Universitat de Lleida

Performance analysis and control optimization of a solar-driven seasonal sorption thermal energy storage system

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TESI DOCTORAL

Performance analysis and control optimization of a solar-driven seasonal sorption thermal energy storage system

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Memòria presentada per optar al grau de Doctor per la Universitat de Lleida

Programa de Doctorat: Enginyeria i Tecnologies de la Informació

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Departament d'Informàtica i Enginyeria Industrial
Escola Politècnica Superior
Universitat de Lleida

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El Dr. Cèsar Fernández, Catedràtic de l'Escola Politècnica Superior de la Universitat de Lleida, el Dr. Álvaro de Gracia, professor agregat de l'Escola Politècnica Superior de la Universitat de Lleida,

CERTIFIQUEN:

Que la memòria *Performance analysis and control optimization of a solar-driven seasonal sorption system* presentada per Alicia Crespo Gutiérrez optar al grau de Doctor s'ha realitzat sota la seva supervisió.

Lleida, Setembre 2022

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Dedication

To my parents and my sister.

Summary

Heat is the world´s largest energy end-use. In particular, the building sector is responsible of around 40 % for the consumed heat. Renewable sources are a good solution to mitigate climate change. Nevertheless, the intermittence of renewable sources calls for the need of energy storage systems. Solar thermal collectors coupled with seasonal thermal energy storage (STES) are a good solution to reduce the fossil fuels consumption in climates with high solar irradiation in summer and high space heating demand in winter. Sorption thermal energy storage (TES) is the more suitable technology for STES due to its nearly zero thermal losses during the storage period and its high energy density at material level. Nevertheless, the operation of a sorption STES integrated into a building heating system is not straightforward and must be studied in detail. A non-optimal operation of the system based on transient weather conditions and thermal building demands may lead to low system efficiency. This PhD thesis aims to analyse and enhance the performance of a solar-driven seasonal sorption TES (SDSSTES) system integrated into a building through different control strategies and system designs. The system was composed of solar collectors, a stratified water tank, a boiler, a sorption STES, and its low-temperature heat source (LTHS). Operating the system with an optimized rule based control (RBC) strategy allowed to minimize the operational costs using a lower volume of sorption TES. Moreover, the energy density of the sorption TES was highly impacted by the weather conditions, and by the type and availability of LTHS. The results proved the technical feasibility of the SDSSTES in Central and North Europe. In spite of the low temperatures in winter, the use of winter solar heat was enough to assist the discharge of the sorption TES. However, energy densities increased by 23 % assuming a constant heat source (e.g. geothermal energy). Better results in terms of operational costs were obtained by operating the system with deep reinforcement learning (DRL), in comparison to the optimized RBC strategy. Indeed, the use of DRL allowed operating the system during winter in a near-global optimum. Nevertheless, the implementation of a DRL algorithm require high programming skills and long computational training times.

Resumen

El calor es el tipo de energía final más consumida del mundo. En particular, el sector de la edificación es responsable de alrededor del 40 % del calor consumido. Las energías renovables son una buena solución para mitigar el cambio climático, sin embargo, la discontinuidad de las energías renovable requiere de sistemas de almacenamiento de energía. Los colectores solares térmicos acoplados a almacenamiento de energía térmica estacional (STES) son una buena solución para reducir el consumo de combustibles fósiles en climas con alta irradiación solar en verano y alta demanda de calefacción en invierno. El almacenamiento de energía térmica (TES) por sorción es la tecnología más adecuada para STES debido a sus pérdidas térmicas casi nulas durante el período de almacenamiento y su alta densidad energética a nivel de material. Sin embargo, el funcionamiento de un STES por sorción integrado en una instalación de calefacción de un edificio no es sencillo y debe estudiarse en detalle. Un funcionamiento no óptimo del sistema en función de las condiciones climáticas y las demandas térmicas del edificio puede conducir a una baja eficiencia del sistema. Esta tesis doctoral tiene como objetivo analizar y mejorar el funcionamiento de un sistema de almacenamiento por sorción estacional impulsado por energía solar (SDSSTES) integrado a un edificio mediante diferentes estrategias de control y diseños de sistemas. El sistema estaba compuesto por colectores solares, un depósito de agua estratificada, una caldera, un sistema STES por sorción y su fuente de calor de baja temperatura (LTHS). Operar el sistema con una estrategia RBC optimizada permitió minimizar los costes de operación usando un menor volumen de almacenamiento por sorción. Además, la densidad energética del SDSSTES se vio muy afectada por las condiciones climáticas y por el tipo y la disponibilidad de LTHS. Los resultados demostraron la viabilidad técnica del sistema en el centro y norte de Europa. A pesar de las bajas temperaturas en invierno, el uso del calor solar durante el invierno fue suficiente para descargar el sistema STES. Sin embargo, se obtuvieron densidades energéticas 23 % mayores suponiendo una fuente de calor constante (p.ej., energía geotérmica). Además, se consiguieron menores costes operacionales controlando el sistema con deep reinforcement learning (DRL), en lugar de con una estrategia RBC optimizada. El uso de DRL permitió operar el sistema durante el invierno cerca del óptimo global. Sin embargo, el desarrollo e implementación de un algoritmo de DRL requiere altas habilidades de programación y largos tiempos de entrenamiento computacional.

Resum

La calor és el tipus denergia final més consumida del món. En particular, el sector de l'edificació és responsable del voltant del 40% de la calor consumida. Les energies renovables són una bona solució per mitigar el canvi climàtic. Tot i això, la discontinuïtat de les energies renovable requereix emmagatzematge d'energia. Els col·lectors solars tèrmics acoblats a l'emmagatzematge d'energia tèrmica estacional (STES) són una bona solució per reduir el consum de combustibles fòssils en climes amb alta irradiació solar a l'estiu i una alta demanda de calefacció a l'hivern. L'emmagatzematge de calor (TES) per sorció és la tecnologia més adequada per a STES a causa de les pèrdues tèrmiques gairebé nul·les durant el període d'emmagatzematge i la seva alta densitat energètica a nivell de material. Tot i això, el funcionament d'un TES estacional per sorció integrat en una instal·lació de calefacció d'un edifici no és senzill i s'ha d'estudiar detalladament. Un funcionament no òptim del sistema segons les condicions climàtiques i les demandes tèrmiques de ledifici pot conduir a una baixa eficiència del sistema. Aquesta tesi doctoral té com a objectiu analitzar i millorar el funcionament d‟‟un sistema d‟‟emmagatzematge per sorció estacional impulsat per energia solar (SDSSTES) integrat en un edifici mitjançant diferents estratègies de control i dissenys de sistemes. El sistema estava compost per col·lectors solars, un dipòsit d'aigua estratificada, una caldera, un SoTES estacional i la font de calor de baixa temperatura (LTHS). Operar el sistema amb una estratègia RBC optimitzada va permetre minimitzar els costos d'operació usant un menor volum d'emmagatzematge de sorció. A més, la densitat energètica del SDSSTES es va veure molt afectada per les condicions climàtiques i pel tipus i disponibilitat de LTHS. Els resultats van demostrar la viabilitat tècnica del sistema al centre i al nord d'Europa, malgrat les baixes temperatures a l'hivern, l'ús de la calor solar hivernal va ser suficient per descarregar el STES. No obstant això, es van obtenir densitats energètiques 23% més grans suposant una font de calor constant (p.ex., energia geotèrmica). A més, es van aconseguir menors costos operacionals en controlar el sistema amb deep reinforcement learning (DRL), en comparació de l'estratègia RBC optimitzada. L'ús de DRL va permetre operar el sistema durant l'hivern prop de l'òptim global. No obstant això, el desenvolupament i la implementació d'un algorisme de DRL requereix altes habilitats de programació i llargs temps d'entrenament computacional.

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Abbreviations

COP	Coefficient of performance	NZEB	Near zero emissions building
CSPM	Composite salt porous matrix	PCM	Phase change material
DHW	Domestic hot water	PV	Photovoltaic
DRL	Deep reinforcement learning	PVT	Photovoltaic-thermal
GHG	Global greenhouse gases	RBC	Rule based control
GTL	Gross temperature lift	RL	Reinforce learning
HTF	Heat transfer fluid	SH	Space heating
IAM	Incidence angle modifier	STES	Seasonal thermal energy storage
IEA	International energy agency	SWS	Selective water sorbent
IPCC	International panel climate change	SDSSTES	Solar-driven seasonal sorption TES
KPI	Key performance indicator	TE	Temperature effectiveness
LTHS	Low temperature heat source	TES	Thermal energy storage
MAPE	Mean average percentage error	UK	United Kingdom
MPC	Model predictive control	ZEB	Zero emissions building

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Chapter I

1 Introduction and PhD objectives

1.1 Introduction

1.1.1 Statement of the problem and motivation

The industrial revolution entailed an improvement in human life quality. Nevertheless, that industrial development promoted an energy dependency of the current society, which led to air pollution, soil contamination, and global warming. Indeed, human activities have caused around 1.0 ºC of global warming above pre-industrial levels [1] as depicted in Figure 1. According to the International Panel on Climate Change (IPCC) [2], at the present warming rate, global temperatures would reach 1.5 ºC above pre-industrial temperature levels in 2040.

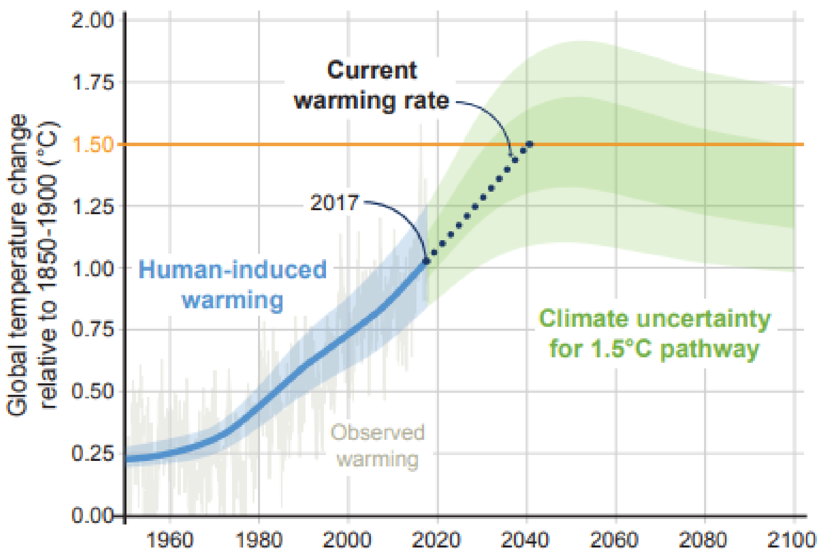

Figure 1: Global temperature change relative to 1850-1900 [2]

The main cause of this change in climate conditions is the emissions of greenhouse gases, which blanket the Earth, causing an increase in the global temperature. According to the IPCC, global greenhouse emissions (GHG) [3] have grown since pre-industrial times by 70% between 1970 and 2004. The energy sector is responsible for almost three quarters of the global emissions, therefore it has to be at the heart of the solution to climate change [4]. In addition, it is estimated that the world population will continue to rise, reaching 10.4 billion by 2100 [5]. This population growth will cause an increase of the global energy demand [3], especially in developing countries. An estimation of the energy demand increased for the period 1980-2030 is shown in Figure 2.

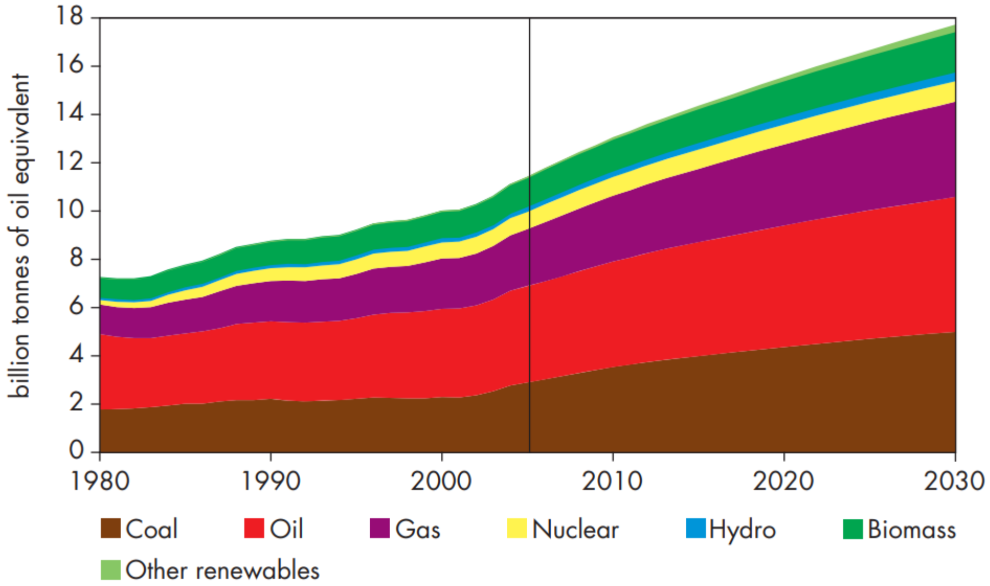

Figure 2: Energy consumption trend [6]

Due to the extreme situation in which we find ourselves several countries pledged to the Paris agreement in 2015 [7]. There, the participant countries agreed among other actions to reduce global emissions as soon as possible to decelerate the global warming rate and reach a maximum temperature of 1.5 ºC above pre-industrial levels. In addition, the International Energy Agency (IEA) has set a challenging goal to tackle the problem by moving on to a Zero Emissions Buildings (ZEB) Scenario by 2050 [4], aiming to decrease the CO_2 emissions by 40% by 2050. The governments and international organizations must approve a road map defining the actions to alleviate the effects of high energy consumption. Renewable energy sources have been identified as the backbone of any energy transition to achieve net zero emissions [8]. Indeed, the growth of renewable energies capacity is forecasted to accelerate in the next five years, accounting for almost 95 % of the increase in global power capacity through 2026 [8].

According to the IEA [8], heat is the world's largest energy end-use. In particular, the building sector is responsible for almost half (46 %) of the energy consumed for heat, which is mainly consumed for space and water heating. Regardless of the various clean and commercial technologies to generate heat for a building, fossil fuels remain as the main heat source, as depicted in Figure 3.

