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Optimization of thermochemical heat storage systems by controlling operating parameters and using two reactors

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Abstract

Direct CO_2 emissions from space heating and hot water production in buildings has been on a rising trend in recent decades. It is increasingly urgent to develop efficient and low-carbon heating technologies that can reduce energy consumption and shift the load to off-peak times. This work concerns thermochemical heat storage (TCHS), which has the potential to offer flexibility to bridge the energy supply and demand mismatches, and help with load shifting. One of the technical barriers for the use of TCHS is the variation of the outlet conditions for discharge process, which limits the implementation and competitiveness of the technology. Here we propose a new method to overcome the barrier. By using packed-bed based thermochemical reactors packed with silica gel, as an example, we use a Computational Fluid Dynamic (CFD) tool to understand the effectiveness of controlling and optimising the outlet conditions of the TCHS reactor. We demonstrated that, by optimizing the packed bed, a stable outlet temperature could be achieved. Furthermore, the whole TCHS performance could be enhanced, doubling the discharging power and prolonged discharge time by 4 times while keeping the same outlet temperature.

Keywords: Thermochemical heat storage, Silica-gel, Decarbonization, Optimization.

Introduction

Heating and cooling for residential, commercial, and industrial purposes accounts for a significant share of total final energy demand [1]. In the European Union, these systems are responsible for about half of the energy consumed by buildings and industries. In 2021, fossil fuels accounted for over 60% of the energy used for heating buildings, resulting in a new high of 2500 Mt of direct CO_2 emissions [2]. Hence, it is urgent to develop more efficient and low-carbon heating technologies that can reduce energy consumption and shift the load to off-peak times [3]. Many innovative approaches, such as solar thermal heat and heat pumps have been proposed for the provision of options for the load shifting and efficiency improvement of heating systems. However, many of these technologies are unable to overcome the scale of the unbalanced demand with supply.

Thermal Energy Storage (TES) provides a solution to address such a mismatch, which is particularly effective for balancing between energy demand and supply in heating and cooling systems. There are three main categories of TES technologies: sensible, latent and thermochemical. This work is concenred with thermochemical energy storage (TCES), which has the advantages of 5~10 times higher storage capacity [4] and negligibe heat loss during storage period. Such a technology, however, has several technical barriers such as varying outlet conditions, limiting the effectiveness of the technology and system efficiency. Research

efforts are therefore needed to develop new approaches for obtaining a more stable thermal output and a higher efficiency.

Several lab-scale testing rigs and prototypes have been reported in the literature [5–7], but the system efficiency and thermal power were very low. For example, a lab-scale thermochemical heat storage with about 1 kg strontium bromide hexahydrate ($SrBr_2 \cdot 6H_2O$) was established through an European project "thermal battery". The system achieved a thermal capacity of 65 kWh with an efficiency of 0.77 [8]. However, the thermal output power was unstable. Jaehnig et al. [9] tested a closed system containing ~200 kg of silica gel as part of the Modestore project. Their experimental results showed that the system could provide a maximum output heating power of 400 W and achieve a temperature lift of only 5℃ during discharge process. The AEE-Institute for Sustainable Technologies in Austria developed a closed and integrated sorption heat storage system for a single-family house [10]. Their experimental results showed that the storage density was much smaller than both theoretical one and that measured one under the laboratory conditions. Zongdag et al. [11] built an open system based laboratory prototype containing 17 dm^3 of Magnesium chloride ($MgCl_2 \cdot 6H_2O$) for space heating. The system generated a maximum thermal power of 150 W with only 50 W transferred to the load. The low heat transfer might be due to large heat losses of the system. An open sorption system designed by Zettl et al. [12] consisted of a rotating drum reactor filled with 50-53 kg zeolites. The system showed an energy density of 0.55-0.53 GJ/m^3 only when the desorption temperature was higher than 230℃ with very low initial water content in the material.

Two major observations can be drawn from the above on thermochemical heat storage systems: first, the present thermochemical energy storage systems have shown low efficiencies compared to the theoretical one; second, very few studies were found on obtaining a stable thermal output. Here we report our work on controlling and optimising the outlet conditions of a TCHS reactor. A CFD modelling was conducted using COMSOL Multiphysics v6.0 environment. The system was optimized , and we show that a stable outlet temperature could be achieved. Also, we showed that, the whole TCHS performance could be enhanced, e.g. enhanced discharging power and prolonged discharge time while maintaining the same outlet temperature.

