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Compressor-assisted thermochemical sorption integrated with solar photovoltaic-thermal collector for seasonal solar thermal energy storage

Kamon Thinsurat^a, Zhiwei Ma^b, Anthony Paul Roskilly^b, Huashan Bao^{b,*}

^a Walailak University, School of Engineering and Technology, Nakhon Si Thammarat 80161, Thailand
 ^b Durham University, Department of Engineering, Durham DH1 3LE, UK

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ABSTRACT

This paper studied the performance of a compressor-assisted thermochemical sorption energy storage (CATSES) system with a solar photovoltaic-thermal collector (PV/T) to support the domestic space and hot water heating. The heat from the PV/T drives endothermic desorption, whilst the electricity from the PV/T powers the compressor to assist the low-temperature desorption. The main aim of this study was to demonstrate that the integrated system can flexibly and maximally utilise solar energy, and store solar energy in a high energy–density system with minimum loss over long-term storage. The parametric investigation on the CATSES system using SrCl₂/NH₃ working pair was conducted for a case study in the city of Newcastle upon Tyne in the UK, which has long wintertime with high heating demand. Two different system operation modes (Case 1 and Case 2) with different strategies of solar energy usage (direct usage / storage) were studied. By using 30 m² PV/T collector with the CATSES reactor that contains 22 m³ (450 kg/m³) composite adsorbent and a compressor with 11.5 compression ratio, the system that operated Case 1 could achieve 100% solar fraction of annual heating demand. The achieved material-based energy storage density was around 0.6 GJ/m³ and the storage efficiency was 0.88 with the net electricity consumption of 180 kWh (around 5% average consumption of an ordinary UK household). The system that operated Case 2 stored less heat than that of the Case 1 but was able to output more electricity.

1. Introduction

Heat is globally the largest energy end-use, however, heating is still mainly provided by fossil fuels with only 10% from renewable, inevitably leading to a substantial CO_2 emission. International Energy Agency suggests a modest increase in the share of renewable heat is foreseen, but robust growth in total heat demand is expected due to the climatic changes, continuous economic and population growth [1] and dramatically increased building number [2]. To meet the continuously increasing demand without negative impact on energy security and environmental sustainability, it is crucially essential to boost the integration of renewable resources in the energy mix for heating. However, one of the key challenges of rolling out renewable sources is their fluctuations which leads to the difficulty of alignment of renewable energy supply and energy demand.

During the warm summer days, solar energy can produce ample thermal and electrical power that sometimes substantially exceeds the actual heat and electricity demands. However, most of the heating demand, which shares 40 \sim 50% of the final energy consumption in the UK and mostly satisfied by natural gas, is in winter time [3]. Without proper seasonally energy storage, solar energy is desperately wasted, and the so-called "wrong-time" renewable electricity causes technical challenges in balancing supply and demand across the power transmission and distribution system [4]. Therefore, one of the most promising solutions is seasonal storage of surplus renewable thermal and/or renewable/cheaper electricity and meet the peak heating demand in winter.

The photovoltaic/thermal (PV/T) collector has undergone rapid developments in recent decades [5,6]. The basic PV/T is obtained by simply attaching PV cell(s) to a solar thermal collector to simultaneously generate electricity and heat. The extracting of heat from PV cell(s) is detrimental to electrical efficiency of PV, and the heat can be used for certain end-user applications, mostly space heating or direct hot water [7]. The generation and usage of both of electricity and heat from PV/T leads to higher solar energy conversion and utilisation efficiency, compared to that achieved by using independent PV and solar thermal collectors. Such integration also reduces the costs of production and

* Corresponding author. E-mail address: huashan.bao@durham.ac.uk (H. Bao).

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ArArrhenius constant (1/s)Subscripts C_p specific heat capacity (J/(kg K))adadsorptionCRcompression ratio (-)adsadsorbentEelectrical energy (J)ambambient E_0 activation energy (J/mol)comcompression / compressorfmass fraction (kg/kg)dedesorption	Nomenclature			density (kg/m ³)		
nneat transfer coefficient (W/(m ⁻ K))heaterH, henthalpy (J/mol)heaterAHreaction enthalpy (J/mol (NH ₃))NH3Llength (m)elecMmolar weight (kg/mol)eqmmass (kg) / reaction pseudo-order (-)evammass (kg) / reaction pseudo-order (-)evammass flow rate (kg/s)metnnumber of mole (mol)outvmetsage constant (8.3144598 J/mol•K)s, saltPpressure (Pa)RRuniversal gas constant (8.3144598 J/mol•K)s, saltSFsolar fraction (-)sumUuseful energy (J)WinUAuseful energy (J)betaviousUAoverall heat transfer coefficient (W/K)betaviousVmolar volume (m ³ /mol)betaviousX, xglobal conversion (-)DHWGreek lettersEGexpanded graphite δ thickness (m)HTF λ thermal conductivity (W/(m K)) ρ prosity of the adsorbent (-) η efficiency (- /%)	ArArrhenius c C_p specific hea CR compression E electrical er E_0 activation er f mass fractic h heat transfe H, h enthalpy (J, ΔH reaction end L length (m) M molar weigl m mass flow r n number of r P pressure (Pa Q heat / therr R universal ga SF solar fractic t time (s) T temperature U useful energ UA overall heat v molar volur X, x global conv $Greek$ letters δ thickness (r λ thermal cor ε porosity of η efficiency (-	onstant (1/s) t capacity (J/(kg K)) n ratio (-) hergy (J) nergy (J) nergy (J/mol) on (kg/kg) rr coefficient (W/(m ² K)) /mol) thalpy (J/mol (NH ₃)) ht (kg/mol) reaction pseudo-order (-) ate (kg/s) nole (mol) a) nal energy (J) as constant (8.3144598 J/mol•K) on (-) e (K or °C) gy (J) t transfer coefficient (W/K) ne (m ³ /mol) ersion (-) n) nductivity (W/(m K)) the adsorbent (-) $\cdot / %$)	Subscripts ad ads amb com de f heater NH3 elec eq eva met out r <i>R</i> s, salt sum w Win <i>Abbreviat</i> CATSES DHW EG HTF PV/T SPH	adsorption adsorbent ambient compression / compressor desorption heat transfer fluid auxiliary heater ammonia electrical equilibrium evaporation metallic output from the reactor reactant reactive part, reaction reactive salt summer wall winter tons compressor-assisted thermochemical sorption energy storage domestic hot water expanded graphite heat transfer fluid Photovoltaic/thermal space heating		