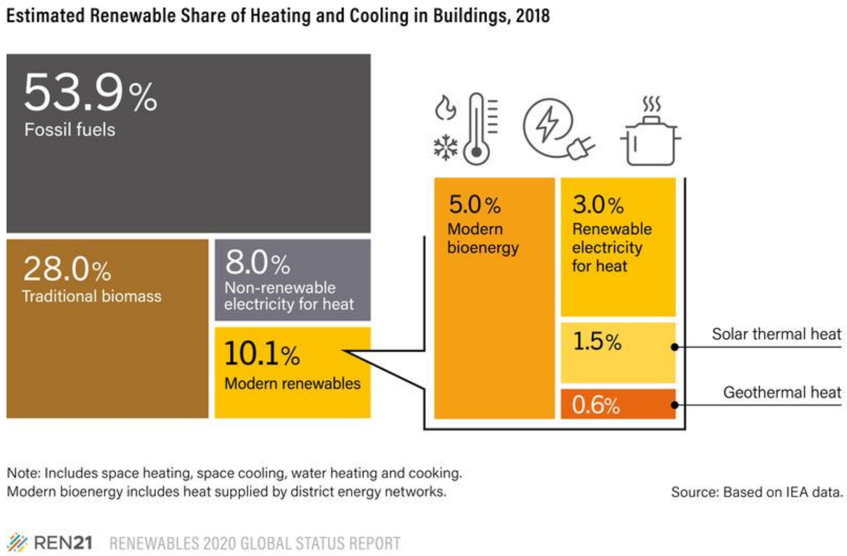

Figure 3: Estimated renewable share of heating and cooling in buildings [9]

Bearing in mind the energy crisis caused by the war in Ukraine, the reduction of fossil fuels consumption is a need not only for environmental reasons, but also from a socio-economic perspective. High gas prices are economically suffocating families both during the winter, mainly in northern Europe, and during the summer, mainly in Southern and Central Europe. A gas-independent and environmentally friendly heat source is necessary. Indeed, the use of renewable heat in buildings is projected to grow by almost 35% [3].

Solar thermal collectors are a mature technology that can greatly contribute to moving on to a decarbonized buildings energy matrix. Nevertheless, as was shown in Figure 3, just 1.5 % of the total heat demand of a building was supplied by solar thermal energy. One of the main drawbacks to profit solar thermal systems is the time mismatch between solar availability and space heating demand. Especially in regions such as Central and Northern Europe, where high solar radiation during summer does not coincide in time with the high space heating demand during winter. Seasonal thermal energy storage (STES) is a great option to solve the time mismatch problem between energy source availability and thermal demand. As explained throughout this section, we are facing an environmental problem caused by human activity, mainly by the energy sector. My doctoral thesis contributes to moving toward a scenario with lower CO_2 emissions and therefore the mitigating of global warming. This fact motivated me to move my professional career toward research, so that my doctoral thesis can have a beneficial impact on society, particularly on future generations' quality of life.

1.1.2 Seasonal thermal energy storage

STES systems facilitate the replacement of traditional fossil fuels heat sources by alternative heat sources, such as solar thermal energy, geothermal energy, and waste heat [10]. STES systems have been extensively used in the building sector, either integrating the system into an individual heating system or into a district heating system to supply heat to a community. Especially in climates with relatively high solar irradiation during summer and high space heating demand during winter, e.i, in Central or Northern Europe, STES allows to exploit solar heat during the period of greatest heat need when solar radiation is inexistent or not enough to cover the thermal demand. There are three types of STES depending on the storage principle, which are presented in the following sections.

1.1.2.1 Sensible thermal energy storage

Sensible thermal energy is stored by an increase or decrease of the temperature of a material (solid, liquid, or gas). In sensible heat storage systems, no phase change occurs in the material used to store or release the heat. The sensible heat stored in a material can be expressed as:

$$Q_{sen} = m\, C_p\, \Delta T = V\, \rho\, C_p\, \Delta \mathrm{T} \tag{1}$$

where Q_{sen} is the sensible energy stored, C_p is the specific heat of the material, m is the mass of the material, and ΔT is the temperature range of the storage, which depends on the material, the heat source, and the application. Since the mass is equal to the product density (ρ) by volume (V), a good material for sensible heat is the one with high density and specific heat capacity.

There are four types of sensible thermal energy storage (TES): tank, pit, borehole, and aquifer TES. All the technologies are mature and have been already implemented into individual or district heating systems [11–14]. Nevertheless, the main disadvantages of this type of TES are the lower energy density compared to latent and thermochemical storage technologies [10].

1.1.2.2 Latent thermal energy storage

Latent heat storage materials store heat by undergoing a phase change at a nearly constant temperature. This type of materials have higher energy density compared to sensible heat materials [15], which means, that latent heat storage materials require less volume to store the same amount of heat. This fact is very important for most of the applications, such as, residential and industrial applications. The latent heat stored in a material can be expressed as the enthalpy variation (ΔH) between two phases at the phase change temperature:

$$Q_{latent} = m\,\Delta H \tag{2}$$

Active latent TES systems are more suitable for seasonal thermal energy storage compared to passive latent TES systems, due to the possibility to control the operational parameters. Some studies have analysed seasonal latent heat storage systems [16,17]. Nevertheless, they still present some drawbacks, such as, potential corrosion, toxicity [10], the lack of economic commercial phase change materials (PCM), and low thermal conductivity. Indeed, Xu et al. [15] identified in several projects that no significant improvements were achieved using PCM storage systems compared to conventional water stores. Indeed, PCM present high thermal losses to the ambient during the storage period, which hinders its use as seasonal TES.

1.1.2.3 Thermo-chemical or sorption heat storage

Thermo-chemical or sorption heat storage materials store heat by undergoing a reversible (de) composition reaction [18] between a sorbent, which can be a solid or a liquid, and a sorbate, which is in vapour state. The (de) composition reaction can involve either physical or chemical bonds and it can be expressed as:

$$A + B \underset{\text{Charging}}{\overset{\text{Discharging}}{\rightleftharpoons}} AB + \Delta H_{sorption} \tag{3}$$

The charging/discharging sorption process is carried out as follows: the sorbent (A) is heated up to its regeneration temperature, at which, the sorbent and the sorbate (B) are separated (charging phase), usually the sorbate is then condensed to the liquid state by rejecting condensation heat to the ambient. The stored energy remains unalterable as long as the sorbate and the sorbent are kept separated. To trigger the discharging process, the sorbent material must be at equilibrium temperature (smaller than the regeneration temperature). At that temperature, the sorbent and the sorbate get in touch again by evaporating the sorbate exploiting an external source, reacting and releasing the heat of sorption ($\Delta H_{sorption}$). Figure 4 schematically depicts the sorption cycle.

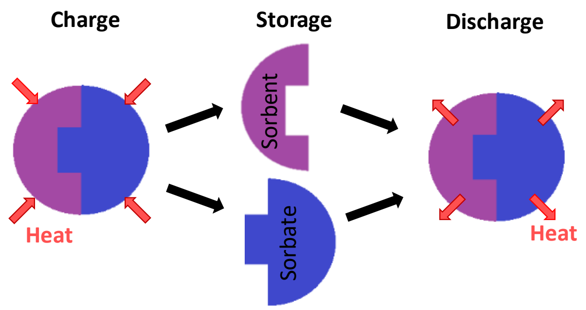

Figure 4: Sorption heat storage concept. Adapted from [19,20].

Sorption heat storage has drawn the attention of the scientific community in recent years because of its nearly zero heat losses during the storage period and its higher energy density compared to sensible and latent TES. Nevertheless, the energy density of a sorption heat storage has a relatively large range (24-1219 kWh/m^3 [21]) since it depends on several factors, such as: sorbent and sorbate materials, the affinity of the working pair, the operating conditions, and the type of system, and its components. Among all the factors involved, the energy density of a sorption storage depends to a large degree on the uptake (*x*), which represents the amount of sorbate (vapour) that can be kept by the sorbent, and is translated into the maximum possible heat of sorption per mass of sorbent material. The amount of adsorbed gas or uptake during the sorption process is function of temperature (T) and pressure (p) as shown in the Clausius-Clapeyron sorption cycle shown in Figure 5.

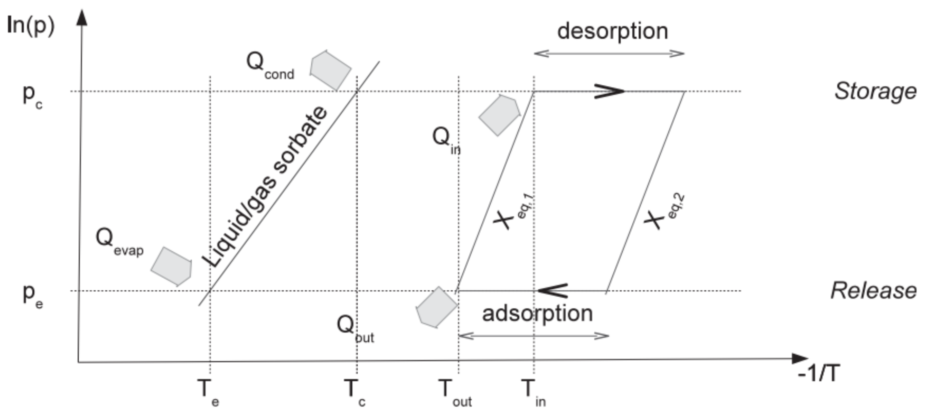

Figure 5: Theoretical Clausius-Clapeyron sorption cycle [22]

A classification of the different sorption heat storage is shown in Figure 6. There are two types of sorption heat storage according to the type of sorption process: absorption and adsorption. On one hand, absorption refers to the materials that undertake a modification in their morphological structure during the sorption process and it usually involves liquid solutions as sorbent medium. On the other hand, adsorption reactions occur at the surface of the adsorbent and therefore, the morphological structure of the material remains invariable. In this section, storage systems based on solid sorption are briefly reviewed.

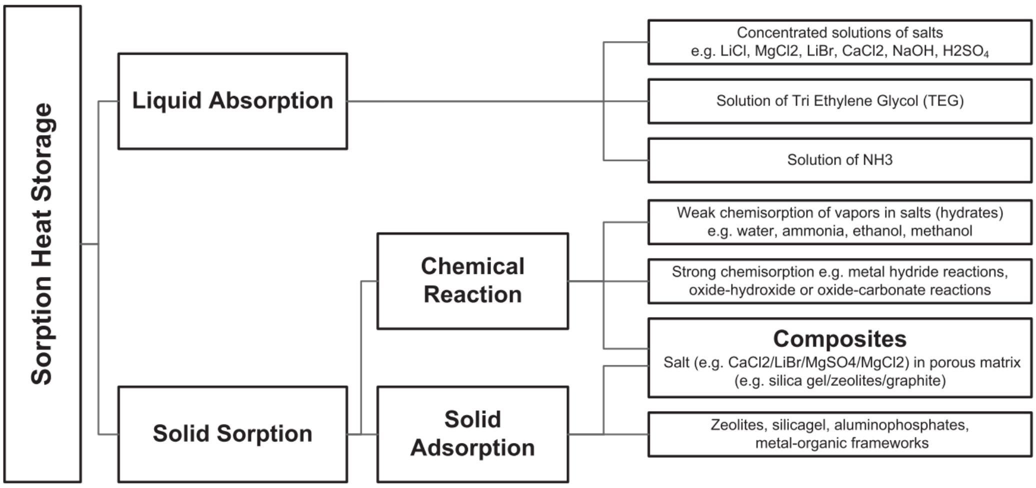

Figure 6: Classification of sorption heat storage [19].

According to the type of sorption mechanism, solid sorption materials can involve a physisorption and/or a chemisorption process (see Figure 6). In a physisorption process, the sorbent and the sorbate are typically related through a weak intermolecular bond, mostly Van der Waals and hydrogen bonding and limited activation energy is required [19,22]. On the other hand, chemisorption consists of strong chemical bonds between the sorbent and the sorbate. In consequence, the energy density of materials that undergo physisorption is lower due to the weaker chemical bonds. Furthermore, solid adsorption materials, such as zeolites, suffer from some intrinsic limitations, such as low water uptake, that limit their energy density [23]. Solid sorbent materials able to exploit chemical reactions, such as salt hydrates, have been also studied. They present high storage density, but they suffer deliquescence, swelling and agglomeration upon reacting with the sorbate, which lead to performance degradation [20]. Composite materials, also known as Composite Salt inside Porous Matrix (CSPMs) or Selective Water Sorbents (SWS) were proposed by Aristov et al. [24] to overcome the drawbacks of both formerly mentioned types of materials. They consist of a salt, embedded into a porous matrix, in which both, chemisorption and physisorption processes, take place. Composite materials present several benefits such as swelling and agglomeration limitation and the improvement of the reaction kinetics due to the confinement of small salt grains inside the matrix pores [25].

In addition to the material classification, sorption heat storage can be classified as an open or closed system. In open systems, a mass and energy transfer between the system and the environment is carried out. The main advantage of an open systems consists of their simplicity, operating at atmospheric pressure [10,26]. However, they also present some disadvantages such as the high material costs and desorption temperatures and lower energy densities at the typical system operating conditions [19]. Furthermore, since they exchange mass with the environment, hazardous materials cannot be used, especially for buildings application. Closed systems are more complex: they require at least an adsorber and evaporator/condenser to keep the adsorbent and the adsorbate always isolated from the environment. Nevertheless, they also present some advantages: their configuration allows combined function: cooling in summer and heating in winter [19,20] and the possibility to work with hazardous materials since there is no mass exchange with the environment. Moreover, one of the main advantages of closed systems is having a higher discharging temperature [27]. In this PhD thesis, we are going to focus on closed sorption TES systems, whose operation and main elements (reactor, condenser, and evaporator) are shown in Figure 7.

