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Numerical modeling of heat transfer during hydrogen absorption in thin double-layered annular ZrCo beds

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ABSTRACT

In this work a three-dimensional (3D) hydrogen absorption model was proposed to study the heat transfer behavior in thin double-layered annular ZrCo beds. Numerical simulations were performed to investigate the effects of conversion layer thickness, thermal conductivity, cooling medium and its flow velocity on the efficiency of heat transfer. Results reveal that decreasing the layer thickness and improving the thermal conductivity enhance the ability of heat transfer. Compared with nitrogen and helium, water appears to be a better medium for cooling. In order to achieve the best efficiency of heat transfer, the flow velocity needs to be maximized.

Introduction

The escalating growth of the human population and rapid development of heavy industries have led to a drastic increase in energy demands. In order to bridge this energy deficit, the hydrogen energy has received much attention due to its clean energy carrying capability for both transportation and stationary applications [1]. The International Thermonuclear Experimental Reactor (ITER) that is based on the generating hydrogen fusion by burning isotopes (i.e. deuterium and tritium), generates tremendous amounts of energy with no harmful waste, and this is regarded as a key approach to solve energy problems in future. As deuterium and tritium are fuels in the fusion reactor, they needed to be stored safely and efficiently. According to the plasma operation scenarios, each metal hydride bed needs to fulfill extensive technical requirements, such as a nominal storage capacity of 100 g tritium and a hydrogen delivery rate of not less than 20 Pa•m^3/s [2]. Since these two elements are the isotopes of hydrogen, some methods for storing hydrogen are utilized in order for their storage [3]. Generally, hydrogen storage is divided into three types: compressed gas, liquefied hydrogen that needs to be controlled at temperatures below 20 K and metal hydrogen. Compared with the two former methods, the latter is recognized as being safer and more efficient [4–6].

Due to their faster recovery kinetics, better stability and lower equilibrium pressure, depleted uranium (DU) and zirconium intermetallics (ZrCo) are taken as favorable metals for the hydrogen isotope storage [7,8]. However, compared with the DU, the ZrCo has gained widespread attention as it is not a nuclear material and its reactivity towards impurities characteristic of fusion is low, which are advantageous in storage applications [9]. Also, it exhibits a smaller volume expansion upon hydride formation, in contrast to DU [10,11] where remarkable volume expansion has been found. Therefore, most investigations for storage and delivery system (SDS) in ITER focus on the ZrCo.

In ITER, a metal hydride bed (MHB) is used to store and supply hydrogen isotopes. From a high efficiency viewpoint, the hydrogen recovery and delivery rates are critical targets for MHB [2], and these behaviors are based on an exothermic/endothermic chemical reaction. For example, the reaction of hydrogen gas with a metal is exothermic for the formation of a metal hydride. If the heat released cannot be removed from the system, the resulting rise of temperature in the hydride will reduce the hydrogen absorption rate. Indeed, there is evidence that the reactions are dependent on heat and mass transfer processes. Lee et al. [12] and Kang et al. [13]

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Nomenclature

Latin Symbols

C_a	Rate constant, s^{-1}
C_p	Specific heat, kJ $(kg\ K)^{-1}$
E_a	Activation energy, kJ mol^{-1}
H/M	Hydrogen-to-metal atomic ratio
ΔH	Reaction heat of formation, J kg^{-1}
h	Heat transfer coefficient, W $(m^2\ K)^{-1}$
k	Thermal conductivity, W $(m\ K)^{-1}$
P	Pressure, bar
R	Universal gas constant, 8.314 J $(mol\ K)^{-1}$
t	Time, s
T	Temperature, K
u	Velocity vector, m s^{-1}

Greek Symbols

ε	Volume fraction of the gaseous phase in the porous
μ	Dynamic viscosity, kg $(m\ s)^{-1}$
ρ	Density, kg m^{-3}

