

Research Article

Study of a Thermochemical Heat Storage Reactor Filled with Polyaluminum Sulfate for Low-Temperature Application

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This paper investigates comprehensively the operational dynamics of a thermochemical heat storage (TCHS) reactor for lowtemperature applications using polyaluminum sulfate and takes into consideration a developed simulation model with an experimentation validation. Significant concordances were found between the developed simulation model and the experimental results. Results reveal optimized conditions for the charging process using an electrical heater, with a heating temperature of 120°C at 10 K/min over 500 minutes. This achieves full material charging, with stabilized pressure drops at an equilibrium of 80 mbar, corresponding to a temperature of approximately 108°C, and yielding a thermal power of 950 W. An inlet vapor pressure of 18 mbar at 10°C for 5 hours is sufficient to completely discharge the bed, with pressure drops reaching around 30 mbar and a thermal power of 300 after reaction completion. Insights into conversion extents during both processes are provided, along with a remarkable thermal efficiency of 90% and a coefficient of performance (COP) of 97%, surpassing recommended theoretical values (50%). The study suggests further enhancing system performance through the design and implementation of a dedicated heat exchanger. The achievement of 75% of the targeted thermal power specification represents a significant milestone, offering valuable contributions towards the realization of sustainable technological advancements of both the reactor technology of TCHS and state-of-the-art thermal energy storage solutions. From the research, it is possible to infer further suggestions for enhancing this performance by designing and implementing a dedicated heat exchanger for both heat supply and retrieval mechanisms.

1. Introduction

Within searching for efficient energy storage solutions, reactors built to function as thermal chemical heat storage (TCHS) reactors are emerging as potential candidates that take advantage of accumulative features of reversible chemical reactions [1–5]. Optimal operation of these reactors, however, faces challenges ranging from balancing between charging and discharging to energy consumption provocation linked to conventional heating methods. Despite the progress, a significant gap between simulation and experimental data exists that hampers the large-scale development of this technology. In some instances, challenges arise from implementing simulation results in real prototypes while many of them are not verified under rigorous experimentation set up. This makes relatively large differences between the simulation and experimental data. This study takes a keen look at the balance of interaction between simulation and experimental results that would bring these challenges down. Therefore, the primary objective of this study is to narrow down this gap by combining the two approaches, simulation and experimentation, primarily for improving the performance of TCHS reactors using aluminum sulfate as a storage material, in providing more sustainable thermal energy storage solutions. Accordingly, the inquiry carefully examines concerning the intricate mechanisms governing the behavior of the reactor, validifying the adopted model while providing valuable insights into key aspects of the performance of the reactor.

2. Materials and Methods

2.1. System Analysis and Target Specifications. Before starting the analysis, specifications of the parameters to be targeted in this work are introduced for delineating the studied requirements and constraints, hence allowing the design of an innovative prototype reactor that shall serve as a solution towards overcoming the existing limits of the reactors.

These values are selected based on various prior studies on thermochemical heat storage applications in closed reactor configurations [6–9]. The aim is to generate heat output at around 50°C within the reactor, suitable for direct utilization in the intended application. The formula employed to determine the discharging reaction time using both the released power of the reactor and the stored energy is written as follows:

Power released =
$$\frac{\text{stored energy}}{\text{time}_{\text{disch}}}$$
, (1)

$$time_{disch} = \frac{stored energy}{power released}.$$
 (2)

For this system, the prototype reactor can run for 5 hours during a cold period. The emphasis on discharging time aims to provide justification for the necessary simulation duration in numerical studies. Consequently, a running period of five hours (18000 seconds) has been selected for this purpose. It is important to note that the essential parameters, including permeability, thermal conductivity, specific heat capacity, and kinetic properties, have already been established in a previous study (reference) and will be applied in the current context.

2.2. TCHS Reactor and Experimental Investigation. The Chinese Academy of Sciences has engineered a compact thermochemical heat storage device, depicted in Figure 1, specifically designed for experimental investigations. This system is dedicated to the storage and retrieval of thermal energy, employing reversible chemical reactions with thermochemical heat storage (TCHS) material.

In the laboratory reactor, the objectives outlined in Table 1 serve as the target. Throughout the instrumentation process, effectively handling the vacuum state and maintaining the pressure within the reactive bed pose a significant challenge. The lab setup of the reactor is shown in Figure 2.

The reactor is constructed from titanium, and preliminary corrosive tests have been conducted on this material. Results indicate that, within a 24-hour time frame, aluminum sulfate does not adversely affect the metal. However, extended exposure beyond five days begins to degrade the structure. Given that the cycle tests in the reactor typically do not extend beyond a day, it is anticipated that corrosion issues are unlikely to arise during these operations. The device is made with essential components, including a cylindrical reactor, two control boxes—one for managing temperature and pressure and another for overseeing weight—a support adjustment block to stabilize the assembly of system components, a centrally located heating tube for supplying heat, temperature measurement probes, and a mass sensor for accurate weight measurements. Figure 3 shows a simplified schema of the storage circuit.

During the dehydration or charging mode, the thermochemical material (TCM) underwent an energetic charging process. In this mode, the operational principle was as follows:

- (i) Material loading
 - (a) The lid is removed using a hexagonal wrench key, and once the material sample is loaded into the reactor cavity, the top of the reactor is securely sealed
- (ii) Initialization
 - (a) Calibration and initialization of the weight sensor are performed
 - (b) The main power button is activated, and the data collection line is connected to the control boxes
 - (c) The program for monitoring the temperature of the reactive bed is then initiated, and the control values (heating temperature, fluid pressure, and volume flow) are input
 - (d) The valve between the water storage tank and the vacuum pump is opened, and the vacuum pump is activated to establish the vacuum
- (iii) Heat input
 - (a) The desorption heat is supplied from the laboratory power unit through the heating tube
- (iv) Desorption
 - (a) Water vapor released from the salt hydrate is condensed and subsequently pumped into the water container beneath the reactor jacket
- (v) Measurement
 - (a) Following the completion of each experiment, the data is meticulously recorded
 - (b) The experiments are then replicated multiple times to ensure the establishment of equilibrium within the system

The discharging mode or hydration process is as follows:

(i) Water discharge



FIGURE 1: Compact thermochemical heat storage reactor.

TABLE 1: System requirements and target values.

Parameters	Target value
Energy storage density	90 kWh
Storage capacity	95 kWh
Thermal power	1.2 kW
Bed temperature range	25-120°C
Bed pressure range	10-100 mbar
Thermal conductivity of the bed	0.44 W/m/K
Permeability of the bed	2×10^{-9}
Heating rate	10 K/min

- (a) Water from the container is pumped into the flow controller
- (ii) Steam production
 - (a) Inside the steam generator, the pumped water undergoes a process to produce steam
- (iii) Vapor adsorption
 - (a) The produced steam is carried to the reactive bed
 - (b) The storage material in the reactive bed adsorbs the vapor
- (iv) Heat of adsorption
 - (a) During the adsorption process, heat is released
- (v) Temperature and pressure monitoring

- (a) Temperature variations are recorded by the temperature controller box
- (b) Pressure variations are recorded by the pressure controller box

2.3. System Simplification and Description. The reactor configuration relies on radial heat conduction and utilizes a cylindrical vessel designed to operate under atmospheric pressure and steady-state conditions.