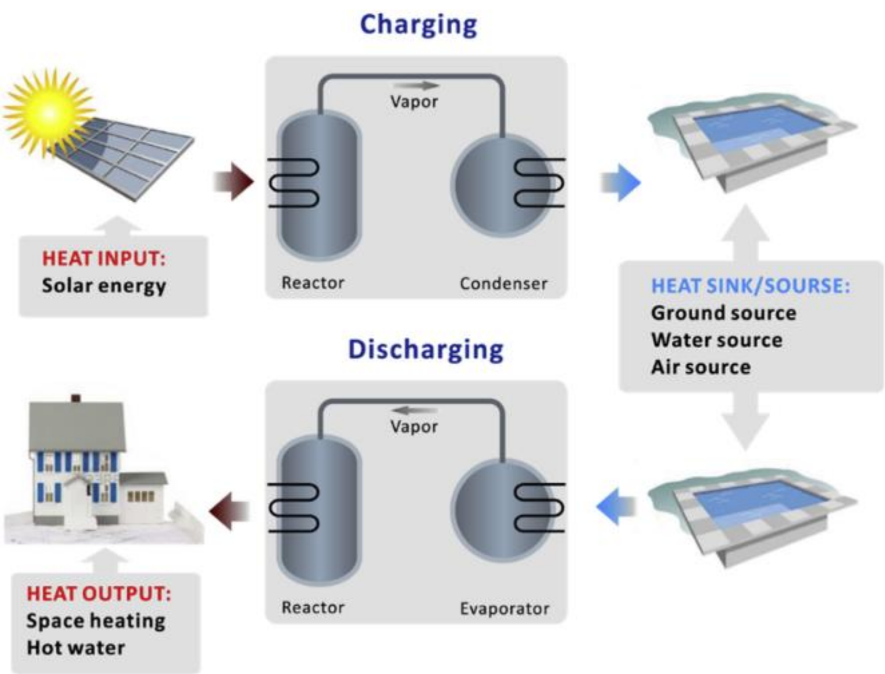

Figure 7: Scheme of a closed sorption TES system [21]

Regardless of the relatively large amount of publications about sorption TES technology, especially at material level [28–31], but also at lab-scale component level [29,32], sorption heat storage still stands in research stage. Nevertheless, some prototypes have been already tested. Bearing in mind that there are many types of sorbent materials and working pairs combinations, in this review I will only highlight sorption heat storage prototypes based on pure adsorption materials and composites since their charging (i.e. 80-120 ºC) and discharging temperatures are more suitable for buildings applications [33]. This fact allows the use of commercial non-concentrated collectors, which are cheaper and easier to install on building roofs. As shown in Table 1, just seven closed sorption TES systems using solid pure adsorption or SWS materials were studied at prototype level. In particular, just three of them explored composite materials. Thus, there is a literature gap in the thermal performance analysis of sorption TES systems using SWS materials.

Active material	Sorbate	T_{des} [ºC]	T_{sorp} [ºC]	Sorbent amount	Storage capacity	Ref
Silica gel 127B	H_2O	88	42	200 kg	13 kWh	[34,35]
Zeolite/Composite	H_2O	90-200	40-160	1.5/15 /750 L	160-240 Wh/kg	[36]
Zeolites/Composite	H_2O	85-140	55	-	164 W/kg	[37]
Zeolite 5A	H_2O	103	20	41 kg	3 kWh	[38]
Zeolite 13X	H_2O	180	45	-	2.8 kWh	[39]
AQSOA FAM Z02	H_2O	90	35	4.3 kg	0.62-1.1 kWh	[40]
LiCl/silicagel	H_2O	89	30	8.9 kg	-	[25]

Table 1: Closed sorption TES prototypes using solid pure adsorption and SWS as active material

1.1.3 Integration of seasonal sorption heat storage into buildings

As reviewed, some prototypes of seasonal sorption TES systems have been already studied. Nevertheless, several of them were tested using less than 10 kg of material inside the reactor. Scaling up the reactors from laboratory or pilot scale to real scale entails challenges in the reactor design, manufacturing, transport, and testing. For instance, a larger amount of sorbent salts entails higher challenges to reaching homogenous equilibrium temperature for all the salts or high heat transfer efficiency between the working pair and the heat transfer fluid (HTF). Hence, the key performance parameters (e.g. COP, energy density) of a sorption TES at large-scale may change in comparison with the values measured at laboratory scale. Not only the design, but the configuration and the integration of a large-scale sorption TES systems into dwelling heating systems is not straightforward and must be deeply studied. In seasonal TES, the dynamic climatic conditions and thermal demands thorughout the year have a dramatic impact in the sorption TES system operation. Sorption TES systems need sensible heat to reach the regeneration or sorption temperature. Especially in winter, if adsorption heat is used to heat up the sorbent material, the higher the thermal losses to the ambient, the lower the heat available to supply the thermal demand. Indeed, N´Tsoukpoe et al. [41] reported, that seasonal sorption TES systems are subjected to significant sensible thermal losses, which in turn, impact the system COP and energy density. As Frazzica et al. [42] highlighted, a careful preliminary analysis of the space heating demand and ambient heat source/sink must be performed to avoid overestimating the size of the sorption TES volume. Thus, further research on the integration and operation of seasonal sorption TES into buildings is needed to push the technology into a competitive stage against other thermal energy storage technologies.

Numerical simulations are the best option to recreate real systems and weather conditions before implementing the system into a large-scale real prototype which involves high investment costs and limited adaptation of testing conditions or configurations. Especially when seasonal storage is involved, numerical simulations allow to analyse the performance of the system without fully depending on the ambient conditions throughout the year, which could prolong the experimental campaigns for months.
Some authors have already analysed based on simulations the integration of sorption TES into buildings. Engel et al. [43]. presented a detailed simulation of a seasonal closed solid sorption storage submitted to different building heating demand profiles. The sorption storage, which used zeolite/water as working pair, was charged with evacuated tube collectors at regeneration temperatures around 180 ºC. The sorption model, validated with experimental data, was implemented in TRNSYS. The storage system with 6 m^3 of storage material could reach thermal energy savings of 70-75 % for a single-family house located in Central Europe. Mlakar et al. [44] analysed a solar-driven thermochemical storage using the working pair $AlPO_4$-LTA/water to provide energy demand coverage of a building in Slovenia. TRNSYS was used to simulate the whole system on a yearly basis and MS Excel was used to calculate the thermochemical storage. The results showed that the system was highly dependent on the environmental conditions. Indeed, due to the importance of boundary conditions (i.e climatic conditions) on the performance of

seasonal sorption TES systems, Frazzica et al. [42] proposed a novel methodology to define the reference boundary conditions to analyse the potential of seasonal sorption TES to cover space heating (SH) demand of buildings. The results demonstrated that such methodology allowed to estimate the achievable sorption TES density under certain boundary conditions. For example, considering a composite sorbent as active material in a Swedish building, up to 11.1 m^3 were required to supply 30 % of the SH demand. Nevertheless, the authors highlighted the lack of pure dynamic simulation to deeply analyse the behaviour of the system.

In spite of the toxicity of ammonia, some authors have studied the integration of sorption TES systems using ammonia as sorbate to supply space heating of buildings located in cold winter climates due to the low freezing point of ammonia (below 0ºC). Thinsurat et al. [45] performed a simulated-based analysis of a solar photovoltaic-thermal (PV/T) collector coupled with a thermo-chemical sorption TES system. The results showed that 26 m^2 of air gap PV/T collectors coupled with the sorption TES could fully satisfy the annual hot water demand of a single household in Newcastle with 100% solar sources. Nevertheless, a detailed optimization of the operation of the sorption TES was not performed (the study focused on the PVT collector). Ma et al. [46] analysed the feasibility of using seasonal sensible, latent, and thermo-chemical storage coupled to solar collectors to supply space heating in eight representative UK cities. In the study, a model of the sorption TES and its dynamic behaviour was missing. In a later study, Ma et al. [47] performed a deeper assessment of the potential of a seasonal chemisorption storage driven by solar energy for domestic application in the UK. In this study, the authors used real weather data and models to simulate the space heating demand, the chemisorption storage, and the solar collectors. Using different salts ($CaCl_2$, $BaCl_2$, NaBr) the system showed energy densities in the range of 127-142 kWh/m^3, much lower than the values for pure material (880-1485 kWh/m^3). In addition, Ma et al. [48] studied a solar-driven seasonal thermochemical sorption system assisted with an electric heater or an electric-driven compressor to supplement the thermochemical desorption process when there was not enough solar irradiation. As part of the study, the optimal number of modules for both scenarios was identified. The results showed that the compressor substantially improved the heat storage capacity in comparison to the use of the electric heater. Typically, sorption heat storage systems are used to store solar heat at long-term. Nevertheless, Tzinnis et al. [49] studied the building integration of a liquid sorption TES combined with an air-source electric heat pump driven by solar photovoltaic panels. Winter electricity demand and emission reductions reached values up to 41 %.

Most of the reported studies dealt with a potential analysis of the integration of the sorption TES into a building heating system. Some of them compared different sorbent materials, optimized the number of sorption modules, or characterized the energy density of the sorption TES. Nevertheless, despite the large dependency of sorption TES system on dynamic environmental conditions [44,50], few studies optimized the control of the system based on demand or weather conditions. Indeed, Engel et al. [43], which analysed a sorption TES system under different climatic conditions, reported that for some locations the system oversize could have been avoided by adjusting the control strategy. Hence, performing the optimization of the operation of the system allows to increase its COP and energy density and consequently, positioning the sorption TES technology in a more competitive place against other storage technologies.

1.1.4 Optimal control of sorption TES systems

Optimal control of TES is gaining attention in the last years since it allows to maximize the efficiency of clean and non-continuous energy technologies such as solar or wind energy by storing or dispatching the energy at the optimal period of the day, month, or year. TES optimal control is a complex task since it can be based on multiple variables such as weather conditions, solar availability, energy demand, or electricity prices [51]. The most extended and traditional control strategies are the rule based control (RBC) strategies, which are based on a deterministic approach: an operational mode is selected based on a defined set of rules and control threshold. The control thresholds of an RBC strategy can be optimized in terms of an objective function. The optimization of a RBC policy allows to operate the system in an optimal scenario (under the defined rules) with a relatively simple control and low computational effort and has been already successfully implemented to optimize the control of TES systems [52].

An RBC strategy is not able to foreseen the best operational mode based on forecasted values even being optimized. Hence, smart control strategies for TES systems gained the attention of researchers in the recent years. There are two main types of smart control methodologies applied for TES: model predictive control (MPC) and reinforcement learning (RL). MPC uses a system model to predict the future states of the system and generates a control vector that minimizes certain objective function over the prediction horizon [53]. Even though MPC can achieve optimal or quasi-optimal control of the TES acting passively [54], coupled to CSP plants [55] or to heating systems [56,57], it presents important drawbacks. MPC requires high programming skills, usually specialized solvers [58], and most important, the need of implementing simple models (avoiding non-linearity and iterative processes). Especially, it can imply limitations for the study of complex TES systems, where detailed mathematical models, equation systems with non-linearity or an implicit scheme may be needed to accurately simulate the behaviour of the system and capture the response of the system under different control actions. On the other side, RL technique it is an emerging smart control technique with a different control logic compared to typical control methods [51]. In RL control, the agent (entity that learns which is the optimal operational mode at each state) learns from experience, which materializes with a reward, which can be economic, energetic, or environmental. RL methodology accepts complex mathematical models, as the ones required to simulate a PCM or a sorption storage tank. Nevertheless, the more complex the numerical model, the longer the learning time of the agent. Even though RL is an emerging research field, few studies reported its benefits to optimally control TES systems [58–64].

At this research stage, regarding the development of sorption TES systems, very few studies have studied its optimal control, despite its importance. Among these studies, Scapino et al. [65] presented a techno-economical optimization of a geothermal energy system with sorption TES that supplied heat to an ORC and a district heating system. The authors optimized the STES size and the system operation under different energy markets, concluding that STES integration was suitable just for some scenarios. Bau et al. [66] presented a model-based method to assess absorber-bed design. The methodology consisted of optimizing the design and the control of different adsorber-beds for its application on chillers. The authors optimized the control using direct multiple shooting method. The seasonal modular sorption TES studied by Engel et al. [43] had more than 30 different operational modes. The authors studied the system in different locations, but the control settings were optimized just for one scenario. Tzinnis et al. [49] explored different PV thresholds to determine an optimal operation mode of a sorption storage that minimized the CO_2 emissions. A detailed optimal control was not performed, since the authors identified the optimum based on a parametric analysis. Recently, Curtis et al. [67] experimentally optimized the performance of an open bulk-scale silica/gel water vapour sorption storage system by varying the key operating parameters (relative humidity, particle size, desorption temperature, and flow rate) and observing its impact on the energy density, temperature lift and thermal power. Even though, the work performed by Curtis et al. was very helpful to provide a basis for a future large prototype design, it did not analyse the performance of a sorption TES once integrated into a building and submitted to multiple transient boundary conditions.

To conclude, according to the best author´s knowledge, there is no study that analysed the thermal performance of a seasonal sorption system integrated into a building heating system and operated under a detailed optimal control.

1.2 PhD objectives

The main objective of this PhD thesis is to analyse and increase the performance of a solar-driven seasonal sorption TES (SDSSTES) system coupled to a building through the study of different control strategies and different system designs. The system was integrated into a building heating system and was submitted to dynamic weather conditions and thermal demands on a yearly basis. To accomplish this general objective, several specific objectives were specified:

- To develop the mathematical models of all system components and implement all the system operational modes to simulate the performance of the whole solar seasonal system.

- To develop a 2D numerical model of a PCM tank and analyse the trade-off between results accuracy and computational time to implement it into the simulation of a complex seasonal system which requires low computational time.

- To analyse the impact of an optimized RBC strategy on the performance of a SDSSTES system integrated into a building heating system.

- To identify, through numerical simulations and an optimized RBC strategy, operational and system enhancements during the discharge of the sorption system when it is subjected to transient weather and thermal demand conditions.

- To evaluate through numerical simulations, the potential of a seasonal water-based sorption TES subjected to different climatic conditions by means of an optimized RBC strategy at each climatic location.

- To implement a DRL algorithm by coupling it to detailed numerical models of the system.

- To study numerically the benefits of DRL with respect to an optimized RBC policy on the operation of a seasonal water-based sorption system driven by solar thermal collectors.

Chapter II

2 PhD structure

This PhD thesis is based on five journal papers. Two of them have been already published in SCI journals, one of them has been accepted, and two have been submitted. Figure 8 shows the distribution of the different chapters that composed this thesis.

