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INVESTIGATION OF AN INNOVATIVE THREE-PHASE THERMOCHEMICAL REACTOR FOR BUILDING'S APPLICATION

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ABSTRACT
Increasing the share of renewable energy in buildings sector is essential. While the dynamic nature of the renewables is an obstacle for improving its efficiency. In this context, thermal energy storage technologies are to store the renewables and supply it to meet building's demand. Thermochemical energy storage stands out in advantages including high energy storage density and low thermal loss. However, for a thermochemical energy storage system, the thermochemical reactor is critical. To tackle drawbacks of the reactor, this paper proposes an innovative three-phase thermochemical reactor and investigates its performance through an experimentally validated numerical model. The reactor is integrated with fins and air gaps to enhance heat and mass transfer. Key parameters and the related heat and mass transfer efficiency of the reactor in both charging and discharging processes have been investigated. According to the analysis, the integration of fins has increased the reactor performance by 129% in charging and by 77% for COP in discharging. The effect of fin pitch has been examined and the results show that reducing the fin pitch can increase the reactor performance by up to 14% in charging and 7.5% in discharging. However, the enhancement is not sensitive for fin pitch lower than 30 mm. Additionally, increase the gap size can enhance the charging performance but may reduce discharging efficiency and the optimal gap size range is 3 mm to 5 mm.

Keywords: Thermochemical energy storage, reactor, heat and mass transfer enhancement, reactor performance analysis

NONMENCLATURE

Abbreviations	*Term*
A	contact area, m^2
h_r	enthalpy of adsorption, J/kg_{H2O}
h	convection heat transfer coefficient, $W/(m^2{\cdot}K)$
m	mass, kg
$\dot{m}$	mass flow rate, kg/s
$\dot{q}$	heat transfer rate, W
T	temperature, K
t	time, s
U	thermal conductance, $W/(m^2{\cdot}K)$
ϕ	specific humidity air, $kg_{H2O}/kg_{dry\ air}$
X	water uptake of adsorbent, $kg_{H2O}/kg_{adsorbent}$
Subscriptions	*Term*
a	air
in	inlet
out	outlet
$pipe$	water pipe
s	dry adsorbent solid
w	water

1. INTRODUCTION

The global buildings sector accounts for 30% of final energy consumption [1]. To reduce carbon emissions, the share of renewable energy in buildings should be increased. While a major obstacle is the mismatch between the building's energy demand and supply of renewable energy sources. To secure a continuous green energy source, scholars have been researching in thermochemical energy storage technologies which stores renewables when available and releases the energy for demand such as space heating. However, for

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its performance, one critical component is the thermochemical reactor [2].

Thermochemical reactor is a space where energy storage and release take place. Efforts have been making to investigate and improve the reactor performance. In 2016, Tatsidjodoung et al. have investigated a thermochemical system with 2 segmented reactors in sandwich structure [3]. Air diffusers have been installed at the upper and lower regions. Zeolite 13X is located at the middle region, supported by an oval shaped perforated grating. According to the tests, however, the reactor air pressure drop is relatively large at around 230 Pa due to the supporting structure. In 2016, Rebecca et al. have tested a full-scale thermochemical reactor for a research building in Germany [4]. Using 3200 kg zeolite 13X, the reactor is separated into 4 sub-sectors. Each sub-reactor is divided into 6 layers. Any two layers form a gap as air flow path. Using the configuration, the sub-reactors can be charged and discharged separately. In 2016, Aydin et al. have reported a modular reactor with internal air input [5]. A pipe shaped reactor is integrated with a diffuser pipe which brings in the air and diffuses it across the reactor. A relatively high adsorption and desorption rate at over 10 g/min have been achieved in experimental tests. Overall, the recent studies in thermochemical reactor lead to improvement opportunities as follow:

- Optimise reactor structure to reduce flow resistance and also provide robust material support.
- Enhance heat and mass transfer within the reactor.
- Optimise heat supply and extraction channel.
- Cyclability and reliability is a real issue which shall be addressed.

