Numerical study and structural optimization on thermochemical heat storage performance of packed bed reactor

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ABSTRACT

Thermochemical heat storage has the advantages of high storage density and low heat loss, which has been an important component in energy system. A cylindrical reaction bed with heat transfer fluid as the heat source is established to study the dehydration process of Ca(OH)₂. Some methods are proposed to improve heat storage performance. The effects of strengthening heat transfer, enhancing vapor flow, and simultaneously enhancing heat transfer and vapor flow on heat storage rate and density for the process are analyzed by adding metal foam and fluid channels. The results show that improving heat transfer and fluid flow at the same time is the most effective way to improve thermochemical heat storage performance. During the heat storage process, it shortens the reaction time by 45.8%, while heat storage capacity is only reduced by 6.2%. In short, the effects of both heat transfer and vapor flow should be considered for the design of reaction beds of the thermochemical heat storage system.

Keywords: thermochemical heat storage; Ca(OH)₂; dehydration; numerical simulation

NONMENCLATURE

Abbreviations	
eff	effective
HTF	heat transfer fluid
MF	metal foam
TCHS	Thermochemical heat storage
X	reaction extent

1. INTRODUCTION

Gas-solid thermochemical heat storage (TCHS), which uses the reaction between gaseous and solid reactants to store and release heat, has been extensively

studied and applied in heat storage systems [1-3]. However, because of the low thermal conductivity and large internal resistance of the reaction bed, the reaction rate is too low and the charge and discharge process are delayed, which is a major factor limiting the large-scale application [4]. Based on previous researches, it can be found that the strengthening of the gas-solid system can be divided into two aspects: enhancing heat transfer and improving the gas transmission process. But there are few works that consider the effects of these two methods on heat storage performance at the same time, and compare them.

This research aims to improve the heat transfer and vapor flow performance of the Ca(OH)₂ heat storage bed. Firstly, foamed aluminum is used to carry the heat storage material to increase thermal conductivity, the effects of metal foam and its porosity on heat storage performance are analyzed. Then using metal mesh to separate the heat storage material and form fluid channels to improve the gas transmission, the effects of different fluid channel structures on heat storage performance are also examined. Finally, the comparisons between different performance enhancement methods are performed and evaluated, the optimal structure has been derived, which is significant for the performance enhancement and application of TCHS system.

2. MODEL DESCRIPTION

2.1 Physical model

A three-dimensional cylindrical reactor with heat transfer fluid(HTF, air) as the heat source is filled with Ca(OH)₂ particles for thermochemical heat storage. Fig. 1 shows the longitudinal and transverse sections of the reaction bed. The thin stainless-steel wall separates the fluid channel from the solid particles. The outer wall and the bottom of the reaction bed are also made of stainless

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steel and wrapped with heat-insulating material. The structural parameters of the reaction bed are shown in Table 1, and Table 2 displays the operating conditions.

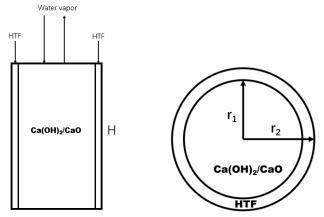


Fig.1 Structure of the reaction bed

Table 1 The structural parameters of the reaction bed

Parameter	Value
H(m)	0.2
r ₁ (m)	0.06
r ₂ (m)	0.05

Table 2 Operating conditions			
Initial pressure	28415 Pa		
Outlet pressure	28415 Pa		
Initial temperature	723 K		
Velocity of HTF	10 m/s		
The inlet temperature of HTF	863 K		
	Initial pressure Outlet pressure Initial temperature Velocity of HTF		

2.2 Mathematical model

The mathematical model provided by Wang et al. [5] is used in this study.

The following assumptions are adopted: (1) The thickness of the stainless-steel inner wall and metal mesh of the reaction bed is ignored; (2) Due to the flow resistance of thermal storage material is much larger than that of metal foam, the influence of metal foam on water vapor flow is neglected.

The Brinkman-Forchheimer extended Darcy model is used to describe the coupling of free media flow with porous media flow in the reaction bed:

$$\frac{\partial(\rho_{\text{vapor}}\vec{u})}{\partial t} + (\frac{\vec{u}}{\varepsilon}\nabla)(\rho_{\text{vapor}}\vec{u}) = \nabla[-\varepsilon p \, \mathbf{I} + (\nabla \vec{u})^{\mathsf{T}}] - \frac{2}{3}\mu_{\text{vapor}}(\nabla \vec{u}) \mathbf{I}] + S_{\mathsf{w}}\frac{\vec{u}}{\varepsilon} - \varepsilon \frac{\mu}{k}\vec{u}$$
(1)

The effective thermal conductivity can be calculated from the model provided by Shen et al. [6]:

$$\lambda_{\text{eff}} = \lambda_{\text{solid ligaments}} + \lambda_{\text{gas}} + \lambda_{\text{gas convection}} + \lambda_{\text{radiant}}$$
 (2)

$$\lambda_{\text{solid ligaments}} = \lambda_{\text{metal}} \cdot \text{relative density} \cdot 0.33$$

(3)

For the HTF, conservation of energy is given by:

$$\frac{\partial ((\rho c_{\rm p})_{\rm HTF} T)}{\partial t} + (\rho c_{\rm p})_{\rm HTF} \vec{u} \nabla T - \nabla (\lambda \nabla T) = 0 \tag{4}$$

3. MODEL VALIDATION

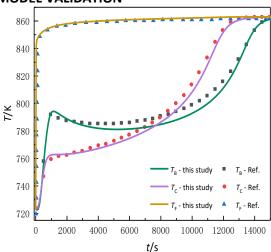


Fig. 2 Model validation

Fig. 2 shows the comparison between the results of the present work and those reported by Wang [5].