System description

Figure 1 and **Table 1** depicts the system diagram and provides process details for controlling operation parameter of a single reactor and using two reactors. The first objective of this paer, controlling the operation parameters of a reactor packed with 0.8 kg silica gel. The system was running in two modes: (a) charging mode, where the inlet air was heated up to 130℃ and passed through the reactor to dehydrate the materials; (b) discharging mode, where the air flows through a humidifier and carries moisture to the reactor for hydration; heat released during this process which can be used for heating applications. Thermochemical materials, such as silica gel, exhibit a peculiar behaviour during discharge process. Initially, the outflow temperature increases sharply before eventually decreasing. However, a more stable output temperature is desirable for practical applications. In the proposed system, if the temperature drops below the desired setting (in our case, 40℃), the inlet relative humidity (RH) is increased or decreasing the flowrate (V) to maintain the outflow temperature.

To investigate the effects of different control strategies on the output temperatures during discharge, we simultaneously studied the following five approaches:

a) Constant_RH_V: Constant inlet relative humidity of 80% and flowrate of 33 LPM.
b) Control_RH: The inlet flow rate held constant at 3 m^3/h while inlet relative humidity varies from 20% to 80%.
c) Control_V: Constant relative humidity at 80%, while flow rate varies from 25 LPM to 87 LPM.
d) Control_RH_V: Firstly, the inlet flow rate held constant at 50 LPM while inlet relative humidity varies from 20% to 80% for a certain time , then, gradually reducing the flowrate (minimum flowrate of 25 LPM).
e) Control_V_RH: Firstly, keeping the relative humidity constant at 80%, while inlet flow rate varies from 25 LPM to 87 LPM for a certain time, then, gradually increacing the relative humidity (to a maximum value of 95%).

The second objective of this paper is using two reactors for optimization, the reactors can be charged or discharged in series or parallel, which controls the flowrate through the reactors. In the proposed cases, during discharge, reactor 1 can be operated first. When the outflow temperature drops below 40°C, the exit air can be introduced to the reactor 2 to continue the discharging process. Using this control strategy, the mass ratio in both reactors can be optimized to achieve a maximum adsorption heat. In this case study, the total mass of materials in 2 reactors was 1.6 kg. The diameters of both reactors were the same while the mass ratio was varied from the heights.

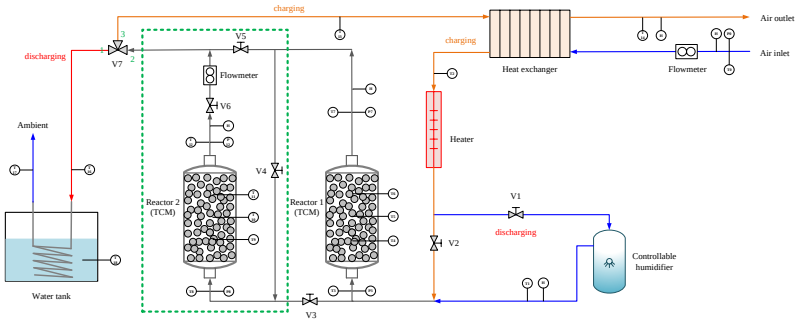

Figure 1 System diagram and operation modes by cotrolling inlet parameters and using two reactors.

Table 1 The operation modes for controlling inlet parameters and using two reactors.

