order to increase the performance of the metal-hydride storage tanks. There has been less concentration on developing models suited to the simulation of practical systems, but it is important to consider all realistic factors which affect a system's smooth running.

Minko *et al.* [9,10] made additions to the basic mathematical model of a $LaNi_5$–H_2 bed for the calculation of the effective thermal conductivity and the bed porosity. A correlation for the hydrogen outlet flow rate was used in the model by Yang *et al.* [11]. Some improvements, including introducing realistic geometry and using validated parameters in the model, were made by Xiao *et al.* [12]. However, some aspects of a practical system, such as injection of hydrogen and a comparison of fixed-temperature *vs* variable temperature cooling systems have not previously been studied.

In the first part of this paper [1], a number of assumptions were tested and improvements made to the usual models. The usual assumption of a metal-hydride system model, which is the treatment of hydrogen as an ideal gas, was examined and found to be a justifiable simplification for pressures up to about 100 bar and at temperatures around 300 K. Experimental data for $LaNi_5$ were used to develop an empirical equation for equilibrium pressure as a function of reacted fraction and temperature. The maximum reacted fraction was also calculated as a function of temperature, in line with experimental observations.

Experimental data for effective thermal conductivity from Pons and Dantzer's study [13] were fitted and used in this model. Hydrogen in-flow and out-flow were modelled to represent realistic conditions and the thermal fluid temperature could be varied according to whether the bed was absorbing or desorbing [1].

These modifications align the model more closely with experimental conditions as well as enabling the investigation of experimental parameters such as hydrogen inlet and outlet flowrate, the amount of hydrogen injected into or withdrawn from the tank, and facilitate an investigation of the effects of varying the thermal management fluid.

The model

A three-dimensional mathematical model [1] based on the work of Hardy and Anton [14,15] was applied to a horizontally-mounted, axially symmetric, cylindrical tank containing 100 kg $LaNi_5$ with a hydrogen capacity of 1.5 kg. The thermal management system consisted of a system of fins embedded in the hydride bed with concentric tubes for inlet and outlet of the temperature controlled fluid. The model was solved by COMSOL Multiphysics 4.3 specifically for the $LaNi_5$–H_2 system but can also be used for all metal-hydride tanks by adapting those equations which depend on the material used for H_2 storage.