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Evaluating design criteria of silica gel based open bed reactor to meet domestic heating demand [#]

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ABSTRACT

The present study conducts a thermal analysis of a silica gel-based open cycle reactor serving as a daily heat storage system. Heat and mass transfer in the reactor during heat discharge are simulated using a transient local thermal non-equilibrium model. The model is validated against experimental data obtained under two different operating conditions, indicating satisfactory agreement between the experimental and the simulated results. Additionally, the study explores the space heating demand on the coldest winter day in London. Design criteria, including the optimal amount of silica gel and the required air flow rate for this open bed reactor to meet this demand, are evaluated and analysed.

Keywords: Thermal energy storage, adsorption, open-bed sorption system, silica gel, numerical study

NONMENCLATURE

Abbreviations	
A_p	Particle Area (m^2)
C_p	Specific heat capacity (J/kg.K)
D_0	Diffusion coefficient (m^2/s)
D_s	Surface diffusivity (m^2/s)
E_a	Activation energy (J/mole)
ΔH	Isosteric heat of adsorption (kJ/kg)
k	Mass transfer coefficient (s^{-1})
K_{eff}	Effective thermal conductivity (W/m^2.K)
m	Mass (kg)
$\dot{m}$	Mass flow rate of air (kg/s)
q	Water uptake in the adsorbent (kg)
Q	Heat demand (kWh)
T	Temperature (K)
$(UA)^{-}$	Overall heat transfer coefficient (W/K)
W	Mass of water (kg)
Subscripts	
da	Dry air
g	gas
ha	Humid air
s	Solid adsorbent
sh	Space heating

1. INTRODUCTION

Efficient and sustainable thermal energy storage (TES) systems are essential for transitioning from fossil fuels to renewable energy sources, particularly in residential heating applications. Thermophysical energy storage technology has received significant attention in these applications due to its non-toxic and non-reactive materials, long-term storage capabilities with no energy loss, and high energy density [1,2]. To leverage the benefits of adsorption TES, a thorough performance analysis is necessary to advance the technology from laboratory experiments to practical applications [3]. Accurate transient models that predict heat and mass flows are required to capture the dynamics of the adsorption process [4]. Previous studies have modeled closed-cycle energy storage systems using silica gel to predict performance in heating applications and energy storage [5,6]. However, open-cycle systems for these applications have not been extensively investigated. The simpler design and reduced number of components in open-cycle systems make them attractive for practical implementation [7].

In this study, we investigate the heating capacity of an open cycle heat storage system utilizing silica gel to deliver heat at a rate of 3 kW during a peak demand period lasting 6 hours, achieving an average temperature rise of 21 K. Section 2 outlines the charging and discharging processes of the reactor for daily heat storage, followed by a subsection describing the modeling of heat and mass transport within the reactor. The simulated temperature profile at the outlet of the bed is validated using two sets of experimental data obtained from an in-house test rig of the heat storage system. The validated model is then employed to estimate the optimal weight of silica gel and the essential air flow rate to achieve the desired heating capacity and

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temperature rise, meeting the space heating demand of a typical semi-detached dwelling on a cold winter day.

2. METHOD ANALYSIS

2.1 System description

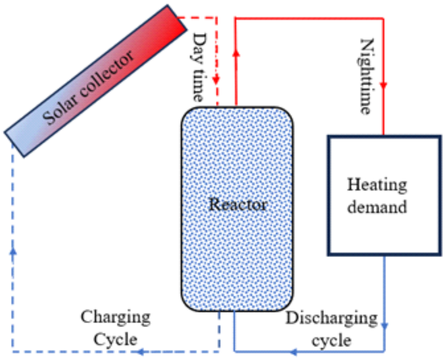


Fig. 1 Schematic of charging and discharging of the bed for daily heat storage system

The schematic of the open cycle adsorption heat storage system is depicted in **Fig. 1**. The primary component of this system is the silica gel reactor. For thermal energy storage, the reactor is connected to the solar collector during the daytime, utilizing solar energy as the heat source to charge the reactor. This energy is retained indefinitely within the material, provided it remains sealed from the environment. As the thermal energy is stored in terms of heat of desorption, not in terms of sensible energy, this technology offers a no-loss heat storage. Subsequently, heat can be released according to the energy demand via an exothermic adsorption process, where water from the air is adsorbed into the pores of the silica gel [8].