To improve the performance of thermochemical reactors, the present study proposes and numerically investigates a novel three-phase thermochemical reactor through an experimentally validated model. The reactor design is given in section 2. The reactor performance through numerical investigations have been demonstrated in section 2 and 3. Highlights have been summarised in section 4.

2. THERMOCHEMICAL REACTOR AND METHODS

This section illustrates the reactor design, numerical model for the reactor performance analysis, and model validation. Zeolite 13X is the thermochemical material for this study.

2.1 Design of the three-phase thermochemical reactor

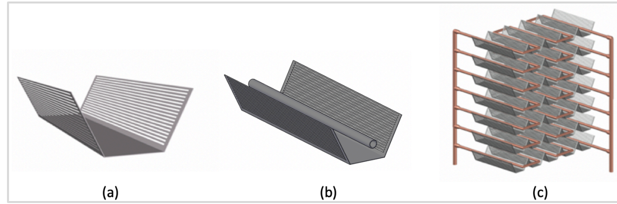

Fig 1 Reactor design: (a) the container, (b) integration with pipe, (c) multiple containers to scale up

The reactor design is depicted in Fig 1. A trapezoid container is proposed with multiple gaps at the sides. To allow heat extraction from the reactor, a water pipe is integrated into the container. The reactor can be scaled up with multiple containers (Fig 1(c)). The reactor dimensions are given in Fig 2 and Table 1. The gaps allow the opening area percentage reach to 38% (the area ratio between the gaps and the side of the container).

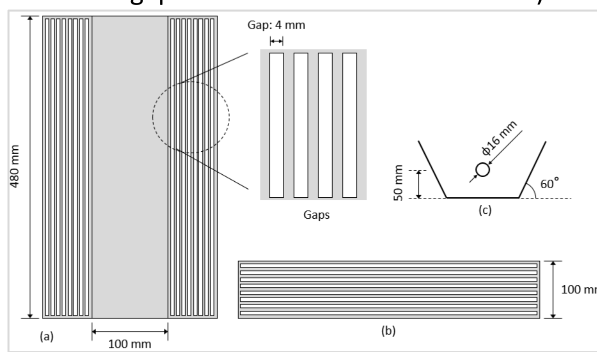

Fig 2 Reactor dimensions: (a) top view, (b) side view, (c) cross section view

Table 1 Reactor dimensions

Gap size	480 mm * 4 mm
Distance between the gaps	4 mm
Water pipe diameter	16 mm
Material	Stainless steel container Copper water pipe

Additionally, to enhance the heat transfer within the reactor, fins have been integrated into the water pipe (Fig 3). In this paper, the reactor with and without fins are named as fin pipe reactor and smooth pipe reactor, respectively.

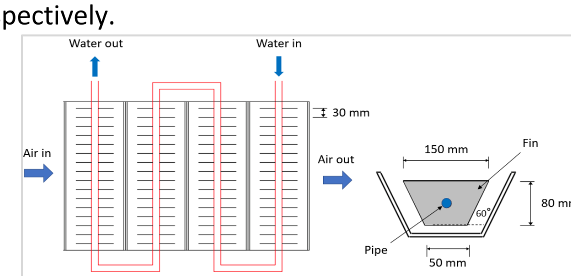

Fig 3 Illustration of the reactor with fin pipe: (a) air flow and water flow, (b) cross section view

2.2 Numerical model of the reactor

To investigate the reactor performance, a numerical model has been developed and illustrated in this section including heat and mass balance equations, adsorption equilibrium, mass transfer resistance, and differential enthalpy of adsorption.