The test material sample was compacted into a powder or granular bed enclosed within a titanium alloy tube, capped at the upper end by a stainless-steel disk lid. A cartridge heater, generating heat flux radially within the cylinder, was employed. Additionally, four Pt 100 temperature sensors were strategically positioned along the diameter of the cylinder, as illustrated in Figure 4.

To ensure exclusively radial temperature gradients, both the top and bottom were effectively insulated using insulating paste (KAIMANN EPDM PL32-R) with a thickness of 32 mm. Calibrating the thermocouples for this apparatus was necessary. The validation experiment involved determining the thermal conductivity of well-known materials and comparing the data to the literature data. The thermal conductivity of the PAS was also determined later, and data were compared to the one previously obtained using the DSC/TGA method [10–12]. A fluid (dry air) and a solid (glass) with a known thermal conductivity to fill the gap were employed. The thermal conductivity of air, a welldocumented parameter varying with temperature, was obtained from tabulated data in [13].

In an experiment conducted with dry air, the determination of heat transfer across the gap relied on the application of Fourier's law of heat conduction, assuming the air within the reactor remained stationary. The heat input to the



FIGURE 2: Reactor prototype during the lab experimentation.



FIGURE 3: Schematic diagram of the reactor during charging/discharging.



FIGURE 4: Simplified schematic of the reactor.

electrical heater was provided by the power unit, and the disparity between the heater and the cylinder jacket indicated heat loss. The experiment was carried out with varying amounts of electrical power input, resulting in different temperature differences across the air layer. This relationship was then represented as a function of the temperature difference across the gap. To achieve this, information on the heater voltage (V), current intensity (I) passing through the heater resistance (R_h) providing the plug-in temperature (T_p) , and the jacket temperature (T_i) maintained at room temperature needed to be known. To determine steadystate conductivity, a constant heat power was applied along the axis of the sample bed, while the external cylinder wall was held at a room temperature of 30°C ±2°C. Temperatures $T(r_i, t)$ at various radial positions were recorded until reaching a stable condition. The sample bed's conductivity was then calculated using Fourier's radial dimensional heat conduction equation.



FIGURE 5: Reactor numerical simulation algorithm.

$$\lambda = \frac{q}{2\pi L} \cdot \frac{d(\ln(r_i + 1/r_i))}{dT},$$
(3)

where q is constant heat power in W, $dT/d(\ln (r_i + 1/r_i))$ is the slope on the temperature fitting curve, and L is the sample axial length. According to Presley and Christensen, inaccuracies in this method can arise from longitudinal heat loss, convection currents, radiation losses, thermal expansion of the sample or core heater, perturbation of the heat flow by the thermocouples, and unsymmetrical heat flow [14]. To mitigate the first three reasons, an insulating paste was applied. The slope and associated uncertainty were determined using the linear fit function in the Origin software. The analysis is based on the following assumptions:

- (i) Heat conduction occurring in one direction
- (ii) Temperature variations along the flow direction
- (iii) The temperature difference being significantly smaller than the mean temperature of the medium

Gurgel et al. scrutinized the uncertainty arising from assuming one-directional heat conduction [15]. They concluded that axial heat losses would minimally affect (less than 1%) the measurement of low thermal conductivity in materials when the ratio of length to the diameter of the sample bed exceeds 2.5. In our case, this ratio was significantly lower than 2.5. Consequently, a calibration was conducted using dry air, as explained in the preceding section, to assess the useful heat transferred in the bed. The wellestablished thermal conductivity of air (as a function of temperature) was employed for this assessment, with a mean value of 0.03 W·m⁻¹·K⁻¹ for a temperature range from 0°C to 327°C [13]. An experiment with dry air was conducted, and the heat transferred across the bed was determined using Fourier's law of heat conduction. Directly evaluating the thermal conductivity based on Eq. (3) proved to be intricate. Therefore, for most practical applications, the parameters were derived from the best fit to the experimental data.

To ensure the accurate measurement of the useful electrical power supplied to the bed, blank measurements were conducted on an empty cylinder. This blank measurement process aimed to eliminate disturbances, address certain systematic uncertainties, and mitigate the impact of buoyancy effects. Within the reactor, the air-filled chamber underwent heating, and thermocouples recorded the temperature variation between the heating element and the outer surface of the jacket. This recorded data served as the heat calibration during the process.

The electrical power device provides heat in the following manner:

$$\mathbf{P} = V \bullet I, \tag{4}$$

where V is the heater voltage and I is the current intensity.

2.4. Numerical Investigation. Hydration is directly linked to discharge, making it a key focus for achieving the required output for the average user. From an engineering standpoint, the question revolves around optimizing the conversion process to deliver excellent performance. The answer lies in determining the ideal vapor flow rate through the bed, determining the bed size, optimizing its porosity, and identifying the optimal hydration time.

2.4.1. Geometry Design. Computational modeling offers approximate solutions to scientific or technical problems. To simplify the system, a simple 2D asymmetric model of the reactor has been considered, as shown in Figure 4.

The geometry consists of three different parts. Domain (2) represents the reactive bed domain (material + reactive gas), domain (3) is the electrical heater tube, and domain (1) is the reactor wall thickness. The outside wall of the reactor is isolated, and the corresponding boundary conditions are set up in the COMSOL model for simulation.

2.4.2. Mathematical Model. Mathematical modeling involves representing the physical phenomena occurring within a reactor through mathematical equations. Solutions to these equations aid in understanding the reactor's operation, identifying issues and irregularities, and proposing innovative or corrective solutions to enhance efficiency. Due to the complexity of the equations governing physics, computational and simulation software are employed to solve them.

Typically, the algorithm depicted in Figure 5 is utilized for problem resolution.

Various literature [8, 16–23] has already investigated the mathematical equations involved in closed or open thermodynamic systems.

In this study, the system under consideration is closed and isolated. Therefore, there is no mass exchange with its surrounding environment. During dehydration, a drop in the mass density of the salt hydrate will increase the mass density of the water vapor in the reactive bed and the reverse process will happen during the hydration.

(1) Charging Phase (Dehydration). In this phase, the motion of water vapor released from the salt hydrate was not considered. Balasubramanian et al. justified this omission of convective heat and mass transfer by highlighting that salt hydrates typically exhibit porosity and voids in their structure, causing the hydrated salt not to occupy the entire volume of the system [24]. Equation (5) is employed in this context for the chemical rate.

$$\frac{\partial \alpha}{\partial t} = A_f \exp\left(-\frac{E_a}{RT}\right) \bullet \alpha^b (1 - \alpha^c) \bullet \left(1 - \frac{p_i}{p_{\text{eq}}}\right).$$
(5)

The parameters *b* and *c* are constants that vary based on the experiment. A_f is the preexponential Arrhenius factor. E_a is the activation energy. The variable α represents the extent of conversion and is defined as follows [25, 26]:

$$\alpha(t) = \frac{m_0 - m(t)}{m_0 - m_f} \text{ (experiment)},$$

$$\alpha(t) = \frac{c_0 - c(t)}{c_0 - c_f} \text{ (simulation)},$$
(6)

where m_0 and m_f are the initial and final mass of the salt hydrate, respectively. Regarding the kinetic equation for this type of reaction, some authors had demonstrated that the parameters in Eq. (5) could be taken as b = 1 and c = 0 for the dehydration [27–30].