installation, resulting in cheaper and more practical applications that require both electricity and heat. The sheet-and-tube flat plate collector is the most common and a highly appropriate option for domestic application of water-based PV/T due to high efficiency, easiest and most affordable configuration to manufacture. In fact, by adjusting the flow rate of the heat transfer fluid (e.g. air or water) with the outlet temperature feedback control, the quality of heat output from PV/T collectors as well as its electrical efficiency are tuneable to meet the specific requirement of the demand side, leading to expanding the spectrum of the application.

Sorption technology has been widely recognised as one of the most promising alternatives of heating technology [8]. The solid-gas thermochemical sorption process has inherent storage function, particularly has huge potential to significantly increase the utilisation of solar energy for domestic heating as it can provide a seasonal shift of demand. The storage using thermochemical sorption process has superiority over other conventional storage methods in terms of high energy density and minimum energy loss over long-term storage [9,10]. Recently, compressor-assisted thermochemical sorption cycle was proposed [11] which can realise the simultaneous storage of low-grade heat and electricity, providing the thermochemical sorption system with additional degrees of freedom, enabling flexible desorption process by balancing between heat and electric energy input. The used electrical compressor can assist the desorption at a relatively lower temperature. This feature not just enables effective use of low-grade heat output from the PV/T collector but also enhances the heat pumping performance in cold winter with additional electricity input when necessary. More interestingly, as it is well known that the solar PV/T collector has trade-off between high temperature heat and electricity, and both scenario of the trade-off perfectly matches with the energy input requirement of the compressor-assisted thermochemical sorption cycle, low temperature heat input plus more electricity input, or high temperature heat input plus less electricity input. Additionally, it also provides a better solution of using the excess electricity instead of trading it back to the grid, which may, in turn, lead to the grid instability issues due to the limited accommodation of the grid. This is a significant capability to copy with the highly variable renewable resources, ultimately substantially increasing the integration of renewable resources in the energy mix and contribute to decarbonisation of heat.

There are rare studies so far on the hybrid vapour compressionthermochemical sorption cycle, either sorption-assisted vapour compression cycle or compressor-assisted sorption cycle. Ferrucci et al. [12] studied a hybrid air-conditioning system that mainly operated the mechanical vapour compression unit for providing continuous cooling power and a standby BaCl₂/NH₃ thermochemical sorption storage unit. van der Pal et al. [13] evaluated a hybrid heat pump system consisting of a low-temperature sorbent reactor, a high-temperature sorbent reactor and a compressor. This study proves the technical feasibility of the hybrid system effectively reducing the temperature requirement of the recoverable waste heat and also increasing the upgraded heat temperature. Bao et al. [14] proposed and investigated an integrated system combining compressor and expander with thermochemical resorption processes, which enables the efficient recovery and storage of low-grade heat source from 30 °C to 100 °C and could achieve temperature lift of 10 °C to 80 °C for heat transformation depending on reactant salts used, the round-trip efficiency for electric energy storage could reach 100% and even higher when the heat source temperature was higher than 50 °C. Ma et al. [11] investigated the energy storage using SrCl₂-NH₃ working pair with electricity as supplementary energy source in two different approaches during charging process, i.e. through electric

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heater or compressor. It was concluded that the usage of compressor was more efficient to enhance the storage capacity as it effectively allowed desorption occurred at relatively lower temperature and ensured that all the heat input required (including sensible heat and desorption heat) could be met by low temperature solar heat.

The present study, for the first time, explored a compressor-assisted thermochemical sorption energy storage (CATSES) system coupling with solar photovoltaic-thermal collector (PV/T) system for seasonal solar energy storage. The proposed system was expected to be capable of (a) flexibly utilising solar energy, including solar heat and solar electricity, in a wide range of weather conditions in summer; (b) efficiently storing the energy with minimum energy loss; and (c) releasing the heat in winter time and achieving 100% solar fraction for annual domestic heating. The current paper modelled the thermochemical sorption process of which the used kinetic equations have been validated by experimental results; the solar PV/T was modelled and the models have been validated against commercial products in our previous work [15]. The system performance and storage efficiency were studied and analysed using the real weather data of Newcastle upon Tyne. The study focused on the optimal operating conditions of the solar PV/T system when coupling with the CATSES system in summer time, two different system layouts regarding the usage of produced hot water by solar PV/T for domestic hot water and/or charging the CATSES system were compared in terms of energy generation and net energy gain. Finally, the overall annual performance of the system was obtained and discussed.

2. Working principle and system operation

2.1. Solar PV/T

Fig. 1 shows the typical flat-plate PV/T design studied in this work because of its simplicity, commercial availability and high overall efficiency [16]. From the top of the device to the bottom in order, the studied PV/T system is comprised of the front cover, air gap, encapsulator, PV cell, ethylene vinyl acetate (EVA) layer, tube-type absorber and the bottom insulation. Each layer was chosen to technical- and economical- effectively maximise the recovery of solar energy and primarily aim at the product of heat.