The first chapter provides the introduction to the research topic and the objectives to be achieved throughout this PhD thesis. In chapter II, the PhD thesis structure is presented. Chapter III describes the methodology applied throughout the thesis, including a detailed description of the SDSSTES system under study.

Chapters IV to VIII include the five papers that comprise this PhD thesis. Each chapter introduces the specific topic, briefly describes the content, and reports the main result findings of the paper. In chapter IV (paper 1) the numerical model of a PCM tank was developed and validated with experimental data. The type of numerical model resolution method (explicit or implicit) and the number of nodes were assessed to identify the best trade-off between model results accuracy and computational time. The developed PCM tank numerical model was implemented into the system simulation model of paper 2. Chapter V (paper 2) studied the annual performance of a SDSSTES system that contained a novel sorbent material (LiCl/Silica gel). The system supplied domestic hot water (DHW) and SH to a single-family house located in Central Europe. Paper 2 assessed the impact of a detailed optimized RBC strategy on the thermal performance of the system. Chapter VI (paper 3) delved into control optimization techniques based on artificial intelligence. The potential of DRL to operate a seasonal sorption system driven by solar collectors was assessed. The smart control policy allowed to minimize the operational costs compared to an optimized RBC policy. As mentioned, chapters V and VI (paper 2 and 3) focused on the impact of optimal control on the thermal performance of a SDSSTES system. On the other hand, chapter VII (paper 4) focused on analysing different scenarios to enhance the discharging process of the sorption TES systems, which has a large impact on the system performance. The last paper, contained in chapter VIII (paper 5), explored the feasibility and quantified the benefits of the solar seasonal sorption system integrated into a building heating system located in different climatic areas.

The ninth chapter contains the description of the global discussion of the attained results. Finally, chapter ten includes the conclusions of this PhD thesis and different proposals in line with this thesis to carry out in future studies.

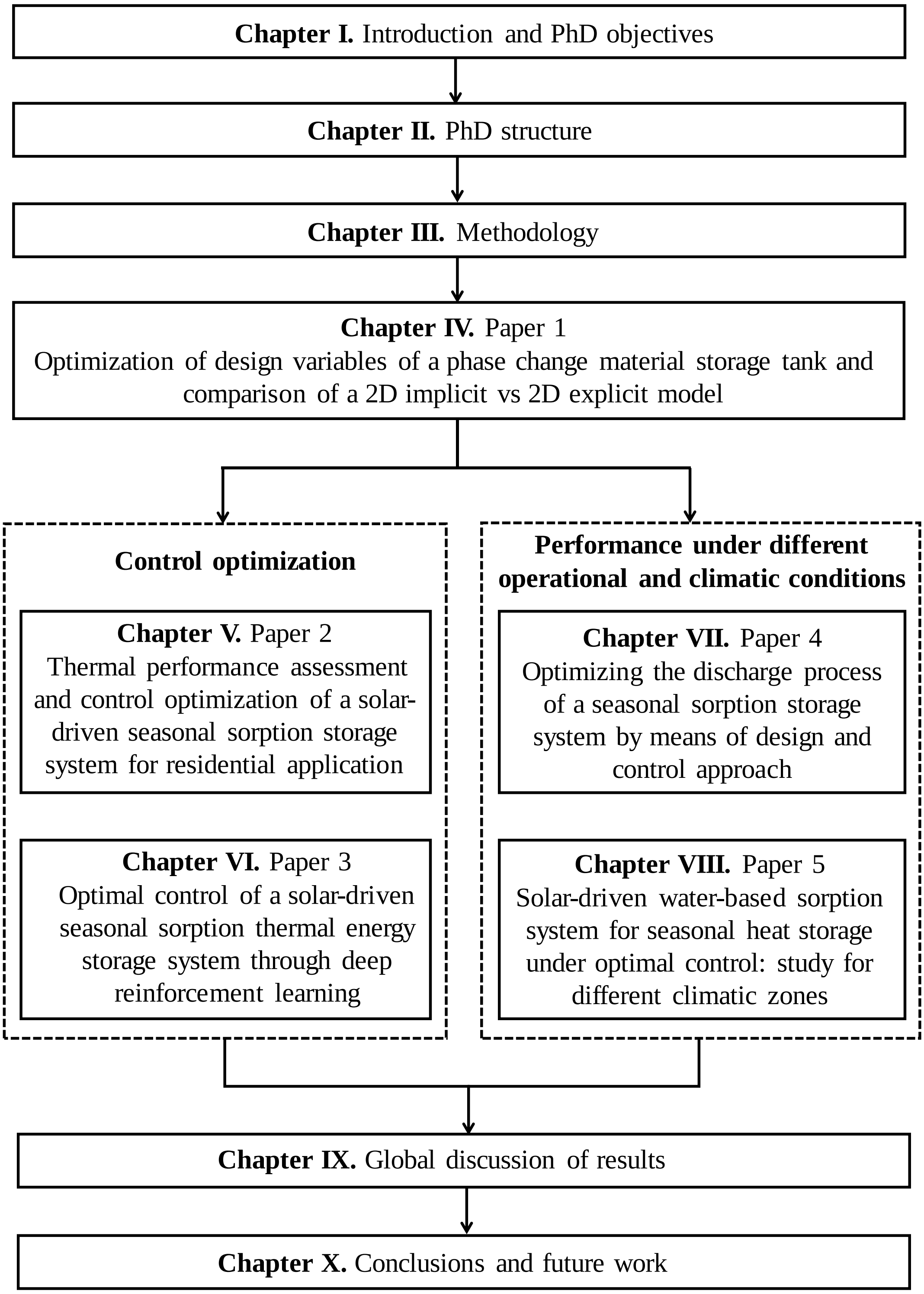

Figure 8: PhD thesis structure

Chapter III

3 Methodology

In this chapter, the methodology followed along the PhD thesis is described. First, the description of the system is presented, which is essential to understanding the rest of the chapters of this thesis. Next, the numerical models and performance maps used to analyse the thermal performance of the system components are described. After that, the features of the system simulation are introduced. Moreover, the operational modes and the implementation of the control strategies are presented. Finally, the key performance indicators (KPIs) used to assess the system performance from a technical and environmental perspective are described.

3.1 System description

The analysed system is shown in Figure 9 and Figure 10 for summer and winter configuration, respectively. It mainly consists of a solar field composed with evacuated tube collectors, a stratified water tank, a seasonal sorption storage filled with 30 wt% (i.e. 30% water uptake) of LiCl embedded in Silica gel, and a backup gas boiler. The system was designed to provide the DHW and SH coverage of a single-family house in Central and North Europe. The seasonal operating principle of the system is as follows: during summer the seasonal sorption heat storage system is charged with high-enthalpy solar heat (around 90 ºC). First, the sorption TES receives solar heat to increase the system temperature up to regeneration temperature. At equilibrium temperature, solar energy is converted into heat of sorption and the system gets charged: water evaporates and is separated from the sorbent material. Energy is stored in form of sorption bonds as long as the sorbent material and the water vapour are kept in different vessels. A condenser is required during charging to condense the water vapour and store it. In the analysed system, one unique piece of equipment (evaporator/condenser) works as evaporator (winter) and condenser (summer).

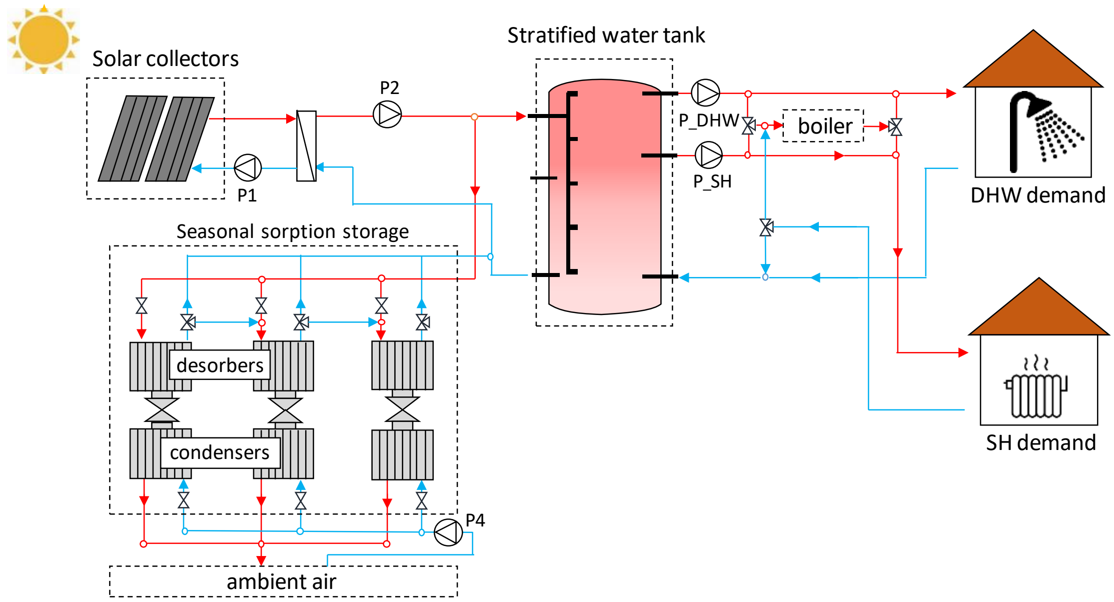

Figure 9: Schematic of the system for summer configuration

Throughout the year, solar heat can also be used to heat up (charge) the stratified-water tank that is able to cover totally or partially DHW and SH demands. Nevertheless, during cold winter days with low solar irradiation, the stratified water tank is not hot enough to supply the SH demand. In consequence, the heat of sorption stored in the seasonal storage is released to the water tank. To discharge the sorption TES, the water stored in the evaporator/condenser must be evaporated and adsorbed again by the sorbent material. A LTHS, that provides heat to the evaporator at temperatures from 5 to 15 ºC, is needed. In cold climates, during certain mild winter days, a dry-heater can take profit from environmental heat (ambient temperature around 15ºC in certain moments) to supply heat to the evaporator. Nevertheless, in cold regions, a sensible or latent storage tank is charged with solar heat at low temperatures to assist the evaporator.

DHW and SH demands are directly supplied by hot water stored in the stratified water tank if its temperature is at the required set point. Otherwise, the system is supported by a natural gas boiler. Furthermore, if the temperature in the middle region part of the stratified water tank is below the return temperature of SH, the boiler supplied the SH demand in close loop mode. The upper part of the stratified water tank is reserved for DHW, since it is at a higher temperature.

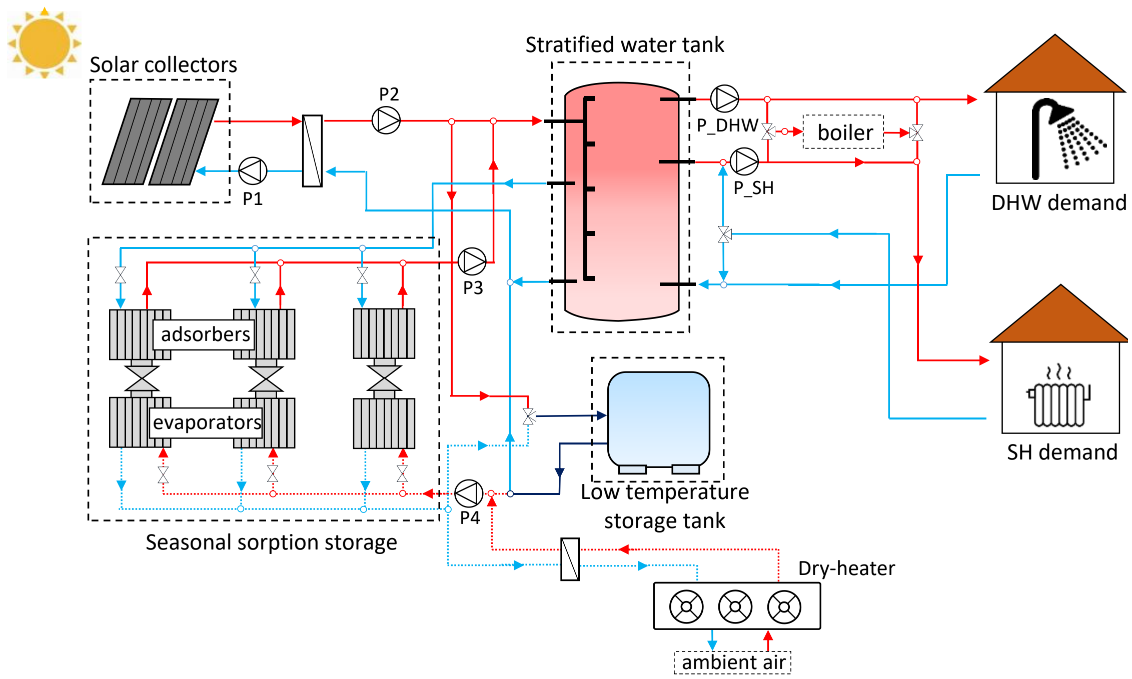

Figure 10: Schematic of the system for winter configuration

3.2 Development and validation of the numerical models

The assessment of the thermal performance of the whole system and each of its components required the development and validation of different numerical models or performance maps. Thus, in this chapter, the developed numerical models of the main components are briefly explained, and the performance maps used are given. All the components models were implemented in Python [68]. Further detailed information about the numerical models and the performance maps is presented in the papers that composed this PhD thesis.

3.2.1 Solar thermal collectors

The general equation of a solar thermal collector presented by Duffie [69] (see Equation 1) is commonly used to simulate the thermal performance of evacuated tube collectors.

$$F_r\ IAM\ E_G\ A_{col} = \dot{m}_{col}\ C_p\ (T_{out,col} - T_{in,col}) + U_{L,col}\ A_{col}\ (T_{ave} - T_{amb}) \quad (1)$$

Equation 1 includes the collector efficiencies through the heat removal factor (F_r), and the heat losses coefficient ($U_{L,col}$). Nevertheless, the collector efficiencies can be also calculated based on the collector overall efficiency ($\eta_{overall}$), whose expression is shown in Equation 2. Thus, the thermal performance of an evacuated tube collector can be also expressed with Equation 3.

$$\eta_{overall} = a_0 - a_1 \frac{T_{avg,col} - T_{amb}}{E_G} - a_2 \frac{(T_{avg,col} - T_{amb})^2}{E_G} \quad (2)$$

$$IAM\ E_G\ A_{col}\ \eta_{overall} = \dot{m}_{col}\ C_p\ (T_{out,col} - T_{in,col}) \quad (3)$$

Where IAM is the incidence angle modifier, E_G is the global irradiation in the title surface, A_{col} is the collector´s area, $\dot{m}_{col}$ is the collector mass flow rate, C_p is the specific heat capacity of the HTF, a_0 is the optical collector efficiency, a_1 and a_2 are the first and second order collector efficiencies, $T_{in,col}$, $T_{out,col}$ and $T_{avg,col}$ are the inlet, outlet, and average collector temperatures, respectively.