Mass balance and transfer. Given the closed and isolated nature of the system, there is no mass exchange with the surroundings. Consequently, a reduction in hydrate mass density results in an increased mass density of the anhydrous substance, water vapor, and the bed. Considering the porosity of the bed, the mass conservation equation for the water desorption system can be expressed as follows:

$$\varepsilon \frac{\partial \rho_g}{\partial t} = -\nabla \bullet \left(\rho_g \bullet \boldsymbol{u}_{\boldsymbol{v}} \right) + D_g \bullet \Delta \rho_g + \chi \bullet \rho_g \frac{\partial \alpha}{\partial t} \bullet \frac{M_g}{M_{s1}}, \tag{7}$$

where ρ_g represents the gas phase mass density of the salt hydrate bed, ε is the total porosity of the bed, u_v and D_g are the velocity and the diffusion coefficient of the water vapor inside the bed, χ is the stoichiometric coefficient of water, and M_g/M_{s1} is the ratio of the molecular mass of water vapor on the molecular mass of the solid phase. The term $\chi \cdot \rho_g(\partial \alpha / \partial t \cdot M_g/M_{s1})$ is known as the mass source term, which accounts for the decomposition rate of salt hydrate from the solid phase to the desorbed phase. Equation (7) is also known as the convective-diffusion-reaction equation where the first term $\varepsilon(\partial \rho_g/\partial t)$ represents the water vapor accumulation in the pores of the salt bed, the second term $-\nabla \cdot (\rho_g \cdot u_v)$ is the water vapor transport out of the salt bed, the third term $D_g \cdot \Delta \rho_g$ is the vapor diffusion through the salt bed, and the last term $\chi \cdot \rho_g (\partial \alpha / \partial t \cdot M_g / M_{s1})$ is the mass desorption rate of water from the solid salt to the gaseous phase. The gas generated during the decomposition reaction is assumed to have the ability to diffuse in and out of the bed. The diffusion coefficient according to [31] can be written as:

$$D_{g} = \left(\frac{0.43(T/100)^{1.81}(1/M_{g} + 1/M_{s})^{0.5}}{p_{eq}(T_{cg}T_{cs}/10000)^{0.1406}\left[(V_{g}/100)^{0.4} + (V_{s}/100)^{0.4}\right]^{2}}\right) \cdot \frac{\varepsilon\delta}{\tau},$$
(8)

where T_{cg} and T_{cs} represent the gas and solid phase temperature at the critical point, respectively, V_g and V_s are the gas and solid atomic volume, respectively, p_{eq} is the equilibrium pressure, τ is the tortuosity characterizing the convoluted nature of the porous pathways followed by diffusing species, and δ is the constrictivity depending on the ratio of the diameter of the diffusing particle to the pore diameter with a value always less than 1.

Energy balance and heat transfer. Heat is supplied to the salt hydrate bed through the electrical heater tube as previously described in Section 2.2. Radiation heat is neglected in this context. Also, there was no need to solve the heat equation for both the solid and gas phases separately since, during the decomposition, the temperatures of the different phases were approximately equal $(T_g \approx T_s)$. In the case of the solid phase, a source term accounting for internal heat generation through chemical reactions was taken into consideration. The energy balance equation is formulated as follows:

Heat accumulation = heat conduction + heat convection + heat source term.

$$\left(\rho \bullet C_p\right)_{\mathrm{eq}} \bullet \frac{\partial T}{\partial t} = \nabla \bullet \left(\lambda_{\mathrm{eq}} \bullet \nabla T\right) - C_{pg} \bullet \rho_g \bullet \boldsymbol{u}_v \bullet \nabla T + \frac{\rho_{\mathrm{eq}}}{M_{s1}} \bullet \frac{\partial \alpha}{\partial t} \bullet \Delta H_r.$$
(9)

In Eq. (9), the source term $\rho_{\rm eq}/M_{s1} \cdot \partial \alpha/\partial t \cdot \Delta H_r$ is presumed to be constant, representing the energy associated with the desorption of water between the solid salt and the gas phase. (C_p) eq and $\lambda_{\rm eq}$ are the heat capacity at constant pressure and the thermal conductivity of the bed at the equilibrium, respectively.

Flow regime of the vapor. The flow regime in the bed is assumed to be Darcy's flow type according to the Reynolds number [32, 33]. When heating the salt hydrate, water vapor is released through diffusion. Mass transfer in the gas phase occurs not only through diffusion but also through advection, where a pressure difference induces bulk motion of the gas. The velocity of the gas leaving the bed is typically expressed as follows:

$$\boldsymbol{u}_{\boldsymbol{v}} = -\frac{k}{\mu} \left(\nabla p_{\text{bed}} - \rho_g \boldsymbol{\bullet} g \right), \tag{10}$$

where μ is the viscosity of the water vapor, k is the intrinsic permeability of porous medium (salt hydrate medium), ∇p_{bed} is the pressure difference across the bed, ρ_g is the water vapor density, and g is the acceleration of gravity. The gas phase is assumed to be ideal, i.e., partial pressure $p = \rho_g RT/M_{\text{H}_2\text{O}}$. R is the constant of the ideal gas.

Boundaries and initial conditions. All variables in any direction inside the reactor were initially considered to be uniform.

At t = 0,

$$T(0, x, y, z) = T_0,$$

 $p(0, x, y, z) = p_i,$ (11)
 $\alpha = 0.$

In the context of the domain depicted in Figure 6, at the boundary where x = 0 (at the top), the pressure gradient was assumed to be zero due to airtight walls, and a convective heat transfer boundary condition is present for the solid phase.

$$\lambda \frac{\partial T}{\partial x} = 0,$$

$$p(t, 0, y, z) = 0,$$

$$\alpha \neq 0,$$
(12)

$$\boldsymbol{n} \cdot \left(-\lambda_{\rm eq} \nabla T \right) = h(T - T_{\rm ext}), \tag{13}$$

where *h* is the convective heat transfer coefficient. At x = L (at the bottom), it was assumed that the vapor pressure equals the evapo-condenser pressure, and there is zero temperature gradient (adiabatic boundaries).

$$\lambda \nabla T = 0,$$

$$p(t, L, y, z) = p_{\text{cond}},$$

$$\alpha \neq 0.$$
(14)

(2) Discharging Phase (Hydration). In this phase, the anhydrous salt undergoes gradual cooling as a result of the flow of water vapor through it. This cooling process, accompanied by the extraction of sensible heat, decreases the salt temperature until it reaches the thermochemical reaction temperature. At this point, hydration is initiated by the combination of salt with vapor, resulting in the production of salt hydrate. The energy needed for this process is contingent on the reaction rate and the enthalpy of hydration. Equation (5) is employed in this context for the chemical rate.