PV cells absorbs specific range of solar spectrum, which is no higher than 23% of the overall incoming solar spectrum [17] (single layer). The rest of the incident energy is absorbed in the form of heat that mainly transfers to the absorber layer. EVA is very suitable for the glass encapsulation layer because it has high thermal conductivity and high optical transmissivity properties. There is another EVA layer between PV cells and the absorber for the purpose of protecting PV cells from moisture, electrical leakage and scratching from neighboring layers. The absorber layer is normally made of high thermal conductivity and lowdensity materials such as aluminum, with circular tubes welded and insulated at the back-layer of the PV/T. Water is normally used as the heat transfer fluid to carry thermal energy out of the collector and the flow rate should be controlled to achieve the desired output temperature.

Solar radiation passes through the front cover to the air layer before reaching the PV cells. The front cover is normally made of tempered glass due to its high strength and coated by the antireflective film such as



Fig. 1. A classic cross-sectional flat-plate PV/T with its components [15].

 SiO_2 to increase the transmittance property [18]. The air–gap layer acts as a thermal insulator to prevent the conduction heat transfer between the PV cell and the front glass cover, therefore it can in turn significantly reduce heat loss. The PV/T can achieve higher thermal efficiency and higher heat output temperature if heat output is required at a temperature higher than 50 °C, especially in cold weather regions, although electrical efficiency is slightly compromised compared to the no-air–gap PV/T [15].

2.2. Compressor-assisted thermochemical sorption energy storage

The thermochemical sorption cycle that uses $SrCl_2/NH_3$ working pair was evaluated in this work as the reversible chemical reactions between $SrCl_2$ ammines and NH_3 , the reaction is expressed in Eq. (1).

$$SrCl_2 \cdot 8NH_3 + \Delta H \leftrightarrow SrCl_2 \cdot NH_3 + 7NH_3$$
 (1)

The basic thermochemical sorption system consists of one solid adsorbent reactor and one refrigerant condenser/evaporator. In the CATSES, one compressor is installed in between the sorbent reactor and the condenser/evaporator. The introduction of a compressor enables the electrical or mechanical-driven pressurisation, consequently, enables comparatively lower temperature heat sources to be used for desorption in the energy charging process. Therefore, with the same heat source, ammines those have relatively higher desorption equilibrium temperature can be used in the CATSES cycle, which indicates that higher temperature heat output in the energy discharging process can be achieved. Such a hybrid cycle enhances heat pumping performance, as it has the collective effect of a thermochemical sorption heat pump and a conventional vapor compression heat pump.

The basic thermochemical sorption cycle and the compressorassisted cycle are plotted in the P-T diagram of Fig. 2 using the working pair SrCl₂ and NH₃. The difference between the equilibrium states and the non-equilibrium conditions shown in the figure is the main driver of the reaction, dominating the reaction rate. This thermodynamic difference is commonly termed as equilibrium drop and can be expressed either in pressure term or in temperature term [14]. The higher the equilibrium drop, the faster the reaction rate. If the equilibrium temperature drop is preset at 5 $^\circ \text{C}$ and the pressure equilibrium drop is at least 1.0 bar, the minimum desorption temperature required is 87 °C (at point A) when ambient air at 15 °C (point B) is used as the heat sink in summer. This temperature will increase to near 100 °C if the available ambient air is at 25 °C. The adsorption temperature can be achieved at 68 °C (point D) if the average ambient temperature is 5 °C in winter (point C), as the A-B-C-D loop represents the basic thermochemical sorption cycle without assistance of compressor.



Fig. 2. P-T diagram of the basic thermochemical sorption cycle (A-B-C-D) and the compressor-assist sorption cycle (E-F-B-C-D).

In the compressor-assisted cycle (E-F-B-C-D loop), if the compression ratio ($P_{\text{outlet}}/P_{\text{inlet}}$) is 4 as the curve E-F represents the electrical or mechanical-driven compression process, and the discharge temperature denoted by point F is controlled no higher than the commonly recommended level of 170 ~ 180 °C, the desorption temperature (at point E) can be effectively reduced by 30 °C to 57.5 °C compared to the basic cycle. This low temperature desorption heat can be effectively provided by solar collectors.

2.3. The integration of PV/T collector with CATSES

The CATSES-PV/T system implements energy charging in summer (Fig. 3(a)) and energy discharging in winter (Fig. 3(b) and (c)).

In summer, as illustrated in Fig. 3(a), the water heated by the solar PV/T heads to the thermochemical reactor and transfers its heat for endothermic desorption. By adjusting the water flow rate, the targeted temperature of water at the outlet of PV/T collectors can be achieved. The adsorbent in the reactor decomposes and releases ammonia vapour, whilst the electricity generated by solar PV/T drives the compressor to pressurise the ammonia vapour to be condensed in the condenser. In this case, both the solar heat and electricity are stored in the form of chemical potential of adsorption, which has minimum energy loss over long term storage.

In winter, the proposed storage system is expected to deliver 100% of the space heating and hot water without extra consumption of natural gas or electricity from the national grid. In the best scenario of making the best use of solar energy, the solar PV/T collectors still produce electricity and heat to boost the energy discharging process if there is useful solar energy available in winter, as shown in Fig. 3(b). In this case, solar heat is used for ammonia evaporation in the CATSES evaporator and simultaneously the electricity drives the compressor to further pressurize the ammonia vapor. The adsorption is then at a relatively higher pressure, leading to the release of adsorption heat at a high temperature for heating purposes. This scenario may not be applicable in the context of the high-latitude regions with weak solar radiation and limited insolation duration during the winter, then the second scenario as illustrated in Fig. 3(c) was studied in this work, as the basic thermochemical sorption heat pump performs and the compressor is bypassed.