Controlling inlet parameters (only reactor 1, reactor 2 in green box is not applicable)							
Valves	V1	V2	V3	V4	V5	V6	V7
Charging	×	√	×	n/a	n/a	n/a	2-3
Discharging	√	×	×	n/a	n/a	n/a	2-1
Using two reactors							
Valves	V1	V2	V3	V4	V5	V6	V7
Charging	×	√	×	√	×	√	2-3
Discharging	√	×	×	T7>40℃, × T7<40℃, √	T7>40℃, √ T7<40℃, ×	T7>40℃, × T7<40℃, √	2-1

Energy conversion and sorption equilibrium

This section presents the energy balance of the system and sorption equilibrium of silica gel. The adsorption heat Q_{ads} for discharging is calculated by

$$Q_{ads} = \int_0^t (\dot{m}_{out} h_{out} - \dot{m}_{in} h_{out}) dt \quad (1)$$

The adsorption rate of packed bed is given by the linear driving force (LDF), expressed as a function of time [13,14]

$$\frac{dw}{dt} = K(w_e - w) \tag{2}$$

where w is the vapor amount absorbed by the absorbents and w_e is the vapor amount absorbed under equilibrium conditions. K is the overall mass transfer coefficient that is calculated by

$$K = \frac{15 D_{so}\, exp(-\frac{E_a}{RT})}{{r_p}^2} \tag{3}$$

where r_p is particle radius, D_{so} is the pre-exponential constant, E_a is the activation energy and R refers to the universal gas constant [14].

The equilibrium water concentration w_e is calculated using Temperature-Dependent Toth isotherm [14]. The fitted Toth parameters are given in **Table 2**.

$$w_e = \frac{aP_w}{[1 + (bP_w)^n]^{1/n}} \tag{4a}$$

$$a = a_0\, exp(E/T) \tag{4b}$$

$$b = b_0\, exp(E/T) \tag{4c}$$

$$n = n_0 + c/T \tag{4d}$$

P_w means the partial pressure of water vapor in the airflow.

The required input parameters to solve the above equations in Comsol model are given in **Table 3**. The model geometry has a cylindrical shape with inlet and outlet ports as shown in the left side of **Figure 2**. The reactor is fully insulated and three thermocouples have fitted in the centre of the reactor at different locations to monitor the temperature.

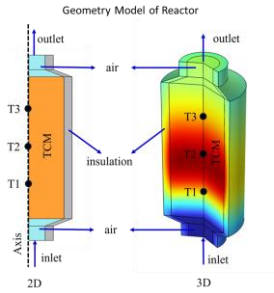

Figure 2 Single reactor geometry of COMSOL modeling.

Table 2 Temperature-dependent Toth isotherm parameters for water vapor on silica gel [14,15].

Parameter	Value
a_0 (mol/kg Pa)	0.1767
b_0 (1/Pa)	2.78E-8
n_0	-0.00119
c (K)	22.13
E (K)	1093

Table 3 Input parameters for the numerical model [13,14,16].

Parameters	Value
Average particle radius (r_p)	1.5 mm
Bed height (L)	200 mm
Bed diameter	86 mm
Activation energy (E_a)	4.2E4 J/mol
Gas constant (R)	8.314 J/mol/K
Pre-exponential term (D_{so})	2.54E-4 m^2/s

Discussion and Results

Figure 3 depicts a temperature contour during discharging in CFD modelling and reactor temperature profiles. The moist air at room temperature flows from the bottom to the top of reactor, heat released during adsorption process and then carried out by air flow for the application. The materials hydrated layer by layer, and the temperature first increases then decreases with absorbing more moisture.

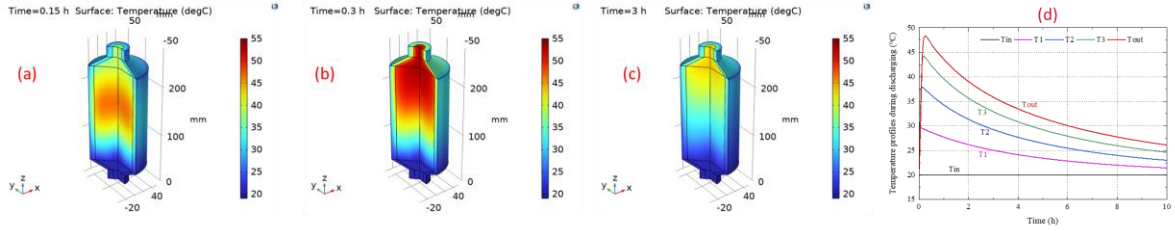

Figure 3 Temperature contours at (a) 0.15 hours, (b) 0.3 hours and (c) 3 hours of discharge; (d) temperature profiles of reactor at discharge process.