2.2 Reactor model and simulation

Humid air with an inlet moisture content W_{in} and temperature T_{in} flows at a mass flow rate $\dot{m}_{ha}$ through the reactor of material thickness L during adsorption or heat discharge process. The water uptake in the adsorbent is denoted as q. Following realistic assumptions are made to simplify the adsorption model [9]

1. Heat from solar collector is adequate to completely regenerate the adsorbent bed before adsorption starts.
2. One-dimensional and steady airflow with a constant flow rate through the bed is considered.
3. The water vapour and heat transport processes within the adsorbent bed are transient.
4. Solid adsorbent and air inside the reactor are not in local thermal equilibrium [10].
5. The homogeneous properties of the adsorbent particles are assumed over the bed.
6. Mass transfer resistance is considered to estimate sorption rate using linear driving force (LDF) model.

Current numerical model, simulating an open cycle adsorption process, is schematically presented in **Fig. 2** which includes initial and boundary conditions for adsorption process.

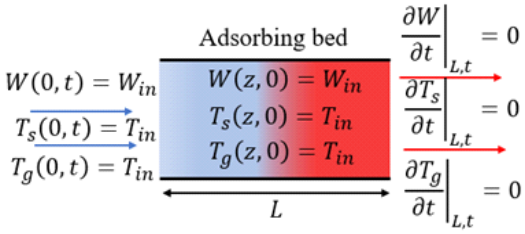


Fig. 2 Schematic representation of the numerical model displaying initial and

Mass transfer of water vapour in the reactor occurs through either advection or adsorption of water by solid material [11]. Governing equation to represent the mass balance inside the adsorbent bed is as follows

$$\dot{m}_{da}(W_{in} - W_{out}) = m_{da}\frac{dW}{dt} + m_s\frac{dq}{dt} \tag{1}$$

Linear driving force (LDF) model is employed to express adsorbed water uptake in above equation [12]

$$\frac{dq}{dt} = k(q^* - q) \tag{2}$$

The overall mass transfer coefficient (k) for adsorption is determined by following equation.

$$k = 15D_s/R_p^2 \tag{3}$$

The surface diffusivity (D_s) in above equation is calculated by

$$D_s = D_0 exp\left[-\frac{E_a}{RT}\right] \tag{4}$$

Equilibrium adsorption uptake (q^*) at any instant in Eq. (2) is given by empirical Toth equation for silica gel water pair and formulated as [5,13]

$$q^* = \frac{K_0 \exp\left(\Delta H_{ads}/RT\right)P}{\left\{1 + \left[\frac{K_0}{q_m}\exp\left(\Delta H_{ads}/RT\right)P\right]^{\tau}\right\}^{\frac{1}{\tau}}} \tag{5}$$

Constants in LDF model [14] and Toth isotherm equation [13] which are applied in this study are summarized in **Table 1**.

Release of heat of adsorption may cause substantial temperature difference between the air and solid adsorbent during adsorption. Therefore, energy balance equations for solid adsorbent and air are formulated separately and expressed as follows [10], respectively

$$m_s C_{ps}\frac{\partial T_s}{\partial t} + K_{eff}A_{bed}\frac{\partial T_s}{\partial z} + hA_p\left(T_s - T_g\right) = \Delta H m_s \frac{dq}{dt} \tag{6}$$

$$m_{ha}C_{pg}\frac{\partial T_g}{\partial t} + \dot{m}_{ha}C_{pg}\left(T_g - T_{g,in}\right) = hA_p\left(T_s - T_g\right) \tag{7}$$

Table 1 LDF model coefficients and Toth isotherm coefficients for silica gel – water working system.

Symbol	Value	Unit
D_0	2.54×10^{-4}	m^2/s
E_a	4.2×10^{-4}	J/mol
K_0	4.65×10^{-10}	kg/(kg kPa)
ΔH_{ads}	2.71×10^{3}	kJ/kg
q_m	0.4	kg/kg
R	8.314	J/mol K
τ	10	-

2.3 Experimental process

This experimental study uses 1 kg of commercial non-indicating white Type A silica gel (SiO_2) manufactured by Brownell Ltd. The bulk density of this silica gel is 720 kg/m^3 and particle diameter is 2-5 mm. An open cycle heat storage system using packed silica gel bed was developed and tested in our lab. Photograph of this set up is depicted in **Fig. 3**.