Results reported by Ayompe et al.[70] were used to validate the numerical model of the solar thermal collectors. The model developed in the frame of this thesis predicted the collector outlet temperature with an average relative error of 1 % compared to the results reported by Ayompe et al. [70].

3.2.2 Stratified water tank

A 1D numerical model was developed to predict the thermal performance of a constant volume stratified water tank. The heat transfer in the water tank domain was analysed through the finite control volume method and was solved with an explicit scheme. The equation system that defined the thermal behaviour of the stratified water tank was already described by Rodriguez-Hidalgo et al. [71]. The following physical processes were considered in the model: heat conduction between adjacent nodes, mass flow transfer between nodes, and thermal losses to the ambient.

Experimental results with a vacuum-insulated water tank (see Figure 11) performed at the laboratories of the GREiA research group at the University of Lleida (Spain) were used to validate the mathematical model. Five temperature sensors were located along the water tank at different heights. To reach a trade-off between results accuracy and computational time, 33 nodes were used for the validation. The average relative error in terms of temperature for the five sensors was 2.14 %.

Figure 11: Picture of the stratified water tank at GREiA laboratory.

3.2.3 Sorption thermal energy storage system

The thermal performance of the sorption TES system was obtained scaling up the results from experimental measurements. The experimental results of an innovative lab-scale adsorber reported by Mikhaeil et. al. [32] alongside the kinetic characterization of the novel adsorbent material [23,72] studied in this thesis (Silica gel impregnates in 30 wt.% of LiCl) were used to define the adsorption/desorption kinetics of the process and were scaled-up to generate the performance maps. The performance maps provide the charging and discharging power of the sorption system as a function of inlet temperatures at the adsorber and evaporator/condenser for defined mass flow rates. Each performance map provided information about a 100 kg of SWS sorption module. The total thermal capacity of the sorption TES was 611.1 kWh. A scheme of one sorption module and its interior is shown in Figure 12.

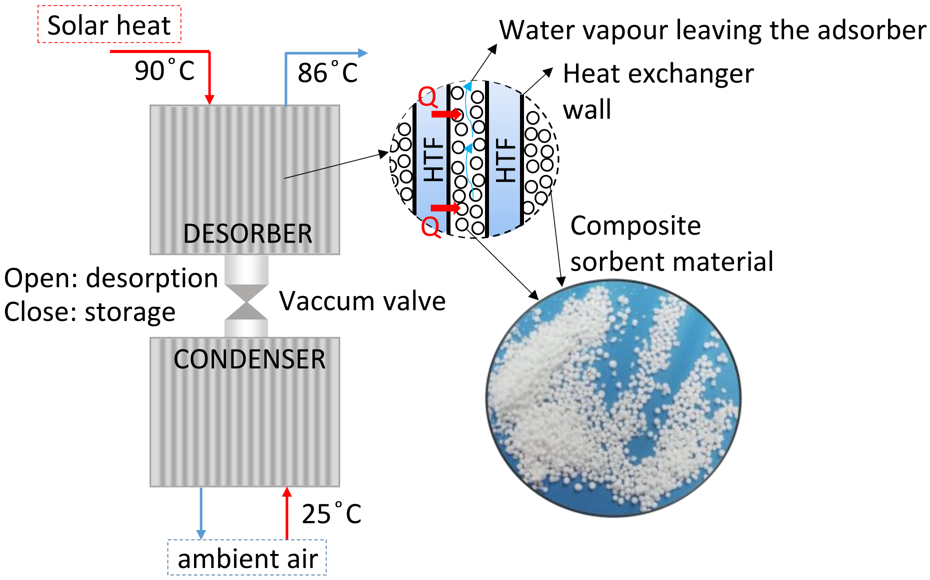

Figure 12: Scheme of a sorption module during charge (dehydration)

In any seasonal TES system, the thermal losses to the ambient highly impact the performance of the system. Nevertheless, in sorption systems, its importance is higher, due to the necessity of the sorbent material to be at a defined regeneration or sorption temperature to drive the reaction. In this thesis, the thermal losses to the ambient of the sorption TES system were analysed assuming the system as a lumped model, representing the composite material, the heat exchanger, and the HTF. Since, the sorption system was assumed to be in a garage or buried underground a constant ambient temperature for summer (20 ºC) and for winter (15 ºC) was assumed. Under this premise, the thermal losses of the sorption module were calculated by an exponential decay equation as a function of the heat transfer coefficient, an equivalent heat capacity, the total mass of the module, and its external heat transfer area. The performance maps can be found in Chapter V (paper 2).

3.2.4 Low temperature heat source

A sorption TES system requires a LTHS to assist the evaporator. In particular, water-based sorption systems require heat at temperatures above 0 ºC. In this PhD thesis, depending on the system analysed in each paper, three LTHS were explored: a PCM storage tank, a water tank, and a dry-heater. It must be mentioned that none of the papers included in this PhD thesis studied simultaneously the three of them.

3.2.4.1 PCM storage tank

The PCM storage tank consisted of a rectangular tank filled with water and stacked PCM with a gap between them to allow the HTF to flow between them. A diffuser was set at the inlet and outlet of the tank to allow the better distribution of the HTF between the water channels. A scheme of the PCM storage tank is depicted in Figure 13.

Figure 13: Scheme of the modelled PCM tank [73]

A 2D numerical model was developed to simulate the heat transfer from the HTF to the PCM slabs and vice versa, and the corresponding storage period. Both, the fully implicit and explicit scheme were implemented (and compared) to solve the system of equations obtained through the finite control volume method. The iterative method Gauss-Seidel was used to solve the set of equations when using the implicit scheme. Further details about the considered assumptions and model description are explained in paper 1 (chapter IV).

(a)

(b)

Figure 14: (a) PCM storage unit; (b) FlatICE PCM slab [73]

Experimental measurements (see Figure 14) performed at the laboratories of the GREiA research group at the University of Lleida (Spain) were used to validate the numerical model. The error in terms of HTF outlet temperate between the numerical model results and the experimental values in the desired working range was ±1%.

The validated PCM tank model using an explicit resolution approach was implemented into the whole system simulation model (paper 2) and consumed, at each iteration, a relevant portion of the total computational time. In consequence, the optimization of the RBC parameters based on system simulations took more than a week. Therefore, in later studies (papers 3, 4, and 5), lumped models were used to model the LTHS.

3.2.4.2 Water buffer tank

A single control volume, also known as fully mixed model, was used to analyse the thermal performance of the water buffer tank. The LTHS was used during winter at short-term to assist the evaporator. Hence, the environmental heat losses were neglected in the model.

3.2.4.3 Dry-heater

Thermal performance of the dry-heater was analysed through the equality between the Fourier´s law of heat conduction [74] and the temperature gradient in the HTF fluid side of the heat exchanger. The UA value of the heat exchanger used in the simulations was 320 W/m^2K [75]. The HTF in the dry-heater corresponds to water with 15% glycol.

3.3 System simulation

The simulation of the whole system was driven in Python by the interconnection of all component models. The convergence of a simulation with many variables requires large computational times, especially if iterative processes are needed and some of the variables must be within a certain range (e.g. collector outlet temperature or collector mass flow range). To speed up the calculation process and facilitate convergence, the following system variables from the previous time-step were used to calculate the system variables for the current time-step (explicit scheme): inlet collector temperature, PCM or water buffer storage tank temperature, temperatures of the stratified water tank and sorption TES tank. In spite of assuming some temperatures from the previous time-step, iterative processes were required to calculate some system variables. The Gauss-Seidel method, assuming an error of 0.01 ºC and 0.01 kg/h was applied.

Moreover, the sizing of the main system components used in the simulations of all the papers is presented in Table 2.

Component	Units	Size
Collector field area	m^2	17.5
Stratified water tank volume	m^3	1
Number of sorption modules	-	20
Mass per sorption module	kg	100
Total PCM mass	kg	220
Water buffer tank volume	m^3	0.39
Dry-heater nominal power	kW_{th}	2.75
Gas boiler power	kW_{th}	9

Table 2: Sizing of the main system components

3.4 Operational modes of the system

As previously mentioned, the system studied in this PhD thesis was composed of a solar field, a stratified water tank, a backup boiler, a seasonal sorption TES, and a LTHS to assist the latter. The type of LTHS used in the different studies was not the same. Paper two (chapter V) analysed the use of a PCM as LTHS. Paper three (chapter VI) analysed the use of a buffer water tank as LTHS and papers four and five (chapters VII and VIII, respectively) analysed the use of both a buffer water tank and a dry heater as LTHS, but never simultaneously. Hence, the studied operational modes at each paper are different and are presented below.

The operational mode (i.e. action) of the system {$\mathcal{A}$} was defined by a vector of sets. Each set defines the operational mode of the corresponding subsystem: 1, solar collectors {$\mathcal{C}$}; 2, the pumps on the consumer side {$\mathcal{P}$}; 3, the seasonal sorption TES {$\mathcal{E}$}; 4, the backup boiler {$\mathcal{B}$}, and 5, the space heating supply {$\mathcal{H}$}. Hence, the vector was defined as $\mathcal{A}$ ={$\mathcal{C}$,$\mathcal{P}$,$\mathcal{E}$,$\mathcal{B}$,$\mathcal{H}$}. The operational modes of the components that composed the vector are presented in Table 3, Table 4, Table 5, Table 6, and Table 7.

ID	Description	Active pumps	PCM or buffer tank
0	No action	P1, P2	Inactive
1	Charging the sorption TES	P1, P2	Inactive
2	Charging water tank for DHW	P1, P2	Inactive
3	Charging water tank for SH	P1, P2	Inactive
4	Charging low temperature heat storage	P1, P2	charge

Table 3: Operational modes of the solar collectors

ID	Description	Active pumps
0	Pumps off	None
1	Pump for DHW on	P_DHW
2	Pump for SH on	P_SH
3	Pumps for DHW and SH on	P_DHW, P_SH

Table 4: Operational modes of the circulation pumps on the consumer side

ID	Description	Active pumps	PCM or buffer tank	Dry heater
0	No action	P1, P2, P4	Inactive	Inactive
1	Charging the sorption TES	P3, P4	Inactive	Inactive
2	Discharging the sorption TES with low temperature heat storage	P3, P4	Discharging	Inactive
3	Discharging the sorption TES with dry heater	P3, P4	Inactive	On

Table 5: Operational modes of the sorption TES

ID	Description	Active pumps
0	Boiler off	None
1	Boiler on	P_SH or P_DHW

Table 6: Operational modes of the circulation pumps on the consumer side

ID	Description	Active pumps
0	SH not supplied	None
1	SH directly supplied from water tank	P_SH
2	SH supplied with assistance of boiler	P_SH
3	SH supplied in close loop with the boiler	P_SH

Table 7: Operational modes of the SH facility

Based on the aforementioned operational modes of the system components, the system operational modes explored in paper 2 (chapter V), whose system used a PCM storage tank as LTHS, are the following: {0:*{0,0,0,0,0},* 1:*{1,0,1,0,0},* 2:*{1,1,1,0,0},* 3:*{1,1,1,1,0},* 4:*{2,0,0,0,0},* 5:*{2,1,0,0,0},* 6:*{2,1,0,1,0},* 7:*{3,0,0,0,0},* 8:*{0,0,2,0,0},* 9:*{0,1,0,0,0},* 10:*{0,1,0,1,0},* 11:*{0,1,2,1,0},* 12:*{2,2,0,0,1},* 13:*{3,2,0,0,1},* 14:*{0,2,0,0,1},* 15:*{2,2,0,1,2},* 16:*{3,2,0,1,2},* 17:*{0,2,0,1,2},* 18:*{0,2,2,1,2},* 19:*{0,2,0,1,3},* 20:*{2,2,0,1,3},* 21:*{3,2,0,1,3},* 22:*{0,2,2,1,3},* 23:*{4,0,0,0,0},* 24:*{4,1,0,0,0},* 25:*{4,1,0,1,0},* 26:*{4,2,0,0,1},* 27:*{4,2,0,1,2},* 28:*{4,2,0,1,3},* 29:*{2,3,0,1,1},* 30:*{0,3,0,1,1},* 31:*{4,3,0,1,1},* 32: {0,1,2,0,0}, 33:*{3,1,0,0,0},* 34:*{3,1,0,1,0},* 35:*{4,0,2,0,0},* 36:*{4,1,2,0,0},* 37:*{4,1,2,1,0},* 38:*{4,2,2,1,2},* 39:*{4,2,2,1,3},* 40:*{4,1, 0,1,1}}.*

In paper four (chapter VII), there was a slight change on the operational modes. Operational modes 0 to 32 were also explored by the system. However, operational modes 32 to 39 were not. Simultaneous charge and discharge of the LTHS turned out to be less efficient than charging and discharging independently. In paper 3, different temperature set points to supply the SH demand and discharge the sorption TES were studied. For this reason, the following operational modes were also explored: {41:*{0,2,2,0,1},* 42:*{0,3,2,1,1}*}. Moreover, paper four also analysed the use of a dry heater to assist the evaporator of the sorption TES. The following operational modes were also explored in paper three: {43:*{0,0,3,0,0},* 44:*{0,1,3,1,0},* 45: *{0,2,3,1,2},* 46:*{0,2,3,1,3},* 47:*{0,3,3,1,1}*}.

Paper two, three, and four explored the system under the weather conditions of Nuremberg. The climatic conditions of this location make it impossible that in winter solar heat can supply DHW and SH without the support of the backup boiler.

Nevertheless, paper five studied also Paris, which presents a warmer climate. Therefore, during mild days also the following operational modes must be explored: {47:*{1,3,1,0,1}*, 48:*{2,3,0,0,1}*, 49: *{0,3,0,0,1}*}.