Mass balance and transfer. In the gas diffuser, the continuity equation accounts for vapor transport, and within the salt, there is a mass source attributed to the reaction. Consequently, the equations are formulated as follows:

$$\frac{\partial \left(\boldsymbol{\varepsilon} \boldsymbol{\rho}_{g}\right)}{\partial t} = \dot{\boldsymbol{m}} - \nabla \boldsymbol{\bullet} \left(\boldsymbol{\rho}_{g} \boldsymbol{\bullet} \boldsymbol{u}_{v}\right) + D_{g} \boldsymbol{\bullet} \Delta \boldsymbol{\rho}_{g}. \tag{15}$$

The resolution of the momentum equation in a porous medium is challenging, primarily attributable to the intricate geometry characterizing the medium. This complexity renders the determination of the local distribution of fluid velocity within the pores generally elusive. According to Fopah-Lele et al., the mass source can be written as follows [34]:

$$\dot{m} = -\chi \bullet \frac{\partial \alpha}{\partial t} \bullet \frac{M_g}{M_{s0}} \bullet \rho_{\rm eq}, \tag{16}$$

where M_g and M_{s0} are the molar mass of the vapor and the dehydrated salt, respectively, and χ is the stoichiometric coefficient of water molecules in the salt.

Mass balance and transfer. Within the reactive medium, the alteration in internal energy arises from both conductive and convective fluxes of water vapor. Consequently, the energy balance equation can be expressed as follows:

$$\left(\rho \bullet C_p\right)_{eq} \bullet \frac{\partial T}{\partial t} = \nabla \bullet \left(\lambda_{eq} \bullet \nabla T\right) - C_{pg} \bullet \rho_g \bullet \boldsymbol{u}_v \bullet \nabla T + \dot{q}, \quad (17)$$

where \dot{q} is the energy source term due to the hydration reaction and is expressed as follows: $\dot{q} = -\Delta H_r \cdot (\partial \alpha / \partial t) (\rho_{eq} / M_{s0.})$.

Boundaries and initial conditions. The reactor wall experiences cooling through a convective heat flux. Therefore, the boundary condition is as follows:

$$\boldsymbol{n} \cdot \left(-\lambda_{\text{eq}} \nabla T \right) = h(T_{\text{ext}} - T). \tag{18}$$

The upper and lower portions of the reactor are assumed to be thermally insulated.

$$\boldsymbol{n} \cdot \left(-\lambda_{\rm eq} \nabla T \right) = 0. \tag{19}$$

As for the fluid distribution is concerned,

At the reactor wall
$$: -n \cdot \nabla u = 0,$$
 (20)

Inlet :
$$-\boldsymbol{n} \cdot \nabla \boldsymbol{u} = \boldsymbol{v}_i,$$
 (21)

Outlet :
$$p = 0.$$
 (22)

For the species transport:

No flux on the reactor wall :
$$-n \cdot N = 0$$
, (23)

$$Inlet: c = c_0, \tag{24}$$

$$Outlet: -\mathbf{n} \cdot D \cdot \nabla c = 0, \qquad (25)$$

where v_i is the inlet velocity of the water vapor and c_0 represents the inlet concentration of the water vapor. For the simulation purpose, the density equation is turned into a concentration equation using the relation: $\rho_g = M \cdot c$.



FIGURE 6: Asymmetric 2D geometry of the reactor.

Assumptions:

- (i) In the considered system, the water vapor is representative of the reactive gas, and the salt hydrate is the storage material
- (ii) Electrical heater is used to supply the heat of dehydration to the salt surface by conduction and then from the surface through the salt by convection and conduction
- (iii) The salt hydrate and the reactive gas are considered pseudohomogeneous mediums with identical temperatures
- (iv) Heat transfer by radiation within the reactor is neglected
- (v) The material is initially loaded into the reactor, and the heat transfer mode is mainly conductive and convective within the reactive bed
- (vi) In this system, as soon as the material is heated, the water vapor released is modeled by Darcy's law in the laminar regime regarding the dimensional analysis of the Reynolds number
- (vii) The thermal conductivity and the heat capacity of the material are assumed constant

2.5. Physics Implementation and Simulation Parameters. Numerical modeling is the systematic approach employed to derive approximate solutions for scientific and engineering challenges. This process requires the utilization of sophisticated software tools tailored to achieve these specific objectives. For this study, COMSOL Multiphysics is used. The present work utilized the chemical reaction engineering and heat transfer modules. The chemical reaction engineering module facilitated the simulation of mass transport and chemical kinetics, whereas the heat transfer module was employed for computing heat transfer processes.

During the charging phase, a nonisothermal flow (NITF) approach, incorporating both fluid and solid heat transfer,

was employed. The study initiation involved the establishment of geometry, allocation of materials to their respective domains, and assignment of physics to corresponding domains and boundaries. Subsequently, meshing was conducted before launching the study [25, 35]. The heat source to heat the bed was estimated at 26 kW. Heat fluxes are applied to the layers between the fluid and the heat exchanger, as well as between the heat exchanger and the bed. Despite the insulation of the shell, there is convective heat transfer to the ambient environment.

For the discharging phase, two physics principles are employed and interconnected using COMSOL. These are the reacting flow diluted species (RFDS) and heat transfer in porous media (HT) modules. The RFDS node handles mass transfer through the Navier-Stokes equations, incorporating kinetic reactions. Its results include concentration, velocity vector, and pressure. On the other hand, the heat transfer in porous media node encompasses conduction and convection heat transfer modes in porous, solid, and fluid mediums. Both physics principles are coupled and resolved in a transient study over a time scale of 5 hours.

From the previous investigation [12, 36], polyaluminum sulfate can be decomposed to $Al_2(SO_4)_3$ at a temperature between 80°C and 125°C.

For the charging:

For the charging :
$$Al_2(SO_4)_3.18H_2O \stackrel{\Delta H_r}{\leftrightarrow} Al_2(SO_4)_3 + 18H_2O$$
(26)

For the discharging : $Al_2(SO_4)_3 + 18H_2O \leftrightarrow Al_2(SO_4)_3 \cdot 18H_2O + \Delta H_f^0$ (27)

From previous study on thermal decomposition of aluminum at 10K/min [37–40]:

$$\Delta H_r = 1490000 \text{ J} \cdot \text{mol}^{-1},$$

$$\Delta H_f^0 = 3440000 \text{ J} \cdot \text{mol}^{-1}.$$
 (28)

TABLE 2: Charging process parameters and thermodynamic properties of the material.