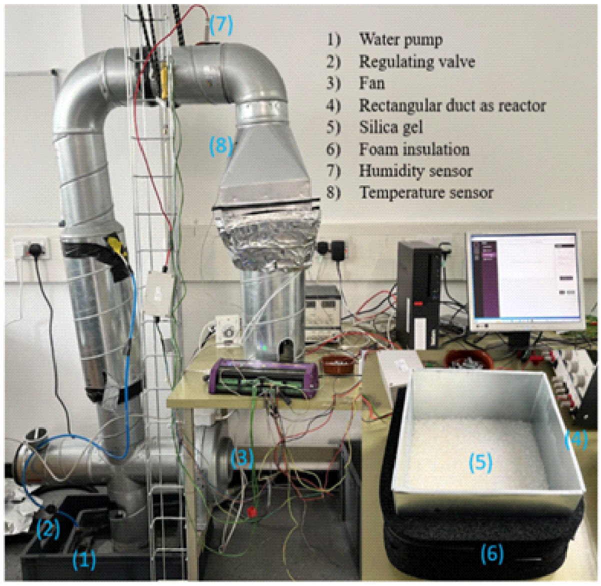


Fig. 3 Photograph of experimental test rig of an open cycle heat storage system

Moist air with specified humidity and flow rate passes through the reactor and after the adsorption process, dry hot air exits through outlet. Heat storage capacity of the material is determined at various operating conditions by monitoring the temperature of the inlet and outlet air. Details of this experiment has been described in previous work [16].

3. RESULTS AND DISCUSSION

3.1 Validation

The numerically simulated temperature profile is validated against experimental data obtained from an open bed heat storage system at two distinct flow rates and inlet relative humidities of the air stream, as depicted in **Fig. 4**. A comparison between the numerical and experimental data reveals a maximum discrepancy of 0.6% when evaluated at an air flow rate of 100 l/min and 80% humidity. Similarly, at a flow rate of 66 l/min and 40% inlet humidity, the discrepancy between the two datasets is only 0.2%. The design properties of the reactor and the operational conditions for model validation are summarised in **Table 2**.

Table 2 Characteristics of adsorption column and working conditions for model validation

Parameter	Value
Column breadth (mm)	200
Column width (mm)	200
Silica gel thickness (mm)	34.7
Ambient temperature (ºC)	21
Inlet relative humidity (%)	80, 40
Air flow rate (l/min)	100, 66
Particle diameter (mm)	2.5

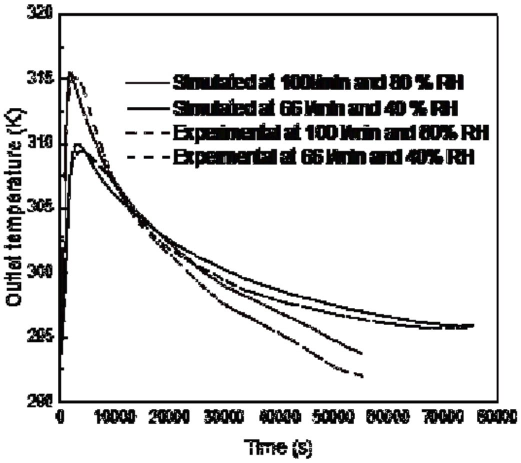


Fig. 4 Validation of numerical model with experimental data at two operating conditions

3.2 Heating demand

The hourly space heating demand (Wh) for a typical residence in London during the coldest December day was estimated using the equation provided by Zhiwei et al. [17], and the results are illustrated in **Fig. 5.**

$$Q_{sh} = \overline{UA}(T_r - T_a) \tag{8}$$

$\overline{UA}$ and comfortable room temperature (T_r) in the above equation have been considered as 150 W/m^2 and 20ºC [18]. Ambient temperature is obtained from photovoltaic geographical information system.