To further increase the efficiency of solar PV/T, two cases of using solar heat produced by solar PV/T in summertime is proposed as illustrated in Fig. 4. In Case 1, as shown in Fig. 4(a), the warm water drained from the reactor is split into two streams, one stream is collected in a reservoir, which will be re-used as heat transfer fluid for the next day operation of solar PV/T; the other one stream is used as domestic hot water for daily usage. Depending on the feed-in temperature of the hot water tank, either a standby electric heater or an inline mixer performs to make sure that the water temperature is in the right range for daily use. The standby electric heater can also be powered by the electricity generated by the solar PV/T. For the second system layout (Case 2) shown in Fig. 3(b), the heated water from the solar PV/T firstly feeds into a hot water tank until it stores for 3-day autonomy in case of no solar energy available. Afterwards, the surplus hot water is used to charge the thermochemical reactor, then the exhaust water from the reactor will be collected in a reservoir and used as heat transfer fluid for the next day operation. In this instance, the daily domestic hot water use is prioritised, and the excess solar heat is stored over seasons. As the same with the Case 1, Case 2 includes a standby electric heater and the inline mixer.

It is worth noting that, in order to meet the energy input required for the desorption, the water flow rate that carries away the solar heat from PV/T collectors is adjustable. In response, the electrical output varies correspondingly as aforementioned that electrical conversion efficiency of PV cell is influenced by its temperature. Hence the PV/T collectors will have compromised electrical efficiency if the heat output is required at relatively higher temperature, vice versa. The CATSES unit can effectively harness low-temperature heat while consuming more electricity for compression process or use high-temperature heat with comparatively less electricity input for compression or even no electrical compression at all. Therefore, it is critical to study the optimal operating conditions of the PV/T collector and the CATSES unit when they integrate with each other, to maximise the solar fraction of domestic heating demands. The key question is how to tactically control the water flow rate to meet the requirement of both heat and electricity by the CATSES unit and at the same time strike the balance between heat and electricity generation from PV/T collectors.

3. Methodology

3.1. Solar PV/T collector

The development and validation of the PV/T models have been reported in detail in our previous work [15]. The PV cells studied in this work is monocrystalline silicon as used in the Siemens SM46 panel. The one-diode model was used to simulate the power output from the 36-series-PV cells which is a function of solar irradiance and cell's temperature with the modified value of series and shunt resistances of the PV panels to achieve higher accuracy at high temperature. The power output function was then interpreted into the full PV/T panel model by using the user define function (UDF) and simulated with the real weather data with 30-minute time-step in ANSYS Fluent. The model was validated with the experimental data from [19].

The used PV/T collector in this work has an area of 30 m^2 , which is the averaged available roof-top area of a domestic household in the UK [20]. Depending on the manufactured panel, the typical panel area is approximately 1.5 m^2 per panel, therefore, 20 panels were connected in parallel in terms of the heat transfer fluid loop. It was assumed that the electrical connection of these panels meets the requirement of the maximum power point controller that controls the connection voltage to obtain maximum power output.

Weather data of Newcastle upon Tyne suggests that there are only around 9 sunny days per month in the summer, and 7–10 sunny days per month in spring and autumn; for the rest of the time, there would be barely recoverable solar energy. Therefore, this work assumed that there was only 9-day-per-month availability of solar energy in three seasons (from March to October) that was converted not just for daily use during this period of time but also to be stored for winter use (from November to February).

3.2. CATSES

The typical water-jacket reactor design as shown in Fig. 5 was used in this study as it can be easily manufactured and experimental results in the previous work [21] can be used to validate the numerical modelling developed in this work. The cylindrical reactor contains the compressed composite adsorbent with an ammonia gas channel in the centre. HTF enters from the top and exists at the bottom of the reactor/heat exchanger. The solid adsorbent studied in this work was a mixture of reactive salt and porous matrixes - expanded graphite (EG), with a bulk density of 450 kg/m³ and the salt/EG mass ratio of 3:1.

For $SrCl_2$ and NH_3 reaction, the global kinetic equations Eq. (2) for the desorption process and Eq. (3) for the adsorption process, reported by Huang et al. [22] were used in this study, while all unknown constants were obtained from fitting the models with experimental data from Yuan et al.'s work [21].

$$\frac{dx}{dt} = Ar \bullet x^m \bullet exp\left(\frac{-E_0}{RT}\right) \bullet \frac{P_c - P_{eq}(T_r)}{P_c}$$
(2)

$$\frac{dx}{dt} = Ar \bullet (1-x)^m \bullet exp\left(\frac{-E_0}{RT}\right) \bullet \frac{P_c - P_{eq}(T_r)}{P_c}$$
(3)



(c)

Fig. 3. CATSES-PV/T system, (a) energy charging in the compressor-assisted mode in summer; (b) energy discharging in the compressor-assisted mode in winter; (c) energy discharging in the basic mode in winter.





(b)

Fig. 4. Two methods of using solar heat in summer. (a) Case 1: the heated water from the PV/T runs through the reactor for energy storage prior to feeding into the DHW tank; (b) Case 2: the heated water from the PV/T fills up the DHW tank then the excessive water is used for energy storage.

where x is the global conversion of the reaction, Ar and m are equation constants, R is gas constant, E_0 is the activation energy. As the global kinetic analysis was considered, the one-dimensional analysis is performed on the longitudinal cross-sectional plane of the reactor. Each layer in Fig. 5 were considered as a single mass with no temperature gradient on its mass.

