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Optimal design methodology of metal hydride reactors for thermochemical heat storage

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ABSTRACT

Metal hydride (MH) is an attractive alternative for thermochemical heat storage. This study proposes an optimal design methodology for MH heat storage reactors (MHHSRs), integrating the optimal design principle (ODP) and a new design procedure. Based on the optimal design methodology, the design of the powder bed with helical heat transfer fluid (HTF) tube is conducted via numerical simulation. A mathematical model is established for the thermal coupling between the powder bed and the HTF tube. The gravimetric exergy-output rate (*GEOR*) is adopted to evaluate the overall discharging performance. First, the helical HTF tube is optimized and improved based on the ODP, which increase the *GEOR* from 198.4 to 255.4 W kg^{-1}. The optimal helical diameter is 30 mm and the optimal improved structure is determined as a U-shaped double helical tube. Then, the structural improvement of the reaction bed is supplemented, achieving reductions of material and energy consumption by 12.2% and 11%, respectively. The final design of the powder bed with helical tube based on optimal design methodology improves the *GEOR* from 198.4 to 306.1 W kg^{-1}, which constitutes a significant increase of 54.3%. This optimal design methodology is validated and efficiently guides the design of advanced MHHSRs.

1. Introduction

Due to excessive carbon emissions, haze, and other environmental problems, developing renewable energy has become an urgent task throughout the world, which also is the focus of China's 13th Five-Year Plan. Most renewable energy sources, such as solar and wind energy, are intermittent and unstable; therefore, energy storage becomes the key problem. In recent years, concentrating solar power (CSP) attracted substantial attention due to the rapid development of heat storage technologies. In particular, sensible heat storage has been successfully applied to commercial CSP plants [1,2]. However, the low energy density of sensible materials limits the cost-reduction space of such a heat storage system. Latent heat storage has a relatively high energy density and a small output temperature range. The applications of latent heat storage are widely investigated in building energy saving and CSP [3–5]. However, the high cost and the detrimental corrosion of phase change materials limit their high-temperature application for CSP plants [6]. In addition, thermochemical heat storage has received much attention due to its outstanding energy density; examples are metal hydrides (MHs), carbonates, and hydroxides [7–9]. In particular, Mg-based hydrides provide an attractive option for thermochemical heat storage due to their low cost, good reversibility, and good stability [10].

Heat transfer in the MH bed is one of the major controlling steps during the hydrogenation/dehydrogenation process [11]. Meng et al. [12] indicated that the overall performance of MH heat storage system was mainly controlled by the heat transfer performance of the reactor. Thus, specific design improvements of MH reactors are constantly developed. According to the filling conditions of the reaction bed, MH reactors can be divided into two categories: powder bed and compact bed. The powder bed formed by natural filling of MH powder has a low effective thermal conductivity (ETC) but no restriction for the use of either a straight or curved heat transfer fluid (HTF) tube. The design of the powder bed mainly involves the optimization of heat exchangers such as the heat pipe [13], the finned tube [14,15], and the helical tube [16–18]. Chung et al. [13] designed a novel MH reactor combining powder bed with heat pipes and reported that heat pipes enhance both the hydrogenation and dehydrogenation rates by ~50%. Nyamsi et al. [15] calculated the optimum dimensions of annular fins based on minimizing the overall thermal resistance under the constraint of a constant fin volume. The results showed that the metal fins reduce overall thermal resistance and hydrogenation time by 13% and 42%, respectively. Raju et al. [16] conducted a systematic numerical study on the optimization of multi-tube heat exchangers with Al fins, helical tube heat exchanger, and shell-and tube heat exchanger, respectively. The

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Nomenclature

Abbreviation

CSP	concentrating solar power
GEOR	gravimetric exergy-output rate
MH	metal hydride
ODP	optimal design principle
ETC	effective thermal conductivity
HTF	heat transfer fluid
MHHSR	MH heat storage reactor