Convective heat transfer of zeolite 13X and air:

$$\underbrace{d\dot{q}_{s\rightarrow a}}_{Heat\ transfer\ rate} = \underbrace{(T_s - T_{a,in})/\left(\frac{1}{U_{s,a}}\right) dA_{s,a}}_{Heat\ transfer\ from\ zeolite\ to\ air} \quad (1)$$

Heat transfer rate of air and water flow:

$$d\dot{q}_{a\rightarrow pipe} = (T_{a,in} - T_{pipe,in}) / \left(\frac{1}{h_{w,pipe} \cdot dA_{pipe}} + \frac{1}{h_{pipe,a} \cdot dA_{pipe,a}}\right) \quad (2)$$

Conductive heat transfer of water pipe and zeolite 13X:

$$d\dot{q}_{pipe\rightarrow s} = (T_{pipe,in} - T_s)/\left(\frac{1}{h_{w,pipe} \cdot dA_w}\right) \quad (3)$$

Mass balance between air and zeolite 13X:

$$\underbrace{\dot{m}_a\left(\phi_{a,out} - \phi_{a,in}\right)}_{Change\ of\ mass\ for\ air} = \underbrace{-\frac{dX}{dt}m_s}_{Change\ of\ mass\ for\ zeolite} \quad (4)$$

The adsorption equilibrium of zeolite 13X is calculated using the Dubinin-Astakhov equation [6,7]. Additionally, to calculate the mass transfer resistance, liner driving force model is utilised [8]. Moreover, measured and validated by Kim et al. [9], the correlation between the differential enthalpy of adsorption h_r and the water uptake of zeolite X is used.

$$h_r = 7\times10^7X^6 - 7\times10^7X^5 + 3\times10^7X^4 - 7\times10^6X^3 + 899951X^2 - 69983X + 6491.3 \quad (5)$$

Additionally, to evaluate the reactor performance, the applied performance indicators are heat transfer efficiency (HTE), mass transfer efficiency (MTE), and coefficient of performance (COP) of the reactor.

$$HTE_{charging} = \frac{Q_{stored}}{Q_{in}}$$
$$HTE_{discharging} = \frac{Q_{release}}{Q_{equilibrium}} \quad (6)$$

MTE is the change of water uptake at any time divided by the maximum water uptake change (the initial state minus the equilibrium state), given as:

$$MTE = \frac{(X_{initial} - X)m_s}{(X_{initial} - X_e)m_s} \quad (7)$$

For a discharging process, COP of the reactor is the ratio of reactor energy generation and energy input by a discharging process, given as:

$$COP_{reactor} = \frac{Q_{gen}}{Q_{a,in}} \quad (8)$$

2.3 Numerical model validation

The numerical model has been validated to demonstrate the intended applicability. Experimental tests have been conducted for the model validation process. Fig 4 shows the built reactor in the experiment.

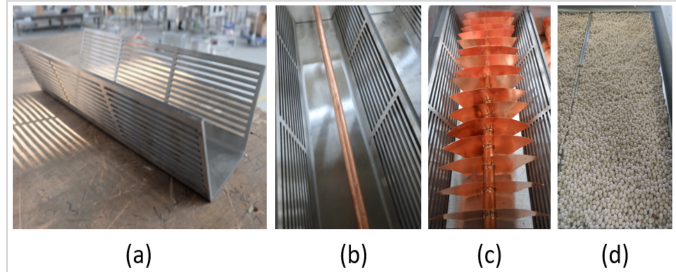

Fig 4 Pictures of the built reactor: (a) the container, (b) reactor without fins, (c) reactor with fins, (d) the container filled with zeolite 13X

By comparing the reactor outlet air temperature in charging and discharging processes, a good agreement has been obtained between the numerical modelling and experiment (Fig 5(a) and Fig 5(b)). The root mean square percent error ranges from 6.02% to 12.29%, within the acceptable error range [10,11].