Last, paper three focused on the system management during the winter period. Therefore, the operational modes dealing with the charging of the sorption TES were not explored. Moreover, the operational modes that explored the use of a dry heater were not explored either.

3.5 Control strategies

The last step of the methodology consisted of implementing and testing the operational modes and optimizing the system control.

The operational modes described in the previous section, which summed up between 32 to 43 depending on the system version, were implemented and tested through an energy balance to verify their validity. Finally, the optimization of the control strategy was driven.

Two different methodologies were applied to optimize the system control in this PhD thesis. The first methodology consisted of controlling the system through an optimized RBC strategy. The control thresholds of the RBC policy were optimized through a hyperparametric optimization [76] using the TPE algorithm [77]. The second methodology consisted of using a smart control technique (deep reinforcement learning (DRL)) to optimise the control of the system. The Tensorflow library [78] from Python was used in this case. Detailed information about the optimization of the RBC and the smart control strategies is presented in paper 2 (chapter V) and paper 3 (chapter VI), respectively.

3.6 Key performance indicators

The thermal performance of the whole system was evaluated through the solar fraction (SF) and the CO_2 emissions savings. The solar fraction represents the amount of thermal demand supplied by the solar system. It was calculated using Equation (4), where D_{DHW}+ D_{SH} correspond to DHW and SH demand and E_b correspond to the share of the thermal demand supplied by the boiler.

$$SF = \frac{(D_{DHW} + D_{SH}) - E_b}{D_{DHW} + D_{SH}} \tag{4}$$

The CO_2 emissions savings were calculated using an equivalent CO_2 coefficient for natural gas (CO_{2eq}) of 0.18 kg/kWh [79] and a boiler efficiency (η_b) of 0.9:

$$CO_2\ emissions\ savings = \frac{[(D_{DHW} + D_{SH}) - E_b\ ]}{\eta_b}\ CO_{2eq} \tag{5}$$

The performance of the seasonal sorption TES was evaluated through the coefficient of performance (COP), energy density (e_d), discharging efficiency (η_{dis}), and temperature effectiveness (TE). The COP measures the ratio between the net discharged energy (E_{ad}) from the sorption modules versus the total energy required during the charging phase, that is to say, the sum of sensible energy ($E_{de,sen}$) plus desorbed energy (E_{de}).

$$COP = \frac{E_{ad}}{E_{de,sen} + E_{de}} \tag{6}$$

The energy density indicates the net discharged energy versus the volume of the sorbent material (V_{sorb}) and is presented in Equation 7.

$$e_d = \frac{E_{ad}}{V_{sorb}} \tag{7}$$

The discharging efficiency, which measures the performance of the sorption TES system during its discharging process is shown in Equation (9). Where $E_{ad,sen}$ is the amount of sorption energy stored that is used the heat up the sorbent material during the discharge.

$$\eta_{dis} = \frac{E_{ad}}{E_{ad,sen} + E_{ad}} \tag{8}$$

A novel key performance indicator, called temperature effectiveness (TE), introduced by Fumey et al. [52] was also used to assess the sorption TES. TE consists of the ratio of resulting gross temperature lift during adsorption (GTL_{ad}), versus the required temperature lift during desorption (GTL_{de}). The temperature effectiveness was calculated using the following equations [52].

$$TE_{avg} = \frac{GTL_{ad}}{GTL_{de}} \tag{9}$$

$$GTL_{ad} = T_{ad,avg} - T_{e,avg} \tag{10}$$

$$GTL_{de} = T_{de,avg} - T_{c,avg} \tag{11}$$

Where $T_{ad,avg}$ is the sorption temperature during discharge, $T_{e,avg}$ is the evaporator temperature, $T_{de,avg}$ is the desorption temperature and $T_{c,avg}$ the condensing temperature.

Chapter IV

4 Paper 1: Optimization of design variables of a phase change material storage tank and comparison of a 2D implicit vs 2D explicit model

4.1 Overview

Sorption TES systems require a LTHS during the discharging process to assist the evaporator. Water-based sorption systems, ergo, sorption systems that use water vapour as sorbate, require heat at temperatures above 0 ºC to avoid freezing. The sorption TES system studied in this PhD thesis had better performance at inlet evaporator temperatures of 15 ºC rather that at 5 ºC because of the lower temperature difference between the reactor and the evaporator. Hence, keeping the evaporator inlet temperature at 15 ºC allows to achieve higher system efficiency. Latent thermal energy storage systems can provide heat at a nearly constant temperature (melting temperature). Thus, for the first system configuration, a latent thermal energy storage was selected as LTHS.

The performance of a latent TES system depends to a large degree on the thermo-physical properties of the storage material, which usually presents some limitations, such as low thermal conductivity, subcooling, phase segregation, or non-uniform temperature distribution inside the PCM slabs or capsules [73]. In addition to the relevance of the material, the storage design (container material, heat exchange area, amount, and shape of the encapsulation…) also plays a relevant role in the performance of a PCM storage deposit. A detailed numerical model allowed to accurately analyse the thermal performance of a PCM storage tank. Several authors presented numerical models of PCM storage tanks. Most of the authors used implicit schemes to solve the equation systems [80–83], while others used explicit [84] or semi-explicit schemes [85], which are less cost-effective, but also less accurate. The selection of the resolution scheme (implicit, explicit, semi-explicit) can strongly affect the required computational time and the accuracy of the model. If the goal of the paper is to analyse or optimize the latent TES at component level, the computational time is nearly irrelevant. Nevertheless, when the PCM storage tank model, is aimed to be integrated into the simulation of a complex system, composed by several components the trade-off between model results accuracy and computational time must be carefully studied. It is especially relevant when the optimization of design variables or control optimization parameters is carried out, which usually requires a lot of iterations and light models are desired.

4.2 Contribution to the state-of-the-art

In this chapter, a 2D numerical model of a PCM storage tank, based on the finite control volume approach, was developed and validated with experimental results obtained at GREiA research group laboratories at the UdL. Based on the validated model, the optimal configuration of the PCM storage tank (number of PCM slabs and its layout) using two different types of slabs with thicknesses of 35 (Flat-ICE) and 17 mm (Thin-ICE) were defined. The objective function consisted of minimizing the mean average percentage error (MAPE) between the nominal heat power required by the evaporator (Q_{ref}), and the simulated heat power delivered by the PCM storage tank (Q^{t}_{sim}). The nominal heat power required by the evaporator of the sorption TES was 2.1 kW. However, this heat power demand can vary between 1 and 3 kW during the operation of the seasonal sorption TES tank. Hence, an additional constraint was considered: the suitable configuration was the one whose heat transfer rate was in the chosen range (1 to 3 kW) for the longest time.

Moreover, the PCM storage tank under study was designed to be part of a complex SDSSTES system. Simulating and optimizing a complex energy system, which includes 2D numerical models containing several control volumes (nodes), consumes high computational resources. Hence, a comparison between a 2D implicit and 2D explicit model was also carried out by means of optimal trade-off between results accuracy and required computational time.

The results indicated that a thicker PCM slab (Flat-ICE) is more beneficial for the case study because it allowed to deliver heat at a transfer rate between 1 to 3 kW during a longer period compared to the Thin-ICE. This can be explained because for nearly the same PCM total mass in the storage tank, less heat transfer area between the PCM and the HTF is available. Thus, heat is released at lower heat power, but for longer time compared to Thin-ICE, making the LTHS more reliable when required by the sorption module, as shown in Figure 15.

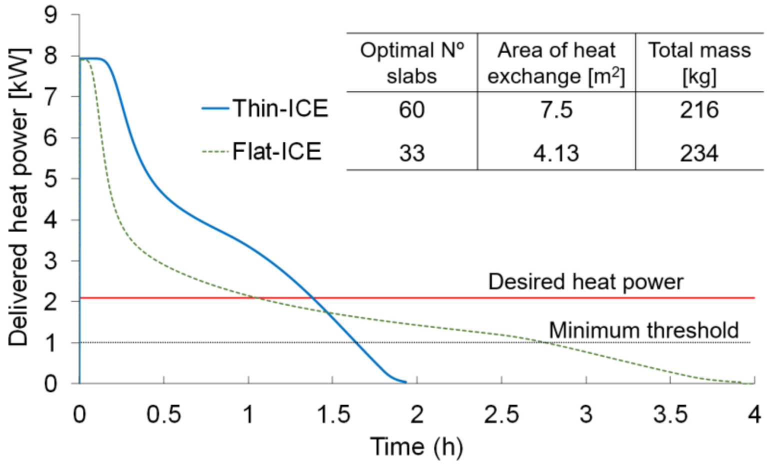

Figure 15: Delivered heat power of the optimal PCM tank configurations

With respect to the comparison between a 2D implicit vs 2D explicit model, the results showed (see Table 8) that it is not worth using an implicit scheme. The explicit model with the same amount of nodes as its implicit version reduced the computational time almost 10 times (428 vs 44 seconds) despite using a smaller time step, while keeping good results accuracy (mean average percentage error (MAPE) of 0.38 %). Furthermore, the accuracy of the model was more sensitive to a reduction in the number of nodes in the x-axis (HTF flow direction), that in the y- axis. It must be mentioned that the most time-consuming control volume was the one containing the PCM, especially during the phase change process.

Table 8: Accuracy and computational time of the different implicit and explicit scheme scenarios

Parameter	Implicit scheme				Explicit scheme			
Time-step (sec)	10	10	10	10	1	1	1	1
Nº nodes in x-axis	25	25	15	15	25	25	15	15
Nº nodes wall (y-axis)	4	3	4	3	4	3	4	3
Nº nodes PCM (y-axis)	9	7	9	7	9	7	9	7
MAPE(%)	Ref	0.08	1.45	1.37	0.38	0.44	1.07	1.00
Computing time (sec)	427.7	237.1	206.6	97.0	43.7	33.64	25.9	22.3

4.3 Contribution of the candidate

Alicia Crespo developed the numerical model, performed the optimization of the design variables, analysed, discussed the results, and prepared the manuscript. Alicia Crespo also collaborated in performing the experiments used to validate the numerical model.

4.4 Journal paper

The scientific contribution from this research work was published in the journal Energies in 2021.

Reference:

Crespo, A.; Zsembinszki, G.; Vérez, D.; Borri, E.; Fernández, C.; Cabeza, L.F.; de Gracia, A. Optimization of Design Variables of a Phase Change Material Storage Tank and Comparison of a 2D Implicit vs. 2D Explicit Model. Energies 2021, 14, 2605. https://doi.org/10.3390/ en14092605

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Optimization of Design Variables of a Phase Change Material Storage Tank and Comparison of a 2D Implicit vs. 2D Explicit Model

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Abstract: In this study, a thermal energy storage tank filled with commercial phase change material flat slabs is investigated. The tank provides heat at around 15 °C to the evaporator of a seasonal thermal energy storage system developed under the EU-funded project SWS-Heating. A 2D numerical model of the phase changed material storage tank based on the finite control volume approach was developed and validated with experimental data. Based on the validated model, an optimization was performed to identify the number, type and configuration of slabs. The final goal of the phase change material tank model is to be implemented into the whole generic heating system model. A trade-off between results' accuracy and computational time of the phase change material model is needed. Therefore, a comparison between a 2D implicit and 2D explicit scheme of the model was performed. The results showed that using an explicit scheme instead of an implicit scheme with a reasonable number of nodes (15 to 25) in the heat transfer fluid direction allowed a considerable decrease in the computational time (7 times for the best case) with only a slight reduction in the accuracy in terms on mean average percentage error (0.44%).

Keywords: phase change material; numerical model; design variables optimization; latent heat thermal energy storage; 2D implicit vs. 2D explicit model comparison

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Citation: Crespo, A.; Zsembinszki, G.; Vérez, D.; Borri, E.; Fernández, C.; Cabeza, L.F.; de Gracia, A. Optimization of Design Variables of a Phase Change Material Storage Tank and Comparison of a 2D Implicit vs. 2D Explicit Model. *Energies* **2021**, *14*, 2605. https://doi.org/10.3390/en14092605

Chapter V

5 Paper 2: Thermal performance assessment and control optimization of a solar-driven seasonal sorption storage system for residential application

5.1 Overview

Some sorption TES prototypes at pilot and large scale have been studied experimentally for heating purposes under specific boundary conditions [34,36–40]. The experimental testing of a large-scale sorption TES system subjected to real transient thermal demands of a residential building or the dynamics of climatic conditions is a very expensive and challenging task. Some authors already studied through numerical simulations the thermal performance of a SDSSTES system integrated into a building heating presenting successful results [43,45,47].

A seasonal sorption TES system requires a high-temperature heat source during the charging process, such as a solar field, and a LTHS during the discharging process. Such a complex energy system requires a carefully preliminary analysis to avoid overestimation of the STES size [42]. In addition to the system complexity, the seasonal sorption system is subjected to high thermal losses [41] which strongly depend on the weather conditions and can limit its operation and affect its performance indicators (COP, energy density). As Engel et al. [43] reported, the adjustment of the control strategy for each scenario, would improve the obtained results. Therefore, a deep study of the control of seasonal sorption TES systems is necessary to maximize its competitiveness against other energy systems, such as those based on fossil fuels. Nevertheless, according to the best author´s knowledge no study has reported a detailed control optimization of a seasonal sorption TES system integrated into a building heating system.

5.2 Contribution to the state-of-the-art

This study analysed, for the first time in literature, the impact of a detailed optimal control on the thermal performance of a SDSSTES system. The system, which was operated under an RBC policy, delivered DHW and SH to a single-family house located in Central Europe (Nuremberg). Validated numerical models and performance maps of the different components were used to simulate the energy system performance. The control parameters that defined the RBC strategy were optimized under two different scenarios: 1, Minimization of operational annual cost (minCosts) and 2, Maximization of the sorption TES use (maxSTES_use). The system could operate with 41 different operational modes depending on the season, solar irradiation, ambient temperature, thermal demand, and system state. As mentioned in section 3.5 the evaporator of the sorption TES was assisted by a PCM storage tank.

Figure 16 depicts the main system KPIs for both studied scenarios in absolute (vertical axis) and relative (horizontal axis) values. The maximum assumed absolute KPI (KPI_{max}) corresponds to: the full coverage with renewable energy for the solar fraction, the maximum capacity of the storage for the used capacity, and energy density at material level [23] for the energy density at system level.