Symbols

A_c	cross-sectional area of helical tube, m^2
C_a	H_2 absorption rate constant, s^{-1}
c_p	specific heat, $J\,kg^{-1}\,K^{-1}$
c_{sat}	saturated molarity of H_2 per cubic meter, $mol\,m^{-3}$
D_o	outer diameter of reaction bed, m
d_c	helical diameter of helical tube, m
d_i	inner diameter of helical tube, m
E_a	activation energy of H_2 absorption, $kJ\,mol^{-1}$
E_x	exergy, J
f	Darcy drag coefficient for turbulence
h	heat transfer coefficient, $W\,m^{-2}\,K^{-1}$
ΔH	enthalpy of reaction, $kJ\,mol^{-1}\,H_2$
L	length of reaction bed, m
M	molar mass, $kg\,mol^{-1}$
Pr	Prandtl number
Pt	helical pitch of helical tube, m
p	pressure, Pa
Q_l	line heat source, W
R_g	universal gas constant, $J\,mol^{-1}\,K^{-1}$
Re	Reynolds number
Nu	Nusselt number
t	time, s
t_d	reaction time, s
T	temperature, K or °C
s	length of helical tube
S	molar reaction rate, $mol\,m^{-3}\,s^{-1}$
ΔS	reaction entropy, $J\,mol^{-1}\,K^{-1}\,H_2$
u_0	flow velocity of heat transfer fluid, $m\,s^{-1}$
V	volume of reaction bed, m^3
W_s	weight of material, kg
W_{cost}	room-temperature compression work, kJ
wt	saturated mass content of H in the metal hydride
X	reaction fraction

Greek letters

ε	porosity
λ	thermal conductivity, $W\,m^{-1}\,K^{-1}$
ρ	density, $kg\,m^{-3}$
μ	dynamic viscosity, Pa s

Subscripts

a	ambient condition
con	convective heat transfer
ea	equilibrium for H_2 absorption
g	hydrogen gas
in	intlet of helical tube
out	outlet of helical tube
s	solid phase
tot	total value
bed	reaction bed
e	effective value
f	heat transfer fluid
i	inner diameter
o	outer diameter
ref	reference value
t	tangential of helical tube
w	wall of helical tube

results showed that the reactor with helical tube achieves maximum hydrogen storage under the same hydrogenation time of 10.5 min. Wu et al. [17] reported that the non-dimensional pitch and heat transfer coefficient of the helical tube are two important parameters that affect the hydrogenation time. Moreover, the non-dimensional pitch has a more important effect than the heat transfer coefficient. Recently, Dong et al. [18] reported an experimental prototype that combined 36 g of MgH_2 powder with a helical tube for heat storage. The helical tube was used to improve the contact with the MgH_2 powder. The internal heating mode improve the energy efficiency by increasing the heat transfer area, while simultaneously reducing the characteristic heat transfer distance instead of the external heating.

The compact bed is formed by a periodical arrangement of MH compacts. MH compact for the heat transfer enhancement of the reaction bed is obtained by compressing a mixture of MH and high-thermal-conductivity materials such as metal foam and expanded natural graphite (ENG) into a mold. The experimental results of Ron et al. showed that the ETC of $LaNi_5$ compact reached from 8 to 23 $W\,m^{-1}\,K^{-1}$ in a volume content of aluminum from 0.15 to 0.5 [19]. However, a solid state diffusion processes between MH and aluminum occurred above 300 °C, which stabilizes the solid solution and then reduces its hydrogen absorption capacity [20]. Therefore, ENG is typically used in the high-temperature MH (MgH_2) compact. This combination is very suitable for the high temperature heat storage field. Chaise et al. [20] reported that the radial ETC of MgH_2 compact with 10 wt% ENG reaches 7.5 $W\,m^{-1}\,K^{-1}$. Pohlmann et al. [21] reported that the ETC of MgH_2-ENG compact can be adjusted from 1 to 43 $W\,m^{-1}\,K^{-1}$ by controlling the compression pressure and ENG content. Additionally, Shim et al. [22] investigated the effect of the ENG flake size on the ETC and reported an optimal size of ENG flakes near 200 μm. A reasonable configuration, including compact thickness and gap distance between compacts, significantly enhances the ETC and avoids the degradation of mass transfer [23]. However, the compact bed only uses straight HTF tubing instead of helical HTF tubing due to the compaction structure of the reaction bed. Bao [24] conducted a numerical comparison between different metal fins and MgH_2-ENG compact related to the heat transfer enhancement of the MH heat storage reactor (MHHSR). Based on a comprehensive evaluation that included the weight of the metal fins, the optimal heat transfer enhancement for the MHHSR used the MH compacts entirely without metal fins. The similar conclusion in the experimental study of Chaise et al. was that 20 wt% ENG-MgH_2 compacts obtain a similar reaction time as 5 wt% ENG-MgH_2 compacts added by copper fins [20].

Currently, the target of most MH reactor designs is to minimize the reaction time for hydrogen storage. However, more metrics need to be considered for heat storage applications, such as their output exergy and energy consumption. Moreover, the designs are almost always confined to structural optimizations of the heat exchanger without considering structural improvements of the reaction bed. In fact, structural improvements of the reaction bed can be used to reduce the required material and energy consumption, which is similar to the streamlining of aircraft to achieve drag reduction. A recent study on the