4. RESULTS AND DISCUSSION

4.1 Effects of metal foam porosity

Metal foam is introduced to increase the thermal conductivity of the reaction bed and improve the effects of enhancing heat transfer on TCHS, and the influence of different metal foam porosities is analyzed. Specifically, the four groups of no metal foam, ϵ_{MF} = 0.98, 0.95, and 0.92 are adopted.

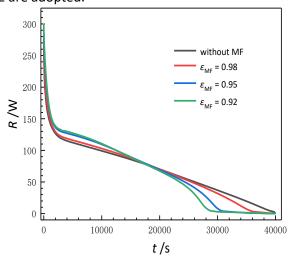


Fig. 3 Heat storage rate over time

Fig. 3 and Fig. 4 show the effect of different metal foam porosities on the heat storage performance. It can

be found that the heat storage time is shortened after adding metal foam. When ϵ_{MF} =0.95, the charging time is about 30826 s, and the heat storage capacity is 2.6 MJ, which means that the charging time is reduced by 21.0% and the total heat storage capacity only decreases by 5.8%. However, as the porosity of the metal foam decreases furtherly, the total heat storage capacity will continue to go down, but the heat storage time will not decrease too much.

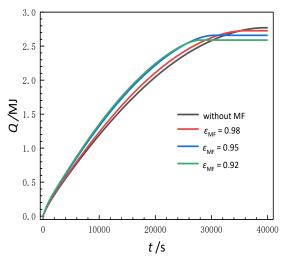


Fig. 4 Heat storage capacity over time

4.2 Effects of the structure of vapor channels





structure A structure B structure C structure D

Fig. 5 Different structures of the reaction bed

To reduce the pressure in the reaction bed during the dehydration process and increase reaction rate, the different structures of the reaction bed are designed. As shown in Fig. 5, structure A represents the reactor without a fluid channel, structure B represents a circular channel with a radius of 0.005 m is set in the middle part of the reactor, and C represents the reactor with a central channel and three extended channels. The width of the extended channel is 0.002 m, and the length is 0.02 m. D indicates that the number of expanded channels is 4. The water vapor can flow out through the fluid channel directly.

Fig. 6 and Fig. 7 show the heat storage rate and heat storage capacity over time. Compared with other structures, structure C is the most competitive one. The heat storage time of the structure C is shortened by about 31.6%, while the heat storage density is only reduced by about 1.8%.

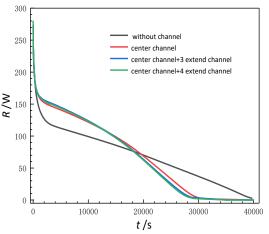


Fig. 6 Heat storage rate over time

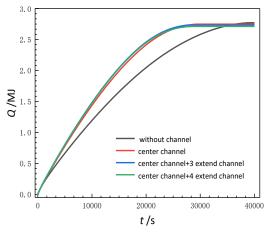


Fig. 7 Heat storage capacity over time

4.3 Combined effects of enhancing heat transfer and fluid flow

In order to analyze the difference between enhancing the thermal conductivity of the reaction bed, strengthening water vapor transport, and improving heat transfer and flow simultaneously on heat storage performance, the following four groups of research results are chosen for comparison in this study. (Four groups are: I. do not enhance heat transfer and fluid flow; II. using metal foam(ε_{MF} =0.95) to enhance heat transfer; III. using structure C to enhance vapor flow; IV. using metal foam(ε_{MF} =0.95) and structure C to enhance heat transfer and vapor flow.)

Fig. 8 and Fig. 9 show the heat storage rate and heat storage capacity over time under four different conditions. It can be found that case IV has a reduction in the total heat storage, but it can increase the heat storage rate the most effectively.

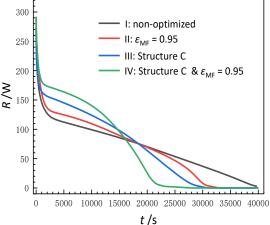


Fig.8 Heat storage rate over time

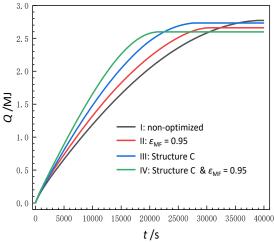


Fig. 9 Heat storage capacity over time

5. CONCLUSION

In this study, the effects of enhancing heat transfer and vapor flow on the heat storage performance of the CaO/Ca(OH)₂ fixed bed reactor are studied. Metal foam and fluid channels are used to improve the heat transfer and water vapor transmission of the reaction bed. The following conclusions can be derived:

- (1) The metal foam helps to increase the heat storage rate. However, a too low porosity of the metal foam will reduce the total heat storage capacity too much;
- (2) After adding fluid channels, the reaction has been promoted significantly, while the heat storage capacity is weakened little, and the recommended structure is C;
- (3) The effect of enhancing heat transfer and vapor flow simultaneously is analyzed. The heat storage time can be shortened by 45.8%, while the total heat storage capacity is only reduced by 6.2%, which is far better than that of unilaterally optimizing one of them.

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