The results indicated that the optimal economic scenario used just 89.6 % of the total capacity of the sorption TES system versus the 99 % used by the maxSTES_use scenario. Nevertheless, from a quantitative perspective, the annual economic difference between both scenarios could be neglected (441.7 vs 442.2 €). Optimizing the control based on operational costs allowed to reduce the size of the seasonal sorption system by almost 10 % obtaining the same annual operational cost. This fact can be explained because, during some periods of the year, when the weather conditions were not optimal (under the RBC strategy) to operate the sorption system, it was more cost-effective to use solar energy to directly charge the stratified water tank, rather than the STES. However, the greater the idle time between two consecutive charges or discharges, the higher the sensible heat required to reach again the sorption temperature, and therefore lower efficiencies of the sorption TES were achieved. Indeed, as Figure 17 and Figure 18 show, the ratio between useful charged heat of sorption versus required sensible heat is higher for the maxSTES_use scenario, which translates into higher COP.

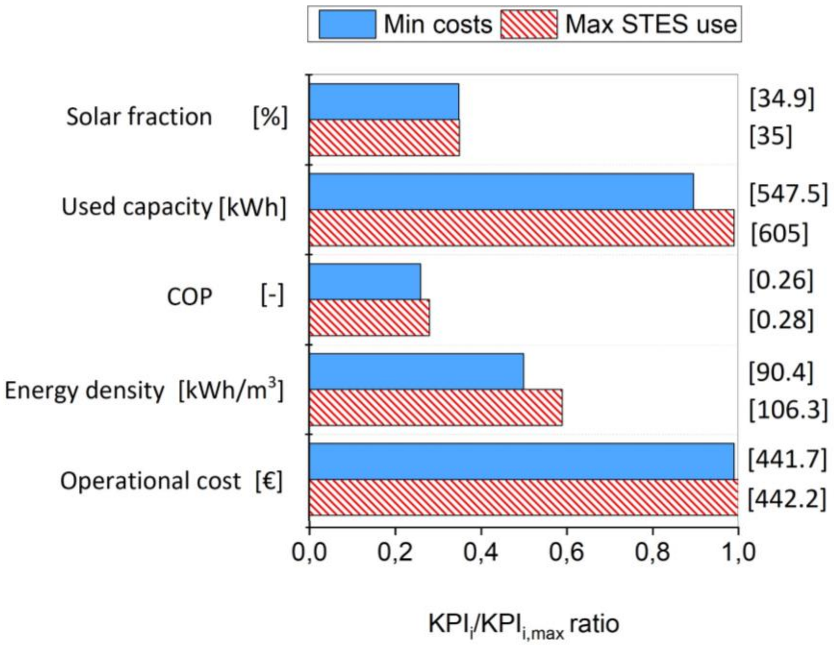
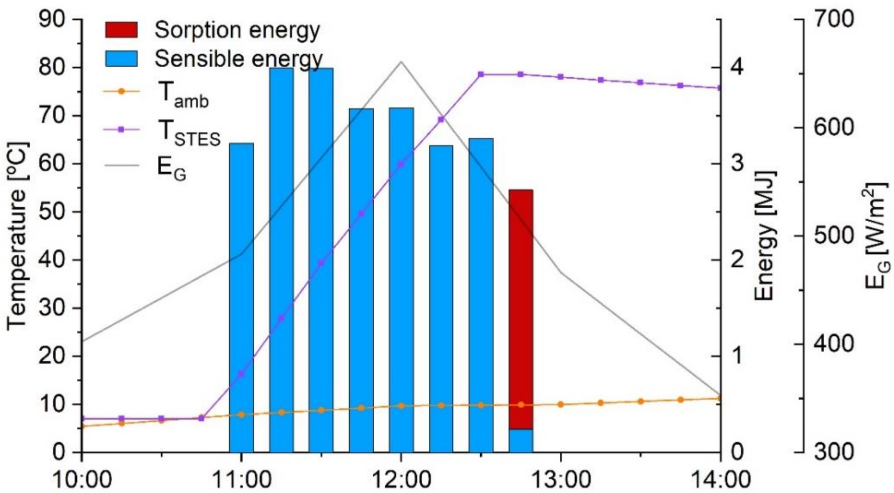


Figure 16: KPIs comparison between both optimal scenarios

One of the main conclusions of this study is that the control optimization of a SDSSTES system is a determining factor to reach a competitive technology level, defining the optimal size in future designs, and therefore maximizing its energy density.



(a) Min costs

Figure 17: Sensible and sorption heat of the sorption TES for the scenario ‘minCosts’ in a summer day

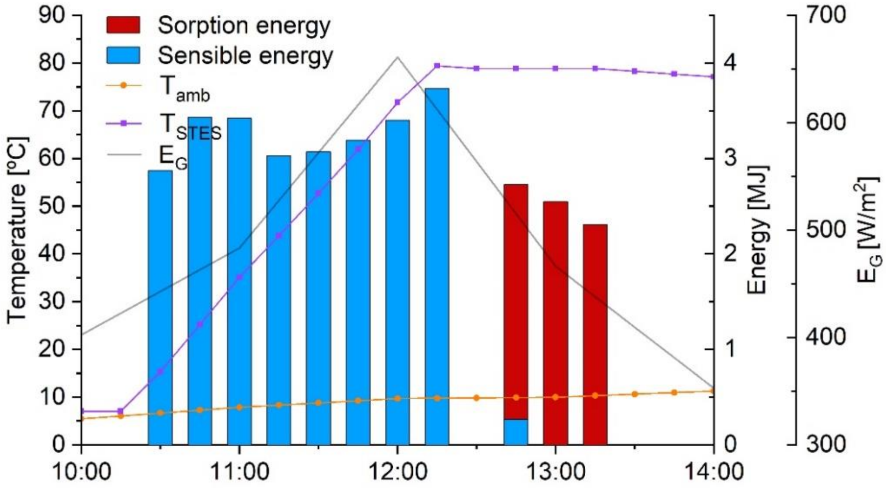


Figure 18: Sensible and sorption heat of the sorption TES for the scenario 'maxSTES_use' in a summer day

The system under study, composed of a solar field of 17.5 m^2 coupled with a sorption TES filled with 3.6 m^3 of SWS reached a solar fraction of 35 %, energy densities of 90.4 kWh/m^3 and COP of 0.26 when optimized according to the economic costs scenario. The obtained energy density was around half of the one reported by Frazzica et al. [23] at material level. This deviation is due to the sensible heat losses suffered during idle periods, the limitation of total capacity use for economic reasons and the lower efficiency when a sorption system is scaled up from laboratory to prototype or real scale (different system design). Moreover, the results also showed that using a latent heat storage tank as LTHS allowed to discharge the sorption TES system during winter with independence from the ambient temperature.

5.3 Contribution of the candidate

Alicia Crespo developed the numerical models of the system components, developed the whole system simulation, implemented the RBC strategy and performed the control optimization. Alicia Crespo analysed and discussed the results and prepared the manuscript. Alicia Crespo also collaborated in performing the experiments to validate the stratified water storage tank.

5.4 Journal paper

The scientific contribution from this research work was accepted by the journal Energy in September 2022.

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Thermal performance assessment and control optimization of a solar-driven seasonal sorption storage system for residential application

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A R T I C L E I N F O

Keywords:
Seasonal thermal energy storage
Control optimization
Numerical simulation
Sorbent water materials
Sorption storage

A B S T R A C T

The present paper analyzed the thermal performance and control optimization of a solar system based on seasonal sorption storage for domestic applications. The system control, which could choose between 41 operational modes, was optimized based on operational costs and maximization of sorption system use. The system was composed by 17.5 m^2 of evacuated tube collectors, 3.6 m^3 of composite sorbents based on lithium chloride and a stratified water tank. High efficiency of a sorption storage system was obtained when continuous charges or discharges occur, which, in this study, depended on weather conditions (ambient temperature and solar irradiation). The operational economic benefits were maximized using a sorption system with 9% less capacity and, therefore, less storage volume. The sorption thermal energy storage system obtained energy densities of 90 and 106 kWh/m^3. The whole system could supply 35% of the total thermal demand of a single family house in Nuremberg. The study concluded that the control optimization of a seasonal sorption system is a key factor to make the technology competitive, define its optimal size and, therefore, maximize its energy density in further designs.

Chapter VI

6 Paper 3: Optimal control of a solar-driven seasonal sorption thermal energy storage system through deep reinforcement learning

6.1 Overview

In the previous chapter, the seasonal system was operated with an optimized RBC strategy. An RBC strategy, although optimized, is not capable to take the optimal decision at every time step, as it has to follow previously defined rules. Thus, in recent years control techniques based on artificial intelligence are standing as promising alternatives to control HVAC systems. Many studies have already reported successful results using MPC to control HVAC systems as reviewed by [53,86], some of them especially focused on the control of TES systems [87]. Regardless of optimal or quasi-optimal solutions reached by MPC, its implementation in complex systems is challenging [58]. MPC formulations usually required linear and non-iterative models. However, to obtain adequate accuracy of the behaviour of the whole energy systems, 2D numerical models, iterative or non-linear processes are often required. Reinforcement learning is also a smart control technique, which is arising as feasible alternative to MPC in the field of HVAC systems management in buildings because of its successful results. Furthermore, RL accepts any type of numerical models, which is why it was chosen in the development of this PhD thesis. As previously mentioned, the energy system under study was composed of several components and more than 30 operational modes. This means, that the state-action vector of the system is too large to be stored in a Q-table and therefore, the RL model can fall into the curse of dimensionality. To tackle this issue, the DRL technique, which substitutes the Q-table with a neural network, was introduced by Mnih et al. [88]. The use of a neural network reduces considerably the learning time of the agent.

In recent years, some authors used DRL in the management of building energy systems, as reviewed by [89–91]. Nevertheless, according to the best author´s knowledge, just three studies applied DRL to control complex energy system coupled to TES systems, and none of them to a sorption TES. All the studies reached successful results, obtaining operational costs savings of 50 % [58], 11 % [92], and in a range from 40 to 84% [93]. The control of sorption TES systems adds an additional complexity in comparison with the rest of TES systems. The sorbent material must be at the required equilibrium to proceed with the charging or discharging process. The system must be optimally operated to reduce the idle periods between two consecutive charges or discharges, and in consequence, the thermal losses. The use of DRL to operate a seasonal sorption system may be able to maximize its performance under transient weather conditions and thermal demands.

6.2 Contribution to the state-of-the-art

This study analysed, for first time in literature, the potential of DRL as a control strategy of a sorption TES system. In particular, this study analysed the competitiveness of DRL to operate a SDSSTES system submitted to transient weather conditions and thermal demands. The system was analysed during the winter season, which corresponded with the discharge of the seasonal TES. The energy system goals to minimize the system operational costs (consumption of fossil fuels and electricity) by maintaining the user thermal comfort. The same numerical models and performance maps considered in the previous study were implemented to simulate the system, with the exception of the LTHS which was substituted by a water buffer tank.

The policy-gradient learning algorithm called REINFORCE [94] was implemented to train the DRL model. Two different DRL models were trained, one to operate the model when the sorption TES was charged (model_1) and, a second one (model_2) to operate the model when the sorption TES was empty. With these two models in mind, the DRL control could switch from model_1 to model_2 according to the state of charge of the sorption TES. As a training set, 18 random winter days of the years 2009, 2010, and 2019 were selected. Then, the learning progress was tested against 18 random winter days of the years 2011 and 2012. The validation of results was performed using the years from 2013 to 2016. Moreover, two different scenarios were explored: a set of 120 consecutive days and a set of 60 non-consecutive days. The 60-days scenario was studied for three different initial states of charge of the sorption TES: 100 %, 50 %, and 0 %.

To quantify the performance of DRL as a control strategy, the results were compared against an optimized RBC strategy. Table 9 presents the results of the performance of both control strategies. In a 60-days scenario starting with a sorption TES fully charged (model_1 was used), the DRL control reduced the operational costs of the system by 28.4 %. The smart control presented two main operational enhancements with respect to the RBC strategy: 1, better management of the thermal demand supply, which involved higher thermal user comfort and lower costs of penalty; 2, higher discharging efficiencies of the sorption TES, which involved discharging more useful sorption energy. In a 60-days scenario starting with a sorption TES fully discharged (model_2 was used), the performance of the smart control was slightly worse than the RBC strategy, because the DRL model did not learn the optimal management of the thermal demand supply identified by model_1. In consequence, the 60-days scenario starting with a SOC of the sorption TES at 50% reached energy savings of just 11.3%, because it combined model_1 and model_2: at the beginning model_1 was used. As soon as the sorption TES was fully discharged, model_2 started up.

In a 120 consecutive days scenario, which matched the four coldest months of the years, the costs savings of the smart control strategy reached 13.6%. The rapid discharge of the sorption TES during winter and the cost minimization using DRL as control strategy suggested that a bigger sorption storage size could be installed with respect to operational costs. In paper 2 (chapter V) was concluded that the sorption TES size could be reduced by 10 % keeping minimum operational costs. This contradiction is due to the fact that the RBC was not capable to foresee optimal actions at every time step, and therefore using 100 % of the STES storage capacity would have increased the operational costs. These results suggested that the optimal size of the sorption TES may vary based on the selected control strategy.

In conclusion, DRL has demonstrated to find complex rules of behaviour that cannot be foreseen in a RBC policy. DRL control strategy can be successfully used to operate a sorption TES and solar complex seasonal heating systems. Nevertheless, advanced programming skills are necessary to implement a DRL algorithm.

		Operational costs [€]								Average improvement [%]
		2013		2014		2015		2016		
Initial SoC [%]	Days	RBC	DRL	RBC	DRL	RBC	DRL	RBC	DRL	DRL vs RBC
100	120	618	560	462	394	489	428	551	489	13.6
100	60	348	289	272	200	330	261	287	222	28.4
50	60	350	318	273	239	332	298	287	262	11.3
0	60	361	363	288	396	343	346	301	308	-1.6

Table 9: Operational costs of the smart and RBC strategies

6.3 Contribution of the candidate

Alicia Crespo and Cèsar Fernández developed the DRL algorithm and performed its training, validation and testing. Alicia Crespo analysed and discussed the results, and prepared the manuscript.

