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Numerical Simulation of Hydrogen Absorption in Metal Hydride with Internal Fin and Embedded Heat Transfer Fluid Channel

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1. ABSTRACT

Metal hydrides (MHs) offer promising hydrogen storage solutions, yet their slow reaction kinetics due to the low conductivity of MHs hinders absorption time. This study conducts transient heat and mass transfer simulations during MH absorption using computational fluid dynamics. Enhanced heat transfer is introduced through internal fins and heat transfer fluid. The effects of different reactor configurations and a parametric study of cooling fluid for the MHs absorption are explored. The installation of internal fins reduced hydrogen absorption time by 15.6%, while increasing heat transfer fluid flow reduced absorption time by 22.2%.

2. INTRODUCTION

Hydrogen is a promising energy source due to its abundance in the universe, carbon-free emissions, and high gravimetric energy density. However, hydrogen storage presents a significant challenge due to its extremely low density under atmospheric conditions. Consequently, various methods of hydrogen treatment are necessary to increase energy density by volume, such as compression and liquefaction. While these methods are straightforward methods for increasing its storage density, addressing safety concerns and substantial energy consumption during the process pose challenges. Metal hydrides (MHs) for hydrogen storage are emerging as a novel approach, offering high volumetric energy density, operation under moderate temperature and pressure, and enhanced safety. The reaction kinetics of MHs are closely related to temperature and pressure, and the direction of these reaction is determined by the equilibrium pressure [1]. Absorption is dominant when hydrogen gas pressure is higher than equilibrium pressure, while desorption proceeds when the hydrogen gas pressure is lower. The reactions are exothermic and endothermic, respectively. Therefore, temperature and pressure management play a crucial role in determining MHs kinetics. Many researchers have explored effective heat transfer methods to enhance MHs kinetics. In this paper, the effect of internal fins in the reactor to increase heat transfer for reduction of MH absorption time is investigated using Computational Fluid Dynamics (CFD). The governing equations including reaction kinetics, equilibrium pressure, and energy source term are employed to analyse transient mass and heat transfer during the MHs absorption. The numerical model is validated with experimental results [2], demonstrating

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good agreements under two different experimental conditions. Additionally, a parametric study of different internal fin numbers and mass flow rates of heat transfer fluid (liquid water) is conducted to compare cooling effect. Two-dimensional axisymmetric models (**Fig. 1**) are employed to analyse a cylindrical reactor. The numerical simulation is carried out using ANSYS Fluent 2022R1, incorporating a User-Defined-Function (UDF) code.

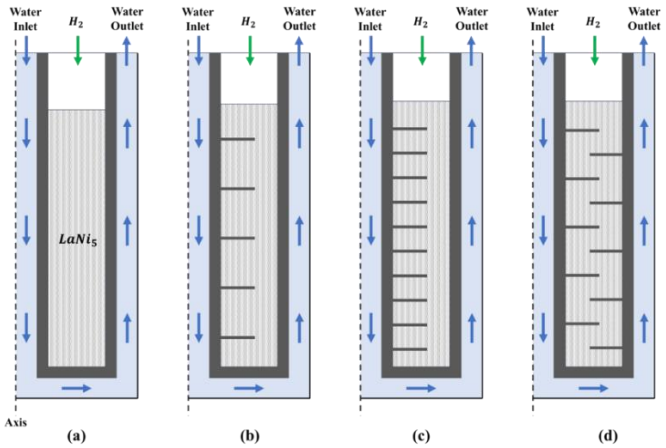

Fig. 1 Schematic diagram of 2-Dimensional axisymmetric cylindrical reactor (a) No Fin, (b) 5 Fin, (c) 10 Fin and (d) Staggered 10 Fin

3. METHODOLOGY

Due to the complexity of chemical reactions of MHs absorption, a few assumptions are applied for the numerical simulation following [2 - 4]: (1) Local thermal equilibrium in porous zone is applied, (2) Hydrogen is regarded as an ideal gas, (3) Thermal-physical properties keep constant during the reaction, (4) Expansion of hydride is neglected, (5) Radiative heat flux is neglected, and (5) Isotropic porosity. The governing equations for the numerical simulation of the MHs absorption are presented below. The $k-\omega$ SST model is selected for the turbulent heat transfer fluid flow.