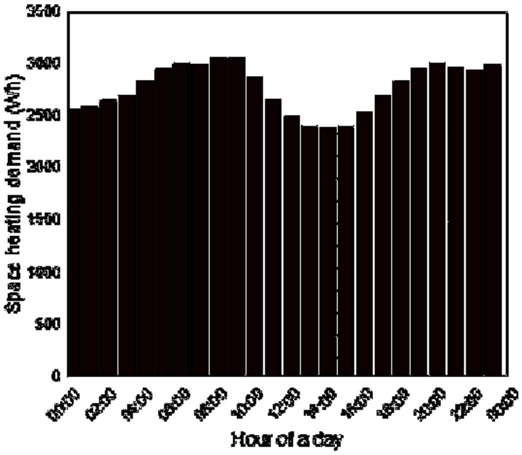


Fig. 5 Hourly space heating demand of a December day in London

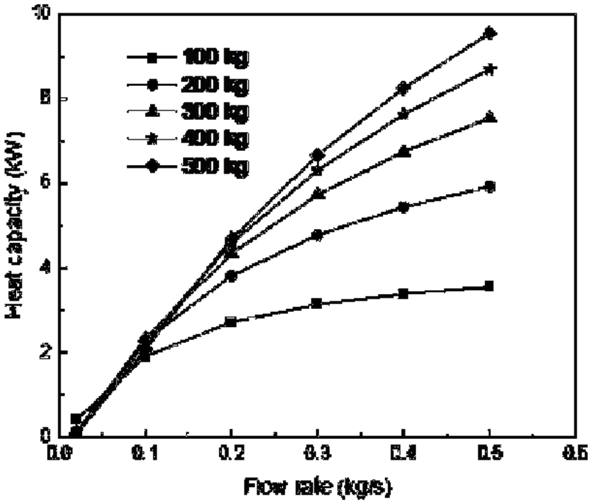
The peak space heating demand is identified to be approximately 3 kWh, occurring between 4 am and 10 am (**Fig. 5**). In the subsequent section, our objective is to determine the optimal bed weight and air flow rate for this system to supply heat at a rate of 3 kW for the duration of the 6-hour peak demand period.

3.3 Selection of optimum bed weight and air flow rate

Heating capacity (W) of the system is estimated using following equation [6]

$$Q_{air} = \frac{m_{air} C_{p,air} \int_0^{t_{ads}} (T_{g,exit} - T_{g,in}) dt}{t_{ads}} \tag{9}$$

The average outlet air temperature is utilized to determine the average temperature lift achieved by the system. The system is intended to be designed to deliver a temperature rise of 21 K, which is adequate for moderate heating applications, in addition to a thermal power output of 3 kW sustained over a period of 6 hours. The heat capacity and average temperature lift obtained from the heat storage system with varying amounts of silica gel are plotted against the air flow rate in **Fig. 6 and 7**, respectively. The heat capacity increases with increasing flow rate and amount of silica gel (**Fig. 6**), while an optimal air flow rate exists at which the system achieves the maximum temperature rise (**Fig. 7**). These two figures collectively indicate that systems with 100 kg and 200 kg of silica gel are unable to simultaneously meet our desired performance criteria. The required air flow rate to meet our demand for different amounts of silica gel is listed in **Table 3**.



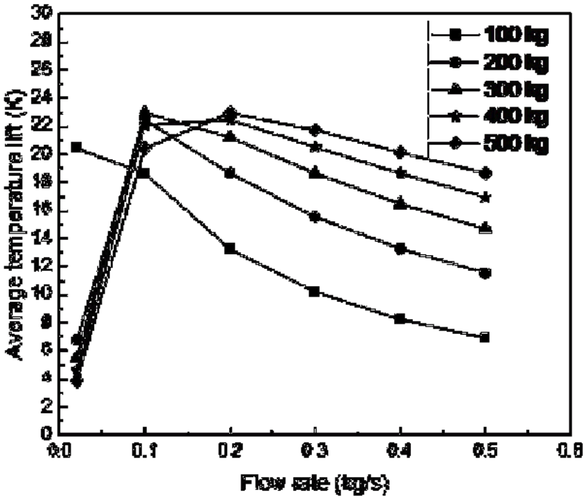


Fig. 7 Average temperature lift obtained from the reactor as a function of air flow rate and amount

Table 3: Optimal amount of silica gel and air flow rate to supply 3kW thermal power for 6 hours at 21 K average temperature rise

Mass of silica gel (kg)	Air flow rate (kg/s)
300	0.14
400	0.13
500	0.12

4. CONCLUSIONS

The energy storage performance of an open cycle silica gel system was examined using a numerical simulation based on a local non-thermal equilibrium model. The model accurately predicted the outlet air temperature, aligning well with experimental data. For a typical residence in London on a cold winter day, it was determined that a minimum of 300 kg of silica gel and an air flow rate of 0.14 kg/s are required to meet the space heating demand.

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