Parameter	Value	Unit	Description	
Charging (dehydratio	on)		···· I · ·	
β	10	K•min ⁻¹	K•min ⁻¹ Heating rate	
ΔH_r	1490×10^{3}	J•mol ⁻¹	Enthalpy of reaction	
A_f	$5.58 imes 10^{50}$	s^{-1}	Frequency factor	
E_a	236×10^{5}	J•mol ⁻¹	Activation energy of the reaction	
$E_{a,w}$	60.30×10^{3}	J•mol ⁻¹	Activation energy of water	
D_q	1×10^{-12}	$m^2 \bullet s^{-1}$	Gas diffusion coefficient	
R	8.314	J•mol ⁻¹ •K ⁻¹	Ideal gas constant	
k	2.89×10^{-11}	m ²	Permeability of the salt bed	
$ ho_{s1}$	1620	kg•m ³	Density of $Al_2(SO_4)_3.18H_2O$	
T_0	303.15	K	Initial temperature of the bed	
$T_{\rm iso}$	304.15	K	External wall insulation temperature	
$\mathcal{P}_{\mathrm{out}}$	38	mbar	Condensation pressure of the vapor	
λ_{s1}	0.78	$W \bullet m^{-1} \cdot K^{-1}$	Thermal conductivity of the bed	
Discharging (hydratic	on)			
m_0	3.095	kg	Initial inlet mass of material	
$C_{p_{s1}}$	240.2	$J \bullet kg^{-1} \cdot K^{-1}$	Heat capacity of $Al_2(SO_4)_3.18H_2O$	
$C_{p_{s0}}$	259	$J \bullet kg^{-1} \cdot K^{-1}$	Heat capacity of $Al_2(SO_4)_3$	
C_{p_g}	$f(T) \approx 2477$	$J \bullet kg^{-1} \cdot K^{-1}$	Heat capacity of the steam	
m_0	3.095	kg	Initial inlet mass of material	
ΔH_{f}^{0}	3440×10^{3}	J•mol ⁻¹	Enthalpy of formation of $Al_2(SO_4)_3$	
ΔS_{f}^{0}	239.200	J•mol ⁻¹ •K ⁻¹	Entropy of formation of $Al_2(SO_4)_3$	
h	3.978	$W \bullet m^{-1} \bullet K^{-1}$	Convective heat flux coefficient	
M_{s0}	0.342	kg•mol⁻¹	Molar mass of $Al_2(SO_4)_3$	
M_g	0.018	kg•mol⁻¹	Molar mass of steam	
$p_{\rm in}$	1800	Pa	Inlet water vapor pressure	
$\mathcal{P}_{\mathrm{out}}$	95	Pa	Outlet water vapor pressure	
$P_{\rm eq}$	95	Pa	Equilibrium pressure	
$T_{\rm in}$	10	°C	Inlet vapor temperature	
ε	0.8	-	The porosity of the bed	
k	0.89×10^{-10}	m ²	Permeability of the bed	
λ_{s1}	0.78	$W \bullet m^{-1} \cdot K^{-1}$	Thermal conductivity of the bed	
λ_g	0.026	$W \bullet m^{-1} \cdot K^{-1}$	Thermal conductivity of the steam	
$ ho_{s0}$	2672	kg∙m ⁻³	Density of $Al_2(SO_4)_3$	
$ ho_{s1}$	1620	kg∙m ⁻³	Density of $Al_2(SO_4)_3.18H_2O$	
$ ho_g$	$f(p, T) \approx 0.015$	kg∙m ⁻³	Density of Al ₂ (SO ₄) ₃ .18H ₂ O	
μ_{v}	$8.90 imes 10^{-4}$	Pa•s	Viscosity of the steam	
χ	18	-	Stoichiometric coefficient	

Materials	Void fraction (%)	Temperature (°C)	Power (W)	Thermal conductivity $(W \bullet m^{-1} \bullet K^{-1})$	Uncertainty on thermal conductivity (W•m ⁻¹ •K ⁻¹)
Glass beads	0.05	27	3.42	1.41	0.097
	0.05	29	3.67	0.82	0.102
	0.05	38	4.81	1.04	0.109
	0.05	40	5.07	1.07	0.073
	0.05	40	5.10	1.06	0.070
Aluminum sulfate	67	80	10.13	0.78	0.104
	53	90	11.4	0.57	0.081
	58	100	12.67	0.65	0.098
	61	125	15.83	0.75	0.108
	64	125	15.87	0.73	0.101

TABLE 3: Experimental validation data.

The parameters used for the simulations are grouped in Table 2.

2.6. Performances Evaluation. Performance analysis of thermochemical heat storage systems is based on the evaluation of thermal power and coefficient of performance of the system as well as their optimization methods. Various mathematical expressions of thermal power are reported in the literature [41–43]. The equilibrium deviation is the condition that expresses what determines the performance of thermochemical reactors.

$$\Delta T_{\rm eq} = T_{\rm HTF} - T_{\rm eq_{\rm hed}}.$$
 (29)

Indeed, both the charging $T_{\rm HTF}$ and discharging temperature $T_{\rm eq_bed}$ of the heat transfer fluid define each operation point of the system for a given pressure value. $\Delta T_{\rm eq}$ has positive values for charging, while having negative values for discharging. This is indicated by the maximum temperature required to execute the chemical reaction and for thermal energy exchange.

2.6.1. Thermal Power Analysis. The average thermal power of the solid-gas heat storage during the discharging and charging processes has been achieved as reported by [44]:

$$P_{\text{aver_dis}} = \frac{Q_{\text{out}}}{t_{\alpha}} = \frac{Q_r + Q_{s_\text{salt}} + Q_{s_\text{:met}}}{t_{\alpha}},$$
 (30)

$$P_{\text{aver_cha}} = \frac{Q_{\text{in}}}{t'_{\alpha}} = \frac{Q_r + Q_{s_\text{salt}} + Q_{s_\text{met}}}{t'_{\alpha}}, \quad (31)$$

where $Q_{\rm in}$, $Q_{\rm out}$, Q_r , Q_{s_salt} , and Q_{s_met} are the overall heat consumed while charging, the effective heat generated when discharging, the heat of reaction of the salt, the sensible heat consumption of salt, and the sensible heat consumption of the metallic part of the reactor depending on the material of manufacturing, respectively, and t_{α} and t'_{α} are the hydration and dehydration times, respectively.

$$Q_r = \alpha. \Delta H_r, \tag{32}$$

$$Q_{s_met} = \int_{T_{HTF_out}}^{T_{HTF_in}} C_{p_{met}} M_{met} dT.$$
(33)

(i) For the charging process:

$$Q_{s_salt} = \int_{T_{HTF}_out}^{T_{eq_cha}} C_{p_{s0}} m_{s0} dT + \int_{T_{eq_cha}}^{T_{HTF}_in} C_{p_{s1}} \alpha m_{s1} dT + \int_{T_{eq_cha}}^{T_{HTF}_in} C_{p_{s0}} (1 - \alpha) m_{s0} dT.$$
(34)

(ii) For the discharging process:

$$Q_{s_salt} = \int_{T_{eq}-dis}^{T_{HTF_in}} C_{p_{s1}} \alpha m_{s1} dT + \int_{T_{eq}-dis}^{T_{HTF_in}} C_{p_{s0}} (1-\alpha) m_{s0} dT + \int_{T_{HTF}-out}^{T_{eq_dis}} C_{p_{s0}} m dT.$$
(35)

In experimentation, the global value of α can be expressed as follows:

$$\alpha = \frac{\Delta m H_2 O_{\text{evap_cond}}}{m H_2 O_{\text{stoichiometric}}},$$
(36)

where $\Delta m H_2 O_{evap_cond}$ is determined by quantifying the water entering by condensation or leaving by evaporation when charging the system it is known as the amount of water absorbed or released during the reaction and $m H_2$ $O_{\text{stoichiometric}}$ is calculated through Eqs. (26) or (27) depending on the process and by using the mole conservation relation. The initial inlet mass during the charging process is given in Table 2.

