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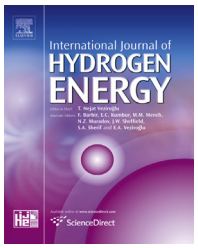

Impact of kinetic reaction models on hydrogen absorption in metal hydride tank modeling

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ABSTRACT

This numerical work presents thermal investigation of transient hydrogen solid storage in $MmNi_{4.6}Al_{0.4}$ metal hydride three dimensional tank. Indeed, thanks to its moderate reaction temperatures and pressure, it is considered among the best hydrogen storage material. The laws governing the chemical and thermal phenomena have been determined experimentally. However, computational simulation allows prediction and understanding of the spatial and temporal evolution of the hydrogen reactions and participates in saving significant time in the design and optimization of hydrogen tanks. Also, an UDF was implemented to FLUENT and used for simulations. In what follows, we describe the contribution to hydrogen absorption process in metal hydride tank in order to consider a better control of the generated phenomena. Finally, results show that because of great sensitivity to time step values and to the very long calculation time, JMAK model is not appropriate for the hydrogen absorption kinetic reaction modeling.

Introduction

Nowadays the most useful methods for hydrogen storage are under high compression 700 bar where (ρ_{H2} = 39 kg/m^3) and through cryogenic form with (ρ_{H2} = 71 kg/m^3). However, a recent promising one is by solid form through metal hydride powder ($\rho_{H2} \approx$ 200 kg/m^3 MgH_2) because of its many advantages such as relative high specific storage capacity, it could be used on a large scale in the near future to enable the rapid development of green and renewable energies especially for nomad applications.

Numerical simulations, allow predicting and understanding the spatial and temporal evolution of the hydrogen storage reaction. In addition, the computational tool saves valuable time in the design and optimization of hydrogen tanks. In this work, we describe the development of a model for filling a specific metal hydride tank for better control of the phenomenon. We are particularly interested in the description of thermal phenomena associated with the process generated by the reaction of hydrogen reaction.

FLUENT software of ANSYS 13.0, was used to perform numerical simulations. One of its specific advantages consists for the most important part on the fact that it attaches to the modeling of thermodynamics and kinetics reactions between the gas and a porous medium. An UDF (User Defined Function) written in C was developed and implemented in "FLUENT" software. The results were validated by those available in the literature. Tridimensional cylindrical tank geometry was used for that modeling.

The obtained equations system was solved with a numerical scheme for fully implicit finite volume. The effect of

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Nomenclature

Cp	specific heat, *J/kg/K*
ΔH	molar enthalpy of reaction at standard conditions, *J/mol*
K	permeability, m^2
M	molar mass of hydrogen, *kg/mol*
P	hydrogen pressure, *Pa*
$P_{eq}(T)$	equilibrium pressure, *Pa*
R	universal gas constant = 8.314 *J/mol.K*
S	source term reaction, *mol/m.s*
ΔS	molar entropy of reaction under standard conditions, *J/mol.K*
wt	maximum weight percentage of hydrogen into material, %

Greek symbols

λ	thermal conductivity, *W/m.K*
ε	porosity
ρ	density, kg/m^3
$d\alpha/dt$	hydriding velocity, s^{-1}

Subscripts and Superscripts

e	*energy*
eff	*effective*
eq	*balance*
f	*final*
g	*gas*
H	*hydrogen*
M	*metal*
m	*mass*
MH	*metal hydride*
i	initial

different kinetic equations of absorption reaction was studied in order to determine which one will be the more adapted for this kind of cases.

State of art

Many experimental and numerical studies have been conducted to improve the performance of hydrogen tanks. A. Jemni and S. Ben Nasrallah [1] conducted one of the first two-dimensional numerical studies of a hydrogen reactor. Their results showed the importance of the geometry of the inlet pressure and the choice of the inlet temperature. A. Dogan et al. [2] presented a mathematical model for the storage of hydrogen in a metal hydride bed; the team concluded that rapid load requires efficient cooling. P. Muthukumar et al. [3] performed a parametric study of a hydrogen storage device in metal hydride; they demonstrated that the increase of overall coefficient of heat transfer is not beneficial. A. Phate et al. [4] realized the analysis of a model of a cylindrical metal hydride bed; their conclusion is that the concentration gradient in the bed is the main driving force of the hydrogen flow. M. Botzung et al. [5] added an experimental validation of numerical simulations of the hydrogen storage tank with metal hydrides; their goal was to obtain performance against the objectives set by a stationary cogeneration system. A CFD model to simulate the storage of hydrogen in a charcoal tank was described by F. Ye et al. [6]; this model showed that the amount of hydrogen adsorbed is greater than that of the compressed gaseous hydrogen. F. Askri and al. [7] as several groups of researchers have proposed to optimize the tank cooling system. They observed that the use of fins enhances heat transfer within the hydride bed and consequently 40% improvement of the time required for 90% storage can be achieved over the case without fins.

Geometry and mathematical model

Modeled geometry

The used geometry in the simulations is an axisymmetric cylindrical canister of hydride bed powder, which is cooled on the surface. For our modeling, we considered the dimensions: (x = 20 mm, y = 20 mm, z = 400 mm or r_0 = 20 mm and z = 400 mm). This model is directly inspired by experimental prototypes available in the literature as shown in Fig. 1.

Formulation of the problem

The hydrogen absorption consists on supplying hydrogen radially in discharged tank at temperature of 300 K with a pressure of 3 MPa. The hydriding reaction is very exothermic ($\Delta H = -28{,}000$ J/molH_2), the temperature should increase very quickly and reach equilibrium temperature then generates a stagnation of the reaction. That's why, an effective cooling becomes necessary in order to allow the continuation of hydrogen absorption.

The following assumptions are made in the heat transfer simulations:

- Hydrogen is considered as a perfect gas between the hydride's pores,

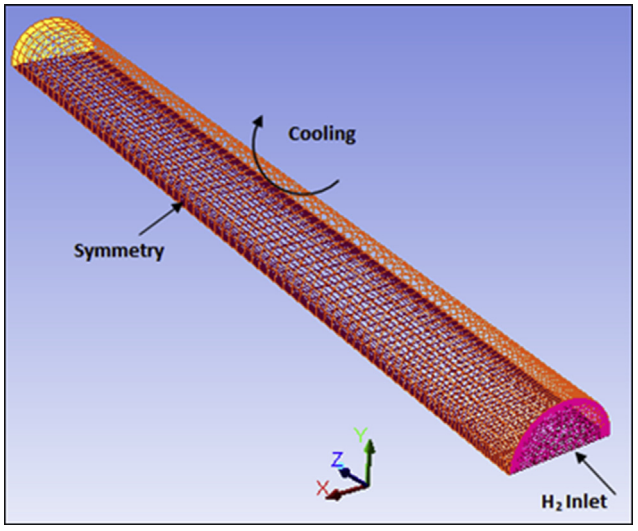

Fig. 1 – 3D tank's geometry based on an experimental tank model.