Superscripts

eff	Effective value
g	Gas phase
s	Solid phase

Subscripts

c	Cooling
eq	Equilibrium
sat	Saturation value
ref	Reference value
0	Initial value

performed a study on the analysis of in-bed calorimetry in MHB with different initial temperatures. Their results showed that a higher temperature could affect the accuracy of in-bed calorimetry. However, the temperature condition led to some other problems, like thermal fatigue and creep [14]. Therefore, the design and optimization of MHB requires a better understanding of heat and mass transfer behavior during hydrogen absorption [15–17]. Shim et al. [18] proposed a design scheme for MHB that had a thin layer with 3 mm of ZrCo powder. It was found that a rapid delivery and recovery rate was achieved by this approach, as a result of the larger area and filer space. Kang et al. [19,20] also proposed a metal hydride bed with thin double layers of ZrCo powder, and the efficiency for both heat and mass transfer was improved significantly. However, an additional requirement was that the heat released needed to be removed quickly.

Numerical simulations are widely used to analyze hydrogen absorption behaviors and identify the key influential factors when designing MHB. For example, Mellouli et al. [21] studied the effects of structural parameters, including pitch, length, thickness and the arrangement of fins, on the heat transfer. A mathematical model was proposed by Nam et al. to investigate the influence of supply pressure and various designs on the thermal behavior of absorption [22]. Valizadeh et al. [23] established a new algorithm based on the lattice Boltzmann method for investigating the dynamic behavior during the process of desorption. Yoo et al. [24] developed a numerical model for simulating the heat transfer process of MHB, and obtained a close fit to the experimental results. However, effects of operational and structural parameters on the heat transfer efficiency of MHB were not considered in that study.

Unfortunately, only a few of these models have been proposed for ZrCo, and there is a need to study the characteristics of heat transfer for such a MHB. The knowledge of the transfer behavior in a thin double-layered bed geometry is fairly scarce to understand the hydrogen absorption mechanism. Compared with previous works, the primary objective of this study is to investigate the effects of ZrCo layer thickness, thermal conductivity, cooling medium and its flow velocity on the efficiency of heat transfer through numerical simulations. The structural and environmental information obtained serves as a guide to the development of MHB in ITER.

Preliminary assumptions

Some assumptions made in the present work are as follows:

(1) Ideal gas suitable for hydrogen.
(2) Negligible radiation heat transfer and viscous dissipation.
(3) Negligible volumetric expansion of ZrCo layer.
(4) Isotropic and homogeneous porous medium for the conversion layer.
(5) Same temperatures for the gas and the conversion layer.

It should be noted that these assumptions are commonly employed in many numerical models [21–24]. Although some items seem to be controversial, such as Assumption (5), a number of studies have been performed to justify the accuracy of these assumptions or approximations [11,25]. Therefore, the above assumptions are taken into account in the model for the analytical purpose.

Modeling

Geometric model

The bed configuration used in this work is shown in Fig. 1. The device is composed of cylindrical-shaped filters and bed walls that are fabricated by stainless steel with thin double annular layers. These filers are primarily used to prevent the ZrCo powders from transferring into gas pipes. A void space that assists gas flow is found between the double filters and cooling fluid tunnels are drilled into the inner and outer walls. In addition, the devices generating heat during the hydrogen recovery and its delivery processes are mounted over the lateral surface and the center of the bed. The input data for simulations is provided in Table 1.

Governing equations and boundary conditions

The model for simulating the heat transfer of metal hydride storage is mainly governed by three equations of conservation: mass, momentum, and thermal energy.

Fig. 2 shows a flow chart of the solution procedure. Before the begin loop, some properties including density, specific heat, thermal conductivity, are provided into the program as inputs. Following this step, the momentum is solved by Navier-Stokes (N-S) equations, and then the velocity that indicates the hydrodynamic condition of the system is updated by solving mass conservation with the continuity equation. To determine the temperature profile in MHB, its distribution is derived from the energy equation that is an extension of the first law of classical thermodynamics.