2.6.2. Coefficient of Performance and System Efficiency. After evaluating the thermal power of the system, there is also a need to evaluate as well the coefficient of performance (COP) and the efficiency (η) of the system in determining whether the system is efficient or not.

$$COP = \frac{\text{useful heat production}}{\text{heat consumption}},$$
 (37)

$$\eta = \frac{P_{\text{aver_dis}}}{P_{\text{aver_cha}}}.$$
(38)

As far already mentioned, there are different ways to evaluate thermal power, and from these kinds of methods, some authors have studied algorithms to optimize the coefficient of performance as well as efficiency in recent works. On the other hand, Stitou developed a simplified technique with a simple operation wherein monitoring the input and output heat flows for heating up the reactive bed along with a mass flowmeter available [45].

$$P_{\text{stored/released}} = \dot{m}C_{p_{\text{HTF}}} (T_{\text{HTF}_{\text{in}}} - T_{\text{HTF}_{\text{out}}}).$$
(39)

According to this formula, an explicit expression of the thermal power and exergy can be used and determined by

(i) For the dehydration phase:

$$\dot{Q}_{\rm des} = \dot{m}_{\rm des_{\rm HTF}} C_{p_{\rm v}} \left(T_{\rm HTF_{\rm in}} - T_{\rm HTF_{\rm out}} \right). \tag{40}$$

Using the same method, the instantaneous thermal energy of the condenser is calculated by the following equation:

$$\dot{Q}_{\text{cond}} = \dot{m}_{\text{cond}_{\text{HTF}}} C_{p_{\text{v}}} (T_{\text{cond}_{\text{out}}} - T_{\text{cond}_{\text{in}}}).$$
(41)

The overall energy released into the bed when charging is:

$$Q_{\text{delivered}} = \int_{0}^{t_{\text{cha}}} \dot{Q}_{\text{des}} dt \dot{Q}_{\text{cond}} = \dot{m}_{\text{cond}_{\text{HTF}}} C_{p_{v}} \left(T_{\text{cond}_{\text{out}}} - T_{\text{cond}_{\text{in}}} \right).$$

$$(42)$$

(ii) For the discharging process:

The instantaneous capacity for hydrating the bed, the total recovered energy during the discharging process, and energy storage density (ESD) are:

$$\dot{Q}_{ads} = \dot{m}_{ads_{HTF}} C_{P_{-v}} (T_{ads_{in}} - T_{ads_{out}}), \qquad (43)$$

$$Q_{\text{recovered}} = \text{abs}(Q_{\text{ads}}) = \text{abs}\left(\int_{0}^{t_{\text{dis}}} \dot{Q}_{\text{ads}} dt\right),$$
 (44)

$$\text{ESD} = \frac{Q_{\text{recovered}}}{m_{\text{adsorbent}}}.$$
(45)



FIGURE 7: 3D bed temperature for the charging process at $t_i = 0$ min and $t_f = 500$ min.

After determining all these parameters, the total energy efficiency of the system is given by:

$$\eta = \frac{Q_{\text{recovered}}}{Q_{\text{delivered}}}.$$
(46)

The above equations describe the method of charging and discharging in a heat storage system, which is applied to the closed system. Since usually the tests are carried out on transient systems, it becomes very essential to perform transient uncertainty analysis for the accuracy of results. This analysis can be numerically computed using the uncertainty propagation algorithm in the Engineering Equation Solver (EES) software [46]

3. Results and Discussion

3.1. Experimental Validation. Making a reference to Section 3.3, the objective of the validation experiment was to determine the thermal conductivity of some materials known before and compare the data that would be acquired from the specific values available in documents in literature among them being aluminum sulfate. An approach to bridge this comprehension gap is to use a fluid (dry air) as well as a solid (glass), which has known thermal conductivities. The aluminum sulfate data obtained are compared to the one obtained by DSC in [12, 25, 47].

The data obtained are organized in Table 2.

The measured results obtained with the reactor are in the range of those established by the values collected from literature, besides their relative uncertainty being less than 11%, summarized in Table 3. This successful alignment goes to the validation of our measurement procedure.

3.2. Bed Temperature and Pressure Drop Analysis during Charging. Regardless of its complexity, 3D simulation offers the advantage of 3D visualization of the physical phenomena occurring within the reactor [35, 48, 49]. The 3D visualization of the temperature as well as the pressure distribution in the reactor is plotted in Figure 7.



FIGURE 8: 1D (a) bed temperature and (b) pressure drops of the reactor during the charging process (simulation).

Figure 7 shows the process of heat storage through a 3D model aiming to be close to reality. The heat transferred from the electrical heater tube helps to dehydrate the salt bed. During this phase of thermal energy storage, water vapor escapes from the bed and these vapors condense at a condenser. This particular step of condensation has not been considered in the present set-up of simulation.

To visualize the distribution within the bed, temperatures and pressure drops at various spatial points of the bed are plotted and subsequently discussed (Figures 8 and 9) for both simulation and experiment. The combined of both 3D and 1D graphics allows the appropriate analysis of the phenomenon occurring in the reactor during the charging process.

Figure 8(a) shows that the reactive bed received almost the quasi totality of the energy provided for dehydration and is fully charged at a temperature around 108° C.

At the reaction onset, before heating starts, the electrical heater is at an initial temperature, while the material in the bed remains at its initial bed temperature of about 30°C. With the continuous supply of heat, the temperature of the reactive bed steadily rises, reaching a value of approx. 100°C around 300 minutes. This temperature increase elucidates the phenomenon wherein water inside the material undergoes a phase transition into vapor, transforming from a liquid to a gaseous state. This can be further illustrated through the pressure distribution in the reactor. In Figure 8(b), the pressure drop exhibits a gradual increase, reaching its initial peak at approximately 60 mbar around t = 50 minutes. This corresponds to the phase change of water into vapor within the bed. Subsequently, a second peak is observed at around 80 mbar at t = 300 minutes, coinciding with the moment when the vapor begins to exit the bed, reaching an equilibrium state. The quasilinearity observed between t = 300 minutes and 500 minutes in both temperature and pressure curves signifies the system's equilibrium. During this phase, the bed is saturated with vapor, resulting in a pressure of around 80 mbar and a temperature of approximately 108°C.

Experimental data for the dehydration process has been plotted to confront with simulation data.

In the experimental setup (Figure 9), the test has been conducted to observe temperature variations between beds. The temperature differences at various measurement points have been graphically represented at 5 different points to provide a comprehensive overview of the temperature changes throughout the experimental process.

As depicted in Figure 9(a), the bed temperature exhibits a rapid increase, reaching its first peak value of 90°C around 100 minutes and a second peak value of 125°C around 250 minutes, followed by a linear trend until 400 minutes. Comparing the experimental data to the simulation results, both temperature profiles follow a similar trend, but the experimental values are slightly higher than those in the simulation. This discrepancy can be attributed to the simplification of heat transfer made in the simulation setup to approximate reality. Specifically, during the initial minutes of heating the bed, there is a sensible heat transfer not considered in the simulation due to simplification assumptions. This additional heat, combined with conductive heat in the bed, leads to an increased bed temperature and a rapid dehydration of the material. The pressure drops across the bed offer further insights into this phenomenon.