Figure 4 shows the reactor outlet temperature and thermal power during discharging under various control strategies. By controlling the inlet relative humidity and flowrate, the system shows more stable output temperatures and higher than 40℃ for longer time though the thermal power reduce. For instance, with a constant relative humidity and flowrate (case a), the outflow temperature drops sharply lower than 40℃ after 1.75 hours that can not reach the target temperature for applications. However, by adopting control strategies (b) and (c), the output temperature remains stable at 40℃ for about 4 hours. Moreover, by applying control strategies (d) and (e), the output temperature remains stable at 40℃ for more than 6~7.6 hours. The discharge period extends more than 4 times compared to the constant inlet conditions, regardless themal power is low during extended period. Thus, the total adsorption heat at acceptable temperature, as shown in **Figure 5**, is increased of 88% to 174% with controlling of inlet relative humidity and flowrate leading to increase the total system effeciency.

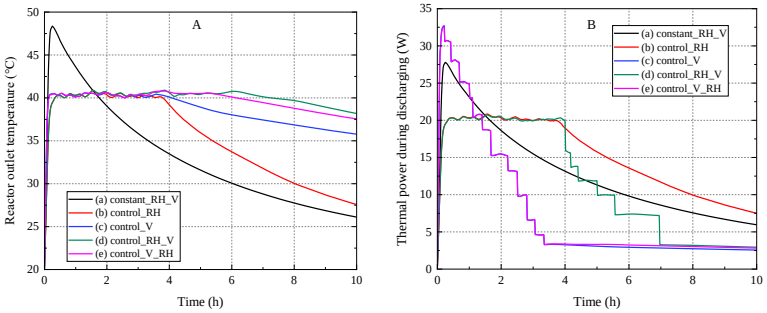

Figure 4 (A) Reactor outlet temperatures and (B) thermal power of discharging under various controlling strategies.

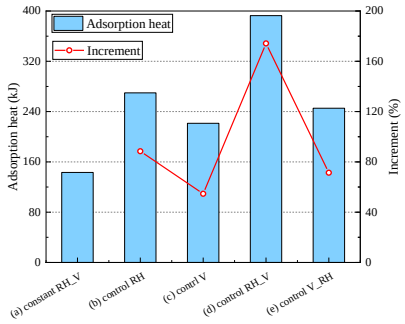

Figure 5 Usable adsorption heat under various control strategies.

By using two reactors, **Figure 6** illustrates the temperature profiles of the reactor outlet and usable adsorption heat under various mass ratios during discharging. Using double reactors with any mass ratio extends the discharge period within the required temperature compared to a single long reactor scenario. For example, while the discharge period with a single reactor is approximately 5.4 hours, it is extended by 22% when using double reactors with mass ratios of (R1:R2) 70%:30%. Because the inlet temperature of reactor 2 is higher than ambient temperature which can activcate the adsorption process of silica gel. Therefore, the adsorption heat of double reactors with any mass ratio is higher than that of a single reactor. Moreover, it foud that the optimum mass ratio of the double reactors system is 40%:60%, that increases the adsorption heat by approximately 14%. This is because of using double reactors can reduce the pressure drop and improves the heat and mass transfer in the system.

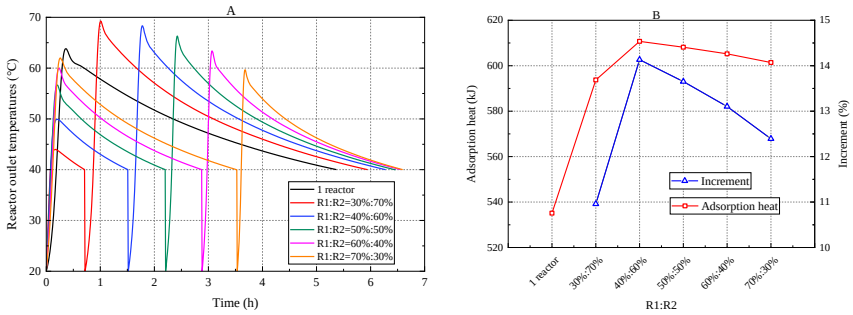

Figure 6 (A) Reactor outflow temperature profiles and (B) usable adsorption heat for various mass ratios durging discharging.