Energy balance equations of HTF, wall and reactant were used as in Eq. (4), Eq. (5) and Eq. (6) respectively.

$$m_f C_{pf} \frac{\partial T_f}{\partial t} = \dot{m} C_{pf} (T_{in} - T_{out}) - (UA)_{fiv} \Delta T_{fiv}$$
(4)

$$m_w C_{pw} \frac{\partial T_w}{\partial t} = (UA)_{fw} \Delta T_{fw} - (UA)_{wr} (T_w - T_r)$$
(5)

$$m_r C_{pr} \frac{\partial T_r}{\partial t} = (UA)_{wr} (T_w - T_r) + n_{NH3-R} \Delta H_R \frac{dx}{dt}$$
(6)

where n_{NH3_R} is the total molar number of reactive ammonia, ΔH_R is the reaction enthalpy change, *UA* is the overall heat transfer coefficient. Logarithm-mean- temperature difference (ΔT_{fw}) was used to represent the average temperature difference between the HTF layer and the wall. The overall heat transfer coefficient between the HTF and the wall



Fig. 5. The physical model of the studied sorption reactor, longitudinal and cross-sectional views.

 (UA_{fw}) can be calculated by Eq. (7) and the overall heat transfer coefficient between the wall and the reactant (UA_{wr}) is obtained from Eq. (8).

$$\frac{1}{(UA)_{fw}} = \frac{1}{h_{fw}A_{fw}} + \frac{2\pi L\lambda_w}{ln\left(\frac{r_w}{r_w - \delta_w/2}\right)}$$
(7)

$$\frac{1}{(UA)_{wr}} = \frac{2\pi L\lambda_w}{ln\left(\frac{r_w - \delta_w/2}{r_r}\right)} + \frac{2\pi L\lambda_r}{ln\left(\frac{r_r}{r_r - \delta_r/2}\right)}$$
(8)

The heat transfer coefficient of HTF, h_{fw} , can be calculated by classic heat transfer correlations [23]. Because the reactant contains multisubstance, the heat capacity and the porosity of the reactant were calculated by Eq. (9) and Eq. (10) [24], respectively.

$$m_r(x)C_{pr}(x) = m_{EG}C_{p,EG} + n_s(1-x)M_{s1}C_{p,s1} + n_s xM_{s8}C_{p,s8} + \varepsilon(x)\rho_{NH3}V_rC_{p,NH3}$$
(9)

$$\varepsilon(x) = 1 - \frac{m_{EG}}{\rho_{EG}V_r} - \left[v_{s1} + (v_{s8} - v_{s1})x\right]\frac{n_s}{V_r}$$
(10)

where n_s is the molar number of used SrCl₂, M_{s1} and M_{s8} are the molar mass of SrCl₂·NH₃ and SrCl₂·8NH₃, v_{s1} and v_{s8} are the molar volume of SrCl₂·NH₃ and SrCl₂·8NH₃, V_r is the bulk volume of the reactant.

The heat input to the CATSES reactor in summer, $Q_{\rm in}$, can be calculated by Eq. (11), which represents the heat released by the HTF. This input heat is used to satisfy the sensible heat load and chemical reaction heat load.

$$Q_{in} = m_{PVT-React}c_{p,HTF}(T_{PVT} - T_{out}) = n_R \Delta x_R \Delta H_R + \int_{T_{amb_sum}}^{T_{out}} \left[m_r(x)C_{pr}(x) \right] dT$$
(11)

where T_{PVT} is the targeted HTF temperature at the outlet of the PV/T collector, i.e., the inlet HTF temperature to the CATSES reactor; T_{out} is the HTF temperature at the outlet of the reactor. $T_{amb,sum}$ is the daily averaged ambient temperature. The total mass of the HTF that delivers heat to the reactor ($m_{PVT-React}$) can be calculated according to Eq. (12) for

two different study cases in Fig. 4, where the amount of HTF (m_{HTF}) produced by the PV/T collector varied because the HTF flow rate was adjusted in order to achieve the targeted T_{PVT} under the varying weather condition; the $m_{PVT-DHW}$ is the total quantity of the HTF that directly fills up the hot water tank.

$$Case 1: m_{PVT-React} = m_{HTF}$$
(12a)

$$\text{Case } 2: m_{PVT-React} = m_{HTF} - m_{PVT-DHW}$$
(12b)

The electrical energy demand for the compressor (E_{comp}) is calculated by Eq. (13) as the enthalpy change of the ammonia gas from the inlet to the outlet of the compressor. The ammonia real gas properties are used for calculation.

$$E_{comp} = m_{NH3}(h_{outlet} - h_{inlet})$$
(13)

The useful heat output (Q_{useful}) of the CATSES reactor in winter is calculated by Eq. (14). The storage efficiency ($\eta_{storage}$) is calculated by Eq. (15).

$$Q_{useful} = n_R \Delta x_R \Delta H_R - \int_{T_{amb_win}}^{T_{release}} \left[m_r(x) C_{pr}(x) \right] dT$$
(14)

$$\eta_{storage} = \frac{Q_{useful}}{Q_{in}} \tag{15}$$

3.3. Domestic heating demands

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The monthly data of domestic hot water consumption (m_{DHW}) in a typical UK household, the monthly average temperature of the cold water supplies (T_{cold}) from the utility and ambient air was reported in the work [20], as presented in.

Table 1. The volume of the hot water tank is designed around 400 L to not only meet the daily use but also have extra capacity for a couple of days autonomy. The heating demand for the DHW can be obtained as Eq. (16), which also includes the electrical input (E_{heater}) if needed. If T_{out} in Eq. 16(a) or T_{PVT} in Eq. 16(b) is already higher than the required T_{DHW} (set at 60 °C), it can be mixed with cold water and the required amount of cold water is calculated by Eq. (17). In winter, the storage system releases adsorption heat which is expected to fully cover the DHW heating without additional electrical input, the needed heat is calculated by Eq. (18).