As depicted in Figure 9(b), the pressure values experience a rapid increase, closely mirroring the rapid increase in bed temperature, and eventually stabilize at an equilibrium value of 80 mbar around 250 minutes. This corresponds to the combined effects of the phase change of



FIGURE 9: 1D (a) bed temperature and (b) pressure drops of the reactor during the charging process (experiment).

water within the material into vapor and the subsequent release of water vapor from the bed. Following this, the pressure values commence a decrease before stabilizing around 60 mbar. This decline is attributed to the bed having received nearly all the requisite heat for material charging by around 250 minutes. Consequently, water vapor undergoes a condensation phase, leading to a reduction in pressure and subsequent stabilization, observed around 450 minutes.

To validate the simulation model, a comparison of pressure drops has been presented, and the data has been juxtaposed with findings from relevant literature.

From Figure 10, the analysis of pressure drops within a reactive bed during the charging process, a comparative examination between simulation and experimental data reveals notable trends. The simulation results closely align with the experimental observations, especially during the equilibrium stage of the process. In the literature for projects on thermochemical heat storage reactor for lowtemperature application in closed system configuration, authors found for the charging process, bed pressure drop varies between 15 mbar and 90 mbar [50-54]. This comparative analysis serves as a crucial step in affirming the accuracy and reliability of the simulation model. The alignment between the simulation results and established literature data adds a layer of credibility to the model's representation of pressure drop dynamics within the system. This validation process enhances confidence in the simulation's ability to accurately capture and reproduce key aspects of the studied phenomenon.

3.3. Bed Temperature and Pressure Drop Analysis during Discharging. In the discharging phase, characterized by hydration, water vapor is introduced into the reactive bed to recover the heat that has been previously stored.



FIGURE 10: Validation using bed pressure drop during the charging process.

Figure 11 illustrates the 3D distribution of bed temperatures throughout this discharging phase.

Figure 12 illustrates the heat release process using a 3D model designed to closely approximate real conditions. At the beginning of the reaction, the reactive bed is initially at a temperature of approx. 90°C. As water vapor enters the reactive bed, the bed temperature undergoes a progressive decrease, ultimately stabilizing around 20°C. This phenomenon is attributed to the adsorption of water vapor by the material. A more comprehensive understanding of this process can be gleaned by examining the combined 1D pressure and temperature evolution of the bed (Figure 13).

At the initial time ($t = 0 \min$), the bed temperature was approximately 90°C, and water vapor entered the bed at a



FIGURE 11: 1D (a) bed temperature and (b) pressure drops of the reactor during the discharging process (experiment).



FIGURE 12: 3D bed temperature for the charging process at $t_i = 0$ min and $t_f = 300$ min.

pressure of 18 mbar. Subsequently, the bed temperature undergoes a progressive decrease, reaching around 20°C after 100 minutes, followed by a linear trend for all measurement points until 300 minutes. However, at t = 100 min, both the bed temperature and pressure experienced a decrease, reaching minimum values of around 20°C and 5 mbar, respectively. This corresponds to the moment when the bed is actively adsorbing the water vapor. Once the bed becomes saturated with vapor, the pressure starts increasing continuously until 300 minutes, marking the phase where the bed is fully discharged.

Experimental data for the discharging process has been graphically presented to compare and validate against simulation data

As evident in Figure 11, the temperature and pressure distribution in the experimental data closely mirror the trends observed in the simulation results. The temperature exhibits a decrease, reaching approximately 20°C within the first 100 minutes, followed by a linear trend until 300 minutes. Concurrently, the pressure drop values decline from 18 mbar to 5 mbar during the first 100 minutes, after which they steadily increase throughout the rest of the discharging process. This alignment between experimental and simulation data reinforces the reliability of the simulation model in capturing the key dynamics of the discharging phase.

In Figure 14, polyaluminum sulfate appears as a powder after the dehydration reaction. At this stage, the particles exhibit small diameters and finer characteristics. Following hydration, agglomeration occurs, albeit with a low percentage of coalescence. It is noteworthy that the material still contains particles with larger diameters, possibly due to water adsorption into the material structure.

3.4. Reaction Conversion Rate. The conversion rate expresses the extent of water adsorption or desorption within a material. It quantifies the degree to which the material undergoes a transformation in its water content, reflecting the effectiveness of the adsorption or desorption process. Certain authors have demonstrated that the conversion rate is likely influenced by the heating rate during the dehydration phase and the inlet water vapor flow during hydration [55–58]. To



FIGURE 13: 1D (a) bed temperature and (b) pressure drops of the reactor during the discharging process (simulation).



FIGURE 14: Topography of polyaluminum sulfate after one cycle of reaction (a) dehydration and (b) hydration.



FIGURE 15: Influence of the heating rate on the reaction conversion during the charging.

investigate this, analyses have been conducted based on variations in the conversion rate as a function of the heating rate for the dehydration process and as a function of the inlet water vapor pressure during the hydration phase. This approach allows to assess how heating rate and water vapor flow impact the transformation of the material in terms of water adsorption or desorption.

In Figure 15, both simulation and experimental data for the reaction conversion exhibit similar trends. Higher heating rates result in a faster reaction, with the maximum conversion rate occurring around 150 minutes, while lower heating rates lead to a more prolonged reaction with a peak value of around 250 minutes. After reaching their highest points, both conversion rates follow a linear trend. This phase aligns with the complete release of water from the material, concurrently allowing heat to be stored until the completion of the reaction. Notably, the conversion rate is higher and more complete for the higher heating rate compared to the lower heating rate. This observation justifies the choice of $\beta = 10$ K/min for the simulation parameters.

For the hydration reaction, the impact of the inlet vapor pressure on the conversion rate has been examined. Two pressure values were selected, with the minimum inlet pressure set at 10 mbar, as recommended by N^TSoukpoe et al. [59].

In Figure 16, it is evident that the extent of conversion is significantly influenced by the inlet vapor pressure, showcasing higher values with increased pressure. At t = 150 min, the reaction achieves a peak conversion rate of 90% when the pressure is 18 mbar, whereas under the same conditions, only 70% conversion is observed with an inlet pressure of



FIGURE 16: Influence of the inlet vapor pressure on the reaction conversion during the discharging.



FIGURE 17: Average thermal power for both charging and discharging process of (a) simulation and (b) experiment.

10 mbar. This discrepancy is consistently reflected in both simulation and experimental data. Subsequently, from 250 minutes to 300 minutes, the conversion rate demonstrates a linear trend for both pressure values, indicating the completion of the hydration process within the reactive bed. Notably, the average pressure p_{avg} is maintained consistently for both simulation and experimental conditions throughout the investigation.

3.5. *Performance Analysis.* The assessment of thermal power in thermochemical heat storage is characterized by a range of expressions, with their applicability strongly tied to the specific process in question. Notably, many of these expressions are primarily centered around the hydration phase. Key to understanding the thermal power in thermochemical reactors is the equilibrium deviation of temperature. This seemingly plays a crucial role in determining the overall performance and efficiency of thermochemical heat storage systems.

From Eqs. (29) and (30), the average thermal power has been plotted.

According to Figure 17, the average thermal power exhibits a similar trend for both simulation and experiment. The thermal power reaches a maximum value of around



FIGURE 18: (a) Thermal efficiency function of the conversion. (b) COP function of the conversion.