Continuity equations for mass balance of MHs:

$$(1-\varepsilon)\frac{\partial \rho_m}{\partial t} = S_m \tag{1}$$

Equilibrium Pressure [3]:

$$ln\left(\frac{P_{eq}}{P_{ref}}\right) = \left(\frac{\Delta S}{R} - \frac{\Delta H}{R \cdot T}\right) + (\phi_s + \phi_0) \times tan\left[\pi\left(\frac{c}{c_{sat}} - \frac{1}{2}\right) + \frac{\beta}{2}\right] \tag{2}$$

Concentration:

$$c = \frac{2(\rho_m - \rho_{m,emp}) \,/\, M_{H_2}}{\rho_{m,emp} \,/\, M_{LaNi_5}} \tag{3}$$

Hydrogen absorption rate per unit volume [4]:

$$S_m = C_a \, exp\left(-\frac{E_a}{RT}\right) ln\left(\frac{P_g}{P_{eq}}\right)(\rho_{m,sat} - \rho_m) \tag{4}$$

Energy equation [4]:

$$\left(\rho C_p\right)_e \frac{\partial T}{\partial t} = \lambda_e \nabla^2 T - \rho_g C_{pg} \vec{u} \, \nabla T + S_m\left[\Delta h_f - T\left(C_{pg} - C_{pm}\right)\right] \tag{5}$$

The outer wall of the reactor is adiabatic condition and no-slip shear condition on the hydride and HTF zone.

4. RESULTS

At the beginning of the absorption, the temperature of the MH rapidly increases due to the heat generated by the reaction. Subsequently, the temperature gradually decreases because of cooling from the HTF. The impact of cooling, influenced by reactor geometry, is assessed by comparing the time required to charge 90 percent of hydrogen in the MH. Specifically, this time is observed to be 616, 581, 536, and 520 seconds for configurations with No Fin, 5 fins, 10 fins, and 10 Staggered fins, respectively (see **Fig. 2 (a)**). Additionally, the effects of HTF mass flow rate of 10 Staggered fins case are shown in **Fig. 2 (b)**, where the red and blue curves represent the average bed temperature and average HTF outlet temperature, respectively.

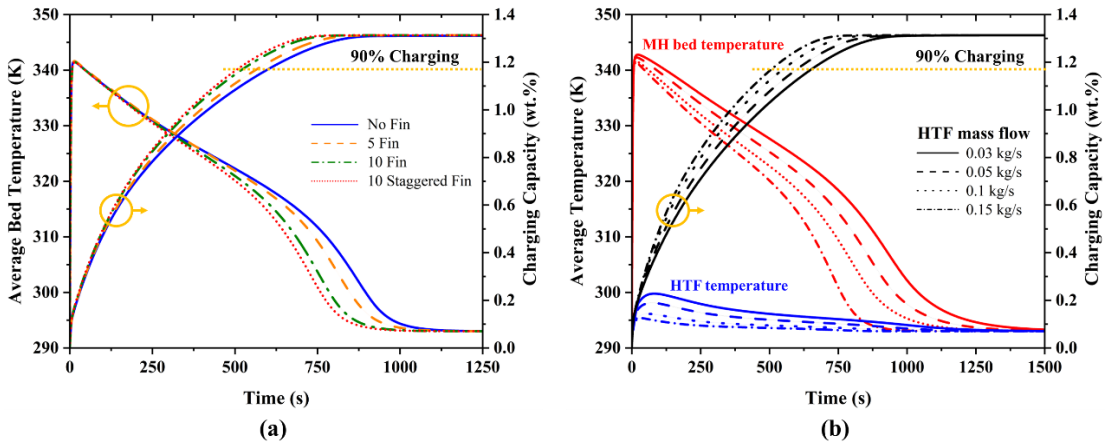

Fig. 2 Temperature and hydrogen charging variation during absorption (a) Parametric results of geometry of 0.15 kg/s mass flow rate and (b) Parametric results of HTF mass flow rate

5. CONCLUSIONS

The numerical simulations conducted in this research explore MH absorption under various reactor configurations and HTF flow rates. Installation of internal fins in the reactor results in a 15.6% reduction in charging time, particularly with 10 staggered arrangements of fins. Furthermore, a higher mass flow rate of HTF leads to a 22.2% reduction in charging time.

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