Case 1:
$$Q_{DHW-sum} = m_{PVT-DHW}c_{p,HTF}(T_{DHW} - T_{out}) + E_{heater}$$
 (16a)

Case 2 :
$$Q_{DHW-sum} = m_{DHW}c_{p,HTF}(T_{DHW} - T_{PVT}) + E_{heater}$$
 (16b)

$$m_{w-cold} = m_{PVT-DHW} \frac{T_{PVT} - T_{DHW}}{T_{DHW} - T_{w-cold}}$$
(17)

$$Q_{DHW-win} = m_{DHW}c_{p,HTF}(T_{DHW} - T_{w-cold})$$
⁽¹⁸⁾

The space heating demand (Q_{SPH}) depends mostly on the overall heat loss coefficient (\overline{UA}) of the household, the ambient temperature and the required indoor temperature, and it can be calculated from Eq. (19).

$$Q_{SPH} = \overline{UA}(T_{room} - T_{amb})t = \dot{m}_{SPH}c_{p,HTF}(T_{RST} - T_{RRT})t$$
(19)

where \overline{UA} varies depending on floor area, insulation and external wind speed and the value ranges between 50 and 300 W/K for the typical UK households [20]. The room temperature (T_{room}) is normally set to approximately 21 °C for most of existing household heating [20]. In this study, the storage is designed to supply at least 60 °C hot water (T_{RST}) to the radiator and the return temperature (T_{RRT}) is considered to be 40 °C. \dot{m}_{SPH} is the mass flow rate of the HTF. The heating time (t) was averagely 10 h per day in winter.

Table 1

Monthly averaged domestic hot water usage and the cold water temperatures in a typical household in the UK [20].

Month	JAN	FEB	MAR	APR	MAY	JUN	JUL	AUG	SEP	OCT	NOV	DEC
T _{w-cold} (°C)	9.62	9.32	10.70	13.70	15.32	17.26	19.3	18.67	17.88	15.55	12.22	10.51
DHW (L/day)	116.9	124.6	125.7	114.7	122.9	116.5	98.4	105.5	112.6	123.6	127.8	133.2
T _{amb} (°C)	3.0	3.1	5.1	7.1	9.9	13.0	14.5	14.4	12.6	9.6	6.0	3.8

3.4. System overall performance

To determine the optimal operating conditions of the solar PV/T collector, the net useful energy gain, U_{neb} is defined as the sum of the heat input to the CATSES unit and the surplus electrical output of the PV/T collector as in the following Eq. (20).

$$U_{net} = Q_{in} + E_{PVT-elec} - E_{comp} - E_{heater}$$
⁽²⁰⁾

where $E_{PVT-elec}$ is the electrical product of PV/T collectors, E_{comp} and E_{heater} are the electricity consumptions of the compressor and the standby electric heater, respectively.

The solar fraction (*SF*) of domestic heating in winter can be calculated from Eq. (21).

$$SF = \frac{Q_{useful}}{Q_{DHW-win} + Q_{SPH}}$$
(21)

4. Results and discussion

4.1. Kinetic models of SrCl₂(8/1)NH₃

As aforementioned, the kinetic equations were obtained by fitting equations, Eq.(2) and Eq. (3), to experimental results, the obtained equation constants are listed in Table 2.

The fitted and experimental results of adsorption and desorption kinetics of $SrCl_2(8/1)NH_3$ were compared in Fig. 6. During the first half hour of the adsorption reaction time, as shown in Fig. 6(a), the deviation is about 10% to 17% which is considerably large, as the global conversion of the simulation indicates the faster reaction rate than the experiment. The main reason is likely to be the rather big thermal resistance at the contact between the adsorbent bulk and the wall of metallic reactor of the experimental test rig, leading to relatively slower heat transfer that negatively affects the reaction rate. After the first half hour, the simulation results fit well with the experimental results with the global conversion rorrelation produces a considerably good match with the experimental results with the parameters shown in Fig. 6(b), the percent deviation is less than 10%.

4.2. Energy generation and storage

Fig. 7 displays the profiles of the electrical and thermal productions from the PV/T collector and energy consumption by other system components, as the HTF temperature (T_{PVT}) varies from 40 °C to 100 °C, when heat sink temperature (i.e., condensation temperature) is at 15 °C and compressor has a compression ratio (*CR*) of 8 as an example. There are three energy output curves, Q_{in} represents the heat that is used for desorption of thermochemical reaction, $E_{PVT-elec}$ is the total electrical output from the PV/T collector, and the U_{net} is the net useful solar energy. There are two energy consumption curves, E_{comp} is for the compressor, and the other one E_{heater} is for the standby electric heater.

Table 2	
Values of constants of kinetic equations.	

	E() (0/ 1101)
9 3.06	1421
2	9 3.06 5 1.52

The intersection point of the Q_{in} curve and the horizontal axis indicates the threshold of desorption temperature of the CATSES cycle, which is 42 °C (i.e., $T_{eq} + \Delta T_{drop}$ in non-equilibrium conditions and equilibrium drop was pre-set as 5 °C) with the assistance of the compressor, reduced by 45 °C compared to that of the basic cycle at 87 °C without vapor compression. Under the same weather condition, the $E_{PVT-elec}$ is only related to the PV/T temperature, represented by the HTF temperature (T_{PVT}), therefore, Fig. 7(a) and (b) have the same $E_{PVT-elec}$ curve.

For the layout of Case 1 shown in Fig. 4(a), the entire HTF carrying thermal outputs from the PV/T collector heats the reactor for desorption prior to being collected in the hot water tank for daily use. When it comes out from the reactor and arrives in the hot water tank, its temperature never reaches the desired level (60 °C) under the conditions that the *CR* is higher than 3. In this instance, the standby electric heater must work which consumes part of the electricity generated by the PV/T collector to lift the water temperature up, and the energy consumption is as depicted by the orange curve (*E*_{heater}) in Fig. 7. In the Case 2, the daily DHW directly comes from the PV/T collector. Once the outlet HTF temperature is controlled higher than *T*_{DHW} (60 °C) there is no need to turn the standby heater on.