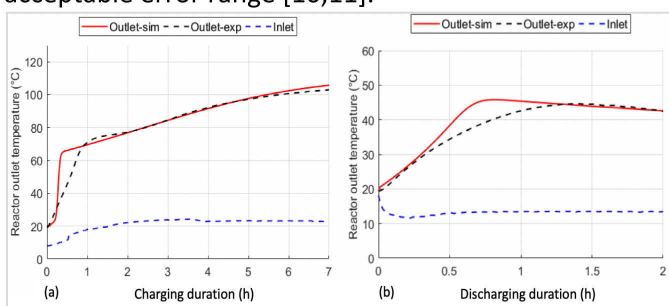

Fig 5 Measured and simulated inlet and outlet temperature of the reactor during (a) charging and (b) discharging processes

3. RESULTS AND DISCUSSIONS

For the reactor performance, effect of critical parameters has been investigated including the gap size, integration of fins, and fin pitches to obtain the optimal performance. The evaluation focuses on air as input and output in charging and discharging. The charging evaluation is conducted with inlet air at 180 °C, 0.048 kg/s, and ambient temperature at 20 °C. The discharging analysis is conducted with inlet air at 20 °C, 0.048 kg/s, and specific humidity at 13.94 g/kg. The ambient is at 20 °C and 60% relative humidity. The thermochemical material is equilibrium with the ambient before a discharging analysis.

3.1 Gap size on the reactor performance

The effect of gap size on the reactor performance is shown in Fig 6 and Fig 7. For charging, both heat and mass transfer efficiency increase with the gap size. However, for discharging, excessive gap size can hinder the performance. Because ambient moist air is driven through the reactor which reduces the thermochemical material temperature and adsorption intensity under relatively large gap. Statistically, COP and mass transfer efficiency peak at 3 mm and 3.5 mm each. Considering both charging and discharging process, the gap is suggested to range from 3 mm to 5 mm.

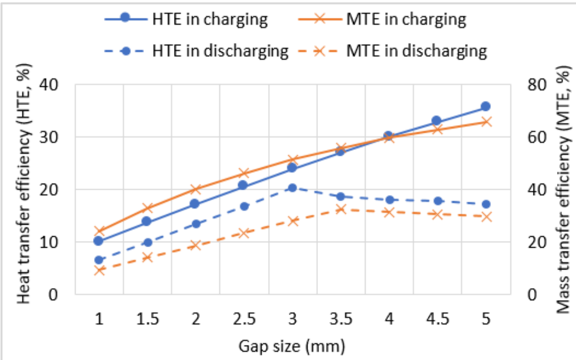

Fig 6 Reactor performance for different opening gap

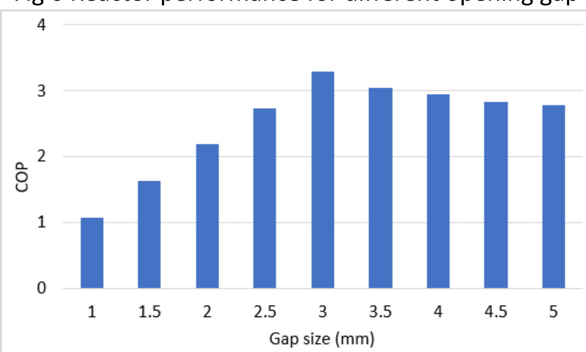

Fig 7 Reactor COP for different opening gap

3.2 Integration of fins on the reactor performance

The performance for the smooth and fin pipe reactor is given in Fig 8 and Fig 9. When comparing charging performance of the two reactors, the fin pipe reactor stands out in both heat and mass transfer efficiency. For instance, in 1 hour, the heat and mass transfer efficiency reach to 71% and 43%, respectively, while the smooth pipe reactor achieves at 31.4% and 20.3%, respectively. Although, the mass transfer efficiency of smooth pipe reactor increases gradually and reaches to 82% in 8 hours while under the same situation the fin pipe reactor reaches to 84% in 3 hours. In average, the fin pipe reactor has improved the heat and mass transfer efficiency by 129% and 55%, respectively.

For the smooth pipe reactor, the heat transfer from air to the reactor is mainly obstructed by the low thermal conductivity of zeolite 13X at 0.2 W/(m·K). However, the integration of the fins has boosted the reactor performance which directs the heat from air throughout the reactor, lifting the thermochemical material temperature. Since the reaction kinetic is closely linked to the material temperature, the mass transfer rate $\frac{dX}{dt}$ is increased, leading to relatively more moisture exchange and adsorption energy storage.