900 W during the charging process and starts decreasing as the reaction progresses. Conversely, in the discharging process, a thermal power of about 300 W is observed, and this value decreases until reaching 0 as the reaction unfolds. The peaks observed at the initial stages can be explained by examining the temperature profiles within the bed, where higher temperatures are present at the beginning of the process.

As observed, the system displays low thermal power during the hydration process. This is attributed to the absence of a specific heat exchanger design aimed at capturing the heat released during the hydration of the bed.

To assess the system's performance, the thermal efficiency and the coefficient of performance have been plotted as functions of the conversion rate.

In Figure 18, a detailed examination of the system's thermal performance reveals noteworthy characteristics. As the reaction progresses and achieves a 60% conversion rate, the system attains a remarkable thermal efficiency of 90%, accompanied by an impressive coefficient of performance reaching approximately 97%. These values significantly surpass the theoretical benchmarks recommended ($\eta = 0.5$, $COP_{th} = 0.5$) [60–68]. Interestingly, as the conversion rate approaches completion, the thermal power experiences a marginal decrease of 80%, while the coefficient of performance follows a linear trend.

3.6. System Analysis and Recommendations. It will be noted that the synthesis of simulation results and experimental data has a tinge of similarity. Improvement would, however, be realized if the recommended implementation is utilized in further work.

Apparently, not all the stored energy was released well. The loss of energy is due to the recovery period of the cooling reactive bed as well as a lack of a dedicated heat exchanger to capture the heat discharge occurrences during such a process. In effect, the system performance obtained would greatly benefit from the introduction of an appropriately designed heat exchanger, which can ensure that one does not require the electrical heater tube to be switched on for heating during the charging phase. The use of the electrical heater results in increased energy consumption and thus in a more expensive system at a larger scale. Perhaps much more sustainable and inexpensive options might be provided by thermal oil circulation in a heat exchanger with industrial waste heat or solar energy as a mean source. Moreover, the improvement in thermal conductivity can improve temperature distribution across the bed, and as a result, availing good movement of heat. For instance, placing thin structures on the reactive bed can improve the temperature distribution within the bed. All these improvements could work collectively on the scheme to increase energy efficiency and also become cost-effective in the process.

Further, without insulation, the reactor wall is made of titanium alloy which has high thermal conducting properties. Heating from the surroundings towards the center of the reactor, the result would be enhanced conductivity of heat and hence better thermal property for the systems. For example, in the previous works [27, 66–74], placing a heating source around the material under treatment facilitates the concentration of heat in its vicinity. Through the synergistic effect of the thermal conductivity of the reactor wall (titanium alloy) and the thermal conductivity of the storage material, significant enhancements in the thermal performance of the reactor can be achieved.

4. Conclusion

A combined simulation and experimental investigation have been carried out to evaluate the operational dynamics of a thermal chemical heat storage (TCHS) reactor. The conclusions drawn from the study are summarized below:

 The suggested simulation model has been well validated by comparing the results to the literature and experimental results

- (2) The proposed simulation model can be used to determine the thermal conductivity of numerous heat storage materials with an experimental validation
- (3) In the charging process using the electric heater, a complete material charge is obtained with a heating temperature of 120°C after 8 h 20 min using a heating rate of 10 K/min. Under these conditions, pressure drops across the bed are stabilized to an equilibrium value of about 80 mbar corresponding to a temperature around 108°C. This represents the specified charging condition for the reactor, wherein a thermal power of 950 W can be attained
- (4) At 10°C and vapor inlet pressure of 18 mbar, during the process of discharging, complete bed discharge is achieved. The process takes 5 hours to fully discharge the material, with a maximum pressure drop reaching the condensation pressure of around 30 mbar. The discharging process reaches a thermal power of 300 W
- (5) Heating rate during discharging and inlet water vapor pressure affects the extent of conversion during the charging and discharging process, respectively. A heating rate of 10 K/min shows rapid and substantial conversion of the material affected in 150 minutes. On the other hand, an inlet vapor pressure of 18 mbar enables a discharging extent of 90% after 150 minutes
- (6) The system performance indicated a thermal efficiency of 90% and a coefficient of performance (COP) of 97%, both surpassing the recommended theoretical values
- (7) The system has successfully reached 75% of its targeted specification in terms of thermal power, signifying a substantial accomplishment in meeting the designated performance goals
- (8) Enhancing system performance is achievable through the design and implementation of a dedicated heat exchanger. This can replace the electrical heater and optimize the provision and retrieval of heat to and from the reactive bed

Nomenclature

- A: Preexponential factor (s^{-1})
- *c*: Concentration of the material $(mol \cdot m^{-3})$
- C_p : Specific heat capacity (J·kg⁻¹·K⁻¹)
- D_q : Vapor diffusion coefficient (m²·s⁻¹)
- E_a : Activation energy (J·mol⁻¹)
- *g*: Acceleration of gravity $(m \cdot s^{-2})$
- *k*: Permeability (m^2)
- *M*: Molar mass $(g \cdot mol^{-1})$
- *m*: Mass of the material (kg)
- *p*: Pression (Pa)
- *P*: Thermal power (kW)
- *R*: Ideal gas constant $(J \cdot mol^{-1} \cdot K^{-1})$
- ΔS_r : Entropy of reaction (J·mol⁻¹·K⁻¹)

- S_w : Sink or source (mol⁻¹·s⁻¹)
- t: Time (s)
- *u*: Velocity vector
- V: Atomic volume (m^3)
- *X*: Advancement of the reaction (-)
- Δh_r^0 : Reaction standard entropy (J·mol⁻¹)
- TCHS: Thermochemical heat storage
- HTF: Heat transfer fluid
- *Q*: Amount of heat consumption (kJ).

Greek Symbols

- α : Extent of conversion (%)
- ε: Total porosity of the material (-)
- η : Thermal efficiency of the system (%)
- τ : Tortuosity (-)
- μ : Dynamic viscosity (Pa·s⁻¹)
- β : Heating rate (K·min⁻¹)
- λ : Thermal conductivity (W·m⁻¹·K⁻¹)
- ρ : Volumetric density (kg·m⁻³)
- χ : Stoichiometric coefficient
- δ : Constrictivity in the porous material (-).

Subscripts

- ads: Adsorption
- avg: Average
- bed: Reactive bed
- *c*: Critical point
- ch, cha: Charging process
- cond: Condenser
- des: Desorption or dehydration process
- dis: Discharging process
- eff: Effective
- eq, eql: Equilibrium state
- evap: Evaporator
- ext: External to the salt bed
- *f*: Final condition
- *g*, *v*: Gas phase or vapor
- *i*: Initial condition
- in: Inlet condition
- *m*: Mean effective
- out: Outlet condition
- *r*: Reaction
- *s*, *s*1: Hydrate form of the material
- 0, *s*0: Anhydrous form of the salt.

Data Availability

Data supporting the results of our study can be provided after request.

Additional Points

Highlights. (i) Comprehensive investigation of TCHS reactor dynamics. (ii) Optimized charging and discharging conditions. (iii) Experimental validation of developed simulation model. (iv) Performance analysis and future enhancements. (v) Thermal conductivity measurement.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Authors' Contributions

Gbenou was responsible for the conceptualization, methodology, writing—original draft and editing, and proofreading and rewording. Kejian Wang was responsible for the outlines, visualization, and funding acquisition.

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