 Q_{in} are determined the HTF temperature at the outlet of the PV/T (T_{PVT}) , the HTF temperature at the outlet of the reactor (T_{out}) , and the $m_{PVT-React}$ (total mass of the HTF delivering heat to the reactor). With a given compression ratio and a given heat sink temperature, the higher the T_{PVT} , the more the thermal input (Q_{in}) , leading to more energy being stored in the form of chemical potential. The E_{comp} curves have their negative peaks when the Q_{in} curves have their positive peaks, as the more the heat is stored by thermochemical reaction, the more compression work is required to assist the desorption and condensation process. Together with larger electricity consumption on the electric heater (E_{heater}), there is no prominent superior of Case 1 over the Case 2 in terms of net energy gain (U_{net}).

However, in the meantime, the higher T_{PVT} not just decreases the electricity efficiency but also abates the thermal efficiency of the PV/T collector with higher energy losses from the collector to the ambient, namely, if T_{PVT} is set too high the $m_{PVT-React}$ reduces considerably. In other words, increasing T_{PVT} generates two conflicting effects on the value of Q_{in} , when the drastic reduction of the $m_{PVT-React}$ outweighs the positive effect of increasing T_{PVT} on the Q_{in} , it results in the decreasing of the Q_{in} curves when T_{PVT} is beyond a certain high point as presented in Fig. 8(a) and (b). Moreover, it indicates there exists an optimal T_{PVT} for the maximum Q_{in}, which is 90.10 °C and 91.51 °C for Case 1 and Case 2, respectively with the CR of 8. However, under the same weather condition, for the maximum U_{net} , there should be another optimal point of T_{PVT} as presented in Fig. 8(c) and (d). For example, with CR = 8, the optimum T_{PVT} are 88.68 °C and 87.27 °C with the maximum U_{net} of 243.06 MJ and 235.09 MJ per 30 m^2 PV/T installation per day in Case 1 and Case 2, respectively, on a typical summer sunny day. The optimal T_{PVT} for the maximum Q_{in} is always required to be higher than the optimal T_{PVT} for the maximum U_{net} , and the temperature difference between these two optimal HTF temperatures get bigger when CR increases.

Fig. 9 presents more comparison between the two cases when the used compression ratios are 4, 8, and 16, respectively. The cumulative summation clearly display the relationship between the energy output and energy consumption, as the light/dark grey zone denotes energy consumption by compressor/electric heater ($E_{comp} + E_{heater}$) and pink-coloured zones represent heat input Q_{in} to the CATSES unit and the



Fig. 6. The comparison between the simulation results in this study and experimental results, (a) adsorption at 20 °C with 0 °C ammonia evaporation; (b) desorption at 110 °C with 20 °C ammonia condensation.



Fig. 7. The energy variation profiles with different HTF temperatures on a sunny summer day when using $SrCl_2/NH_3$ working pair and the compression ratio of 8, (a) Case 1; (b) Case 2.

magenta-coloured area means surplus electricity ($E_{PVT-elec} - E_{comp} - E_{heater}$) that can be used for other appliances, the only one blue strip in Fig. 9(a) suggests the deficit of electricity, meaning the electrical

generation by the solar PV/T collector cannot 100% satisfy the total electricity consumption within the proposed system. The Case 1 can store considerably more thermal energy than the Case 2, suggesting a larger flow of the desorbed ammonia and more electricity consumption by the ammonia compression process. Moreover, the Case 1 always consumes part of the electricity for the standby heater in the hot water tank, whereas the Case 2 only uses the standby heater when the T_{PVT} is lower than 60 °C. If the primary goal is to increase the solar fraction of the domestic space heating, it is noticeable in Fig. 9 that the Case 1 has prominent superiority to the Case 2; nevertheless, the Case 2 surpasses its viral in terms of net electricity generation.

By using higher compression ratio (CR), more thermal energy can be effectively recovered and stored regardless of the operation modes, because it enables the utilisation of the relatively lower temperature heat for endothermic desorption. When the CR is at 4, the optimal HTF temperature is above 90 °C in both cases, and it can be reduced by more than 30 °C if increasing the CR value to 16 when the maximum Q_{in} is needed. Moreover, lower HTF temperature is also favourable in the electrical efficiency and the longevity of the PV/T collector. However, the electricity deficit can occur when the CR is too high (e.g., in Fig. 9 (a)) and the proposed system has to import electricity from the grid to fulfil the energy charging process. Nevertheless it is still a cost-effective and low carbon solution to utilise and seasonally store the grid electricity whilst enabling relatively lower temperature thermal energy storage. Because it shifts the electricity demand over seasons, using cheap electricity generated in the summer with larger share of renewable energy sources rather than the more expensive and high-carbon electricity/gas at the peak hours for domestic heating in winter.

The maximum potential of the net energy gain using different CR values from 1 to 16 is summarised in Fig. 10(a) on a sunny summer day and the corresponding Q_{in} is shown in Fig. 10(b). Again, the Case 1 stores more thermal energy than the Case 2, the storage capacity gap between these two cases expands with the increasing CR values. For the net energy gain, two curves shown in the figure cross over each other at the point of CR = 11.5. The Case 1 can yield more net useful energy than the Case 2 if the CR value is lower than 11.5 and the maximum gap exists when CR = 3-4 as the gap gradually narrows down with the increasing *CR* value; over the point of CR = 11.5, it becomes opposite as the Case 2 marginally beats the Case 1. The operating condition with higher CR enables desorption to occur at a lower temperature, leading to the lower HTF temperature at the outlet of the reactor in the Case 1. In this instance, not just the compressor that consumes more electrical power due to the higher compression ratio but also the electric heater is activated and consumes more electricity for lifting the water temperature to the required level of daily use. For example, for Case 1 with the CR value at 16, the optimum T_{PVT} is around 60 °C when two electricity consumptions combined exactly offsets the electrical generated from the PV/T collector, and the net energy gain is merely represented by the



Fig. 8. The optimum T_{PVT} (a) Case 1 and (b) Case 2 for the maximum reactor heat input; (c) Case 1 and (d) Case 2 for the maximum net energy gain.

amount of thermal energy delivered to the CATSES unit. However, for Case 2, when the T_{PVT} is at 60 °C, there is still considerable amount of net electricity output, plus the Q_{in} to represent the total net energy gain.