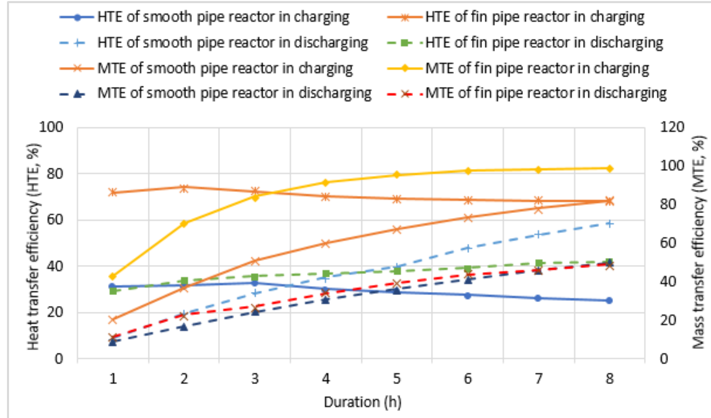

Fig 8 Reactor performance of smooth and fin pipe reactor

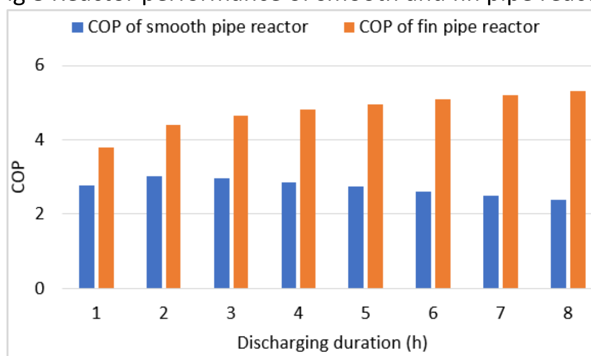

Fig 9 Reactor COP of smooth and fin pipe reactor

When it comes to discharging, both COP and mass transfer efficiency of fin pipe reactor exceed that of the smooth pipe reactor. For mass transfer efficiency, the average improvement is 13%. For COP, the average improvement is 77%.

The reactor COP is lifted by the heat transfer enhancement of the fins. Considering reactor outlet air as the heat supply source, fins direct the released adsorption energy from the air inlet side of the reactor to the outlet, increasing temperature of the thermochemical material and outlet air. This also improves the reaction kinetics across the reactor. However, the relatively small improvement in mass transfer efficiency at 13% is resulted from the humidity of the inlet air. With the heat and mass transfer improvement of the fins, the fin pipe reactor is more likely to achieve adsorption equilibrium with the air. The specific humidity of the air flow shall be increased to further enhance the mass transfer efficiency.

3.3 Fin pitches on the reactor performance

Since fins boost the reactor performance, the effect of fin pitches becomes significant. The reactor performance under different fin pitches from 10 mm to 50 mm is analysed and the reactor performance is shown in Fig 10 and Fig 11. Reducing fin pitches increase both charging and discharging performance, especially for fin pitches from 30 mm to 50 mm. However, for fin pitches below 30 mm, less performance improvement is achieved. The fins direct energy of air and solid material across the reactor. When fin pitches reduce to an extent, the heat transfer between any two fins is dominated by the heat transfer between air and solid material.