Summary/Conclusions

This study focuses on thermochemical heat storage (TCHS) for heating applications. One of the technical barriers for TCHS is the variability of outlet conditions during the discharge process. To overcome this, we proposed a new method of controlling the inlet parameters so that we can control the reaction process, subsequently controlling the outlet conditions. The results show that by optimizing the inlet relative humidity and flowrate, rather than using constant conditions, the discharge period within the desired temperature can be extended by up to four times with a 174% increase in the usable adsorption heat. Additionally, optimizing the mass ratios of double short reactors, rather than using a single long reactor, can also extend the discharge period and increase the released heat. Compared to a single reactor, using double reactors results in 14% more heat released during discharging with optimum mass ratio of 40%:60%.

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References:

[1] IRENA (2021), World Energy Transitions Outlook: 1.5°C Pathway, International Renewable Energy Agency, Abu Dhabi. n.d.

[2] Heating – Analysis - IEA n.d. https://www.iea.org/reports/heating (accessed April 20, 2023).

[3] Ahmad, A., Ding., Y., "A thermochemical energy storage based cooling and heating system: Modelling, experimental validation and lab-scale demonstration", Energy Conversion and Management, 2021.
[4] Jarimi, H., Aydin, D., Yanan, Z., Ozankaya, G., Chen, X., Riffat, S., "Review on the recent progress of thermochemical materials and processes for solar thermal energy storage and industrial waste heat recovery", International Journal of Low-Carbon Technologies, 2019.
[5] Mauran, S., Lahmidi, H., Goetz, V., "Solar heating and cooling by a thermochemical process. First experiments of a prototype storing 60kWh by a solid/gas reaction", "Solar Energy", 2008.
[6] Casey, S.P., Aydin, D., Riffat, S., Elvins, J., "Salt impregnated desiccant matrices for 'open' thermochemical energy storage—Hygrothermal cyclic behaviour and energetic analysis by physical experimentation", Energy and Buildings, 2015.
[7] Michel, B., Mazet, N., Neveu, P., "Experimental investigation of an innovative thermochemical process operating with a hydrate salt and moist air for thermal storage of solar energy: Global performance", Applied Energy, 2014.
[8] Fopah-Lele, A., Rohde, C., Neumann, K., Tietjen, T., Rönnebeck, T., N'Tsoukpoe, K.E., et al, "Lab-scale experiment of a closed thermochemical heat storage system including honeycomb heat exchanger", Energy, 2016.
[9] Jaehnig, D., Hausner, R., Wagner, W., Isaksson, C., "Thermo-chemical storage for solar space heating in a single-family house".
[10] Bales, C., Gantenbein, P., Jaenig, D., Essen, M., Weber, R., "Laboratory tests of chemical reactions and prototype sorption storage units. A Report of IEA Solar Heating and Cooling Programme - Task 32 Advanced Storage Concepts for Solar and Low Energy Buildings".
[11] Zondag, H., Kikkert, B., Smeding, S., Boer, R., Bakker, M., "Prototype thermochemical heat storage with open reactor system", Applied Energy, 2013.
[12] Zettl, B., Englmair, G., Steinmaurer, G., "Development of a revolving drum reactor for open-sorption heat storage processes", Applied Thermal Engineering, 2014.
[13] Deshmukh, H., Maiya, M.P., Srinivasa Murthy, S.,"Study of sorption based energy storage system with silica gel for heating application", Applied Thermal Engineering, 2017.
[14] Helaly, H.O., Awad, M.M., El-Sharkawy II, Hamed, A.M., "Theoretical and experimental investigation of the performance of adsorption heat storage system", Applied Thermal Engineering, 2019.
[15] Wang, Y., LeVan, M.D., "Adsorption Equilibrium of Carbon Dioxide and Water Vapor on Zeolites 5A and 13X and Silica Gel: Pure Components", J Chem Eng Data 2009.
[16] Chua, H.T., Ng, K.C., Chakraborty, A., Oo, N.M., Othman, M.A., "Adsorption Characteristics of Silica Gel + Water Systems", J Chem Eng Data, 2002.