4.2. Overall annual performance

This section focuses on Case 1 to explore the overall system performance. The energy storage efficiency, energy storage density and the potential annual performance of the integrated system has been investigated to determine the required scale of system installation in order to achieve 100% solar fraction of domestic heating for a typical single household in Newcastle upon Tyne. The size of each main component, i. e. solar PV/T panel and thermochemical sorption unit, as well as the compressor specifications was also discussed, as summarised in Table 3. The energy storage density presented in this work was based on the thermochemical material volume, as the adsorbent composite density of 450 kg/m³ and the salt/EG mass ratio of 3:1. Therefore, in order to meet the heating demand in winter with solely solar energy sources (SF =100%) collected by a 30 m² solar PV/T panel in summer, the hybrid thermochemical system potentially requires about 22 m³ SrCl₂(8/1) adsorbent composite and a compressor that has the compressor ratio at least of 11.35. in this case, the integrated system could also have net electricity yield of 180.50 kWh annually.

In another study scenario to explore the threshold of the required area of solar PV/T panel to meet the goal of 100% solar fraction, the performances with the installation area of 23 m², 26 m² and 30 m² are shown and compared in Fig. 11. If the PV/T is installed with the area of 26 m², the SrCl₂(8/1) systems are able to accomplish 100% solar fraction with the CR of 15.9. Because of the reduction of the PV/T panel

area, it produces less thermal energy and less electricity, in the meantime, the standby electric heater has to work and more electricity is consumed to satisfy the DHW use. This leads to the negative value of the electricity output curves in magenta colour in the figure, in other words, the grid electricity is needed to provide DHW heating in summer and simultaneously complete the energy charging process.

If with the fixed *CR* at 16 and no constraint of using the grid electricity, the minimum required PV/T installation area to acquire 100% solar fraction is 25.8 m². For further investigation, it can be an interesting subject to study whether a bigger installation if the roof area allows, or importing more electricity from the grid has a shorter payback time for the overall system.

5. Conclusion

The compressor-assisted thermochemical sorption energy storage (CATSES) unit with the hybrid solar PV/T system was proposed and investigated in this work for the first time. Thermal and electrical energy produced by solar PV/T can be simultaneously stored in the CATSES system over seasons and recovered in winter in the form of heat for domestic space heating and hot water heating. In order to achieve 100% solar fraction of domestic heating demand of a typical household in Newcastle upon Tyne as a case study, the optimal operating condition of the solar PV/T system (in terms of the HTF temperature at the outlet of the PV/T panel) in summer was identified when it is coupled with the CATSES system using SrCl₂(8/1)NH₃ as the ammine adsorbent in two different system layouts. The Case 1 prioritises the storage of thermal energy than the Case 2, but at the same time, it consumes more electricity for the compressor and the standby electrical heater for daily hot







Fig. 9. The energy variation profiles vs different HTF temperatures on a sunny summer day when using SrCl₂/NH₃ working pair and the compression ratio of 4, 8 and 16 in two different operation modes.

water use. The Case 1 has more net energy gain than the Case 2 when the compression ratio is lower than 11.5, but it is the other way around when the CR used is higher than 11.5. Operating the system at higher compression ratio enables the utilization of lower temperature heat generated by the PV/T collector, leading to a positive effect on the life cycle of PV-cells.

(c)

With 30 m² PV/T installation, the CATSES unit requires nearly 22 m³ SrCl₂ composite adsorbent to achieve 100% solar fraction for domestic heating in winter with a storage efficiency of about 88%. If the compressor is able to work at compression ratio of 16, the PV/T panel area can be reduced to 25.8 m² to achieve 100% solar fraction, nevertheless, the grid electricity would be required in the energy charging

stage since less electricity output from the PV/T collector and potentially more electricity demand by the standby electric heater in the hot water tank.

(d)

In the future work, more efforts should be put on the investigation on the performance of other potential ammine adsorbents, the optimal controlling strategies based on the dynamic heating demand, and the cost-effectiveness of different options of system operation optimization.

CRediT authorship contribution statement

Kamon Thinsurat: Writing – original draft, Methodology, Data curation, Software, Investigation. Zhiwei Ma: Validation, Writing –



Fig. 10. (a) CR vs U_{net} and (b) CR vs Q_{in} diagram on a sunny summer day.

Table 3 Preliminary performance for PV/T-DHW-TCSS for 100% solar fraction of domestic heating demands.

	$\eta_{ m storage}^*$	Minimum CR	Energy Density (kWh/ m ³)	V _{ads} (m ³)	$\begin{array}{l} \text{Minimum } A_{PV/T} \text{ for } SF = 1 \text{ and } CR = \\ 16 \\ (m^2) \end{array}$	E _{left} (kWh)	Estimate price of reactive salt (\$/ton)**
SrCl ₂ (8/1) NH ₃	0.8761	11.35	171.65	21.91	25.80	180.50	672–842

*The values presented in this column were calculated from CR = 8.

*The prices are based on the wholesale price per metric ton from https://www.alibaba.com.



Fig. 11. Solar fraction and the net electrical output with different installation areas of the PV/T panels.

review & editing. **Anthony Paul Roskilly:** Supervision. **Huashan Bao:** Conceptualization, Methodology, Writing – review & editing, Visualization, Project administration.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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