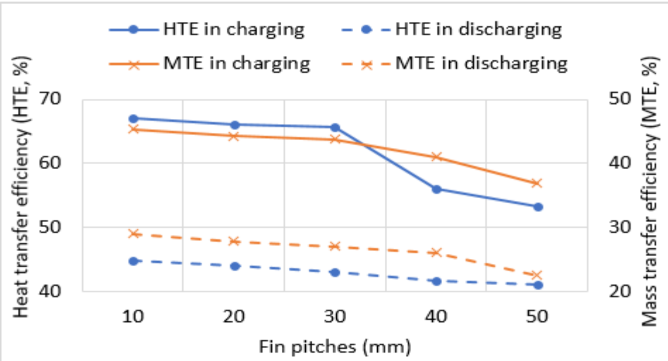

Fig 10 Reactor performance for different fin pitches

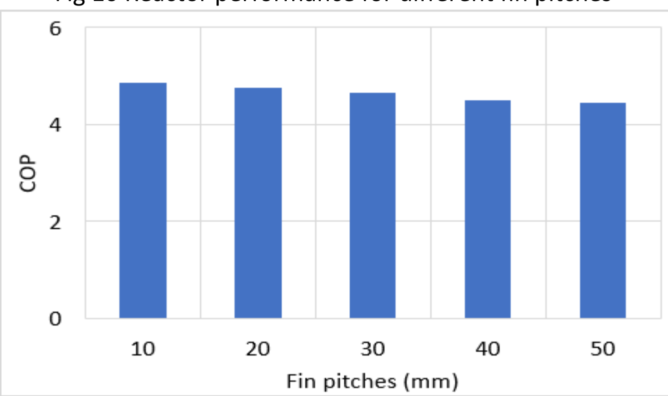

Fig 11 Reactor COP for different fin pitches

3.4 *Comparison of the results to the literature*

Table 2 summarises the investigation results and the comparison with the findings of the other related studies. In this study, the investigation on the reactor gap size is new to the literature. For the integration of fins, the findings in the reactor performance enhancement consist with the other studies especially for the adsorption heat exchangers. However, the findings in the effect of fin pitch are interesting to the literature as they partly consist with the studies where the geometry and operational conditions of the published reactor can differ from the current study.

4. CONCLUSION

The paper proposes a three-phase thermochemical reactor to tackle the current drawbacks of thermochemical reactor with numerical investigations on thermal performance through an experimentally validated model. The highlights of the study are listed as follow.

- The literature gives an insight of the development opportunities in thermochemical reactors, especially for the structure optimisation and heat and mass transfer enhancement.
- The trapezoid reactor with side gap supports the thermochemical material and increases the opening area percentage to 38%.
- Fins have boosted the reactor performance, improving the average heat and mass transfer efficiency by 129% and 55% each in charging and by 77% for COP and 13% for mass transfer efficiency in discharging.
- Critical reactor dimensions to the reactor performance have been evaluated including gap size and fin pitches. The suggested gap size and fin pitches range from 3 mm to 5 mm and 10 mm to 30 mm, respectively.
- The specific humidity of inlet air can be raised to further increase the reactor discharging intensity.

Table 2 Findings and comparison with the other related studies

Investigations in the study	Findings	Contributions and comparison to the literature
Gap size on the reactor performance	• Reactor performance increases with gap size and peak at 3 mm to 5 mm. Excessive gap size reduces discharging performance.	• New to the literature.
The integration of fins on the reactor performance	• Fins have boosted the reactor performance by up to 129% in average.	• Consist with the experimental study on a closed thermochemical reactor [12]. The reactor is composed by copper fins, achieving an energy yield of 60% of the theoretical value.

		• Consist with [13] where flat-tube heat exchangers has achieved high specific cooling power in adsorption chillers. However, authors have called geometry optimisation in fins.
Effect of fin pitches on the reactor performance	• Reducing fin pitches increase reactor performance by up to 14% in charging and 7.5% in discharging. • Less performance improvement is achieved with fin pitch under 30 mm.	• Consist with the studies on finned flat-tube adsorption heat exchangers [14,15] where the specific cooling power increase with reducing fin pitches. However, it is more sensitive at a lower fin pitch. • Conflict with the study on a closed type thermochemical reactor [16] where the fin plate has been placed vertically to the mass transfer fluid. The fin is an obstacle to the mass transfer fluid dynamic and thus a better mass transfer is achieved at larger fin pitch.

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