6.4 Journal paper

The scientific contribution from this research work was submitted to the Journal of Applied Energy in September 2022.

Applied Energy

Optimal control of a solar-driven seasonal sorption storage system through deep reinforcement learning

--Manuscript Draft--

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	Daniel Gibert
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Abstract:	Deep reinforcement learning (DRL) has already been successfully used to control energy systems. Nevertheless, none of the studies used DRL to control seasonal sorption thermal energy storage (TES) systems, whose operation is different compared to other TES systems. This study analyzes the competitiveness of DRL to control during the winter season a seasonal sorption TES system driven by solar thermal collectors and compared it with a traditional optimized rule based control (RBC) strategy. The system, located in Central Europe, supplied domestic hot water (DHW) and space heating (SH) to a single-family house. Two DRL models were developed and trained to operate the system under two different sets of data: 120 winter consecutive days and 60 winter non-consecutive days. The results showed that the DRL control strategy reduced the system operational costs by 28% in a 60 winter days scenario. For a 120 winter days scenario, the operational cost savings decreased to 13% because the smart control performed worst once the sorption TES was fully discharged. These results were obtained for a validation data set of four years, which provides robustness to the results. Thus, DRL successfully controlled a solar-driven seasonal sorption TES system. Future work will consist of implementing the smart control strategy at prototype level to assess its performance.

Chapter VII

7 Paper 4: Optimizing the discharge process of seasonal sorption storage system by means of design and control approach

7.1 Overview

Papers 2 and 3, introduced in chapters V and VI, focused on analysing the benefits of optimal control over the thermal performance of a seasonal sorption system driven by evacuated tube collectors. Papers 4 and 5 focused on analysing the system thermal performance under different operational, design and climatologic conditions.

As previously discussed, sorption TES systems need a LTHS during discharge. A careful analysis of the availability of the LTHS must be considered since it directly impacts the sorption TES system performance. Indeed, the performance of an ammonia-based sorption TES highly depends on ambient temperature, especially during cold winter. The low freezing point of ammonia allows the use of temperature air as an environmental heat source for the evaporator. Nevertheless, low ambient temperatures lead to a decrease in the heat output temperature [50]. Hence, several authors have studied solutions to tackle this issue obtaining successful results [50,95–97].

Water-based sorption TES systems present several advantages over ammonia-based systems: they are non-toxic, suitable for floor SH temperatures and they can achieve higher energy storage density compared to the ammonia-based systems thanks to the higher evaporation enthalpy of water. Nevertheless, they require heat at the evaporator at temperatures above 0ºC, which hinders the profit of ambient temperature as a heat source during cold winter days and pushes to explore for alternative heat sources. As is the case with ammonia-based systems, a deep analysis of the availability and influence of the heat source in water-based sorption TES during cold conditions must be carried out. Indeed, Frazzica et al. [42] highlighted the influence of ambient heat source/sink and Crespo et al. [98] concluded that further research on the outlet temperature of the LTHS of a water-based sorption TES must be performed. Most of the studies of water-based sorption TES systems [99–103] focused on experimental analysis at component level (lab or prototype scale) under defined boundary conditions (e.g. summer or winter temperatures) using representative testing cycles of hours or days. A study that analyses different solutions to enhance the discharging process of a water-based sorption TES subjected to transient annual weather conditions and thermal demands is missing in the literature. Moreover, this study steps forward in comparison with previous studies by optimizing the control strategy for every scenario to avoid the overestimation of the sorption storage volume.

7.2 Contribution to the state-of-the-art

In this chapter, several solutions are proposed to increase the discharging efficiency, and therefore the competitiveness, of a SDSSTES system based on LiCl/silicagel and water vapour. For that purpose, based on annual simulations and, different LTHS and different discharging temperature set points of the sorption modules were explored. The seasonal system was coupled to a dwelling heating system that supplied DHW and SH and operated always under optimized RBC policy. Annual analysis of a seasonal system allows to observe the system dynamics throughout the year, the operational limitations due to weather conditions, and the impact that solar energy stored in summer has during the cold season.

Five different scenarios that combined different LTHS to assist the evaporator and different set-points to discharge the sorption modules were evaluated. With regard to the LTHS the system can choose between two scenarios: 1, Operating just the buffer water tank, 2, Operating the dry heater during mild days or the buffer water tank during cold winter days. The main results found out in this study were:

- The water-based sorption TES system obtained a COP and an energy density of 19 % and 22 % higher using a water tank as LTHS instead of a latent TES tank.
- Higher discharging efficiency, and accordingly also energy density and COP, were obtained when a constant and conservative (35ºC) temperature set point of the stratified tank to discharge the sorption TES was set, in spite of requiring higher sensible heat to reach that temperature. Interrupting the discharge of the sorption TES when the stratified tank reaches the minimum temperature defined by the SH set point (i.e 32 ºC) caused more interruptions during the discharge throughout the winter and therefore more heat losses.

- The integration of a dry-heater to assist the evaporator during winter mild days in a continental climate of central Europe was not justified due to its limited operating hours.
- The optimal scenario of a SDSSTES system composed of 20 modules of LiCl/silica gel supplied 37.4 % of the DHW and SH demand of a nearly zero emissions (NZE) single-family house located in Nuremberg (Germany). An energy density of 106 kWh/m^3 and a COP of 0.3 were obtained.
- The availability of an infinite LTHS would allow reaching a COP and an energy density of the sorption TES of 0.39 and 139 kWh/m^3 respectively, 24 and 23 % higher compared to the best-case scenario. The integration of the sorption TES system into a dwelling that could receive constant and free heat (i.e. waste heat from a nearby factory or geothermal heat) would significantly enhance its competitiveness. Definitely, the COP of the sorption heat storage is limited by the LTHS, which in this study depends on the winter solar heat.

7.3 Contribution of the candidate

Alicia Crespo used the numerical models and system simulation developed in the previous paper. New numerical models (water buffer tank, dry-heater) were developed and implemented in the existing system simulation. The corresponding operational modes of the new components were implemented in the code and tested. The simulations and control optimization of the different system scenarios were driven by Alicia Crespo. She also analysed and discussed the results and prepared the manuscript.

7.4 Journal paper

The scientific contribution from this research work was submitted to the Journal of Energy Storage in September 2022.

Journal of Energy Storage

Optimizing the discharge process of a seasonal sorption storage system by means of design and control approach

--Manuscript Draft--

Manuscript Number:	
Article Type:	Research Paper
Keywords:	seasonal thermal energy storage; sorption thermal energy storage; simulations; solar thermal energy; performance optimization
Corresponding Author:	Alvaro de Gracia SPAIN
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	Andrea Frazzica
	Cesar Fernandez
	Alvaro de Gracia
Abstract:	Sorption thermal energy storage systems have higher energy densities and low long-term thermal losses compared to traditional energy storage technologies, which makes them very attractive for seasonal heat storage application. Although they have a lot of potential at material level, its operation and system implementation for residential application requires further study. The performance of a seasonal sorption thermal energy storage system strongly depends on the discharging process during the cold season. The present study analysed through numerical simulations different scenarios to enhance the thermal performance of a solar-driven seasonal water-based sorption storage, which supplied space heating and domestic hot water to a single-family house in a cold climate region. All studied scenarios were analysed under optimal control policy. The results indicated that the sorption storage could increase by 9 % its energy density if its discharge happens when the temperature at the stratified water tank is below a conservative and constant temperature set point, due to fewer interruptions during the discharge. The energy density of the sorption storage driven by solar energy was highly impacted by the weather conditions, and by the type and availability of low-temperature heat source. Using a heat storage to assist the evaporator of the sorption storage based on water instead of phase change materials increased the energy density by 22 %. Nevertheless, the use of a dry-heater to profit environmental heat to assist the evaporator was not suitable for the climate studied due to the low hours of operation. The sorption storage system composed of 20 modules of LiCl-silica gel could obtain an energy density and a COP of 139 kWh/m 3 and 0.39, respectively, if a constant low-temperature heat source (i.e, geothermal or waste energy) was available.

Chapter VIII

8 Paper 5: Solar-driven water-based sorption system for seasonal heat storage under optimal control: study for different climatic zones

8.1 Overview

In the previous chapters, the thermal performance of a SDSSTES system was studied for one location in Central Europe. As already mentioned, sorption TES systems are subjected to significant sensible thermal losses [41] and their performance depends on the dynamics of climatic conditions [44] and thermal demands of a specific location. Hence, to fully understand its behaviour and push the technology to a commercial level, the system must be analysed under different climatic conditions.

Some studies [43,44,104] already analysed the potential of sorption seasonal storage systems under different climatic conditions. Among them, Engel et al. [43], reported that adjusting the control strategy for each location could have avoided oversizing the system for some locations. Regardless of its relevance, is still missing in the literature an assessment of a seasonal sorption system operated in different climatic zones by means of an optimal control.

8.2 Contribution to the state-of-the-art

In this chapter, a water-based sorption system for seasonal heat storage driven by solar energy was studied for three European climates represented by Paris, Munich, and Stockholm. Three representative European cities were selected as exemplified in the reference framework of the IEA [105]. Optimal control in terms of operation cost minimization was performed for each location optimizing the thresholds of the used RBC as described in Section 3.6. The same nearly zero emissions building (NZEB) was considered for the three different analysed climates. The thermal demands were generated in EnergyPlus for each location using average weather data for the period 1991-2010.
As concluded in chapter VII (paper four), the use of a water tank as LTHS of the sorption TES increased its COP by 19 % in comparison with the use of a PCM storage tank. Thus,

was a water buffer tank was selected as the LTHS to assist the evaporator of the sorption TES during winter days. Moreover, due to the higher ambient temperatures in Paris compared to Munich and Stockholm, the system located in Paris could also operate a dry heater when the ambient temperatures were around 15 ºC. The implementation of the dry heater in Munich and Stockholm was discarded due to the limited operating hours.

The optimizer found for each location the control parameters at which all the energy stored in the seasonal storage during summer could be discharged by the end of the winter period. In this way, the sorption TES efficiency was maximized, and oversizing for future designs was avoided. Under this premise, the seasonal system composed of 17.5 m^2 of evacuated tube collectors and 3.6 m^3 of LiCl/Silicagel reached solar fractions of 44.5, 40.8, and 27 % for a single-family house located in Paris, Munich, and Stockholm, respectively.

The energy density, COP, and temperature effectiveness for the three studied climates are shown in Figure 19. The highest energy density was obtained for Paris thanks to the use of a dry heater which prolonged its operation during mild winter days. As mentioned, the dry heater was suitable for Atlantic climates (Paris), but not for Continental and Boreal climates, due to the low winter ambient temperatures which caused limited availability of this system to be used as LTHS. Stockholm was the location with the highest thermal demand, which could lead to the idea that maximum sorption TES capacity could be profited. Nevertheless, the optimal size for Stockholm according to the operational optimization was 76 % of its full capacity. This fact can be explained by the low solar availability during winter to charge the LTHS. Nevertheless, Stockholm reached the highest COP, thanks to its higher charging efficiency in the summer. With respect to temperature effectiveness, the system obtained average temperature effectiveness of 0.35, which means that relatively low regeneration temperature was required by the sorption system (i.e., below 100 ºC). On the other hand, another study [39] reviewed by Fumey et.al [26] obtained a TE of 0.15, which means that a higher regeneration temperature (around 150 ºC) was required. Regeneration temperatures above 100 ºC call for the need for high effective or concentrated solar collectors and may cause higher thermal losses to the ambient.

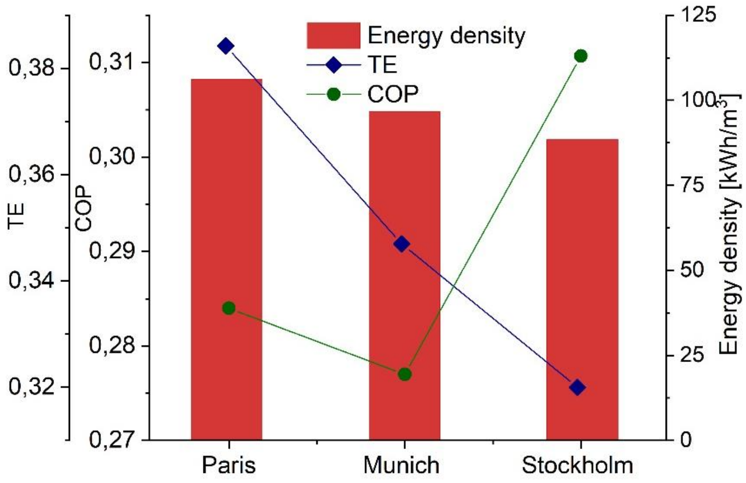

Figure 19: Key performance indicators of the sorption TES system for the different cities

Solar heat could be used to charge or discharge the seasonal sorption TES in summer or winter, respectively, or to charge the stratified water tank. According to the designed RBC strategy, the weather conditions, and the thermal demand, during some periods charging or discharging the sorption TES was not cost-effective due to the high number of idle periods between two consecutive charges or discharges. During those periods, charging the stratified water with solar heat was more efficient. For this reason, in the three locations, the maximum used capacity was limited by the optimal system operation, which aimed to minimize the operational costs. The identification of the optimal storage capacity allowed to avoid oversizing in future designs, and therefore increase the energy density. For instance, the energy density in Stockholm could be increased from 88.5 to 116.5 kWh/m^3 by reducing the storage size while maintaining optimal operational annual costs of the whole system.

The sorption TES system operated at minimum ambient temperatures of -11 and -15 ºC in continental and boreal climates (Munich and Stockholm, respectively), showing independence from ambient temperature during its discharge thanks to the use of low enthalpy solar heat to assist the evaporator.

8.3 Contribution of the candidate

Alicia Crespo generated the space heating demands for each location in EnergyPlus. Alicia Crespo performed the simulation and control optimization of the different climatic zones, analysed and discussed the results, and prepared the manuscript.

8.4 Journal paper

The scientific contribution from this research work was published in the journal Energies in 2022.

Reference:

Crespo, A.; Fernández, C.; de Gracia, A.; Frazzica, A. Solar-Driven Sorption System for Seasonal Heat Storage under Optimal Control: Study for Different Climatic Zones, Energies 2022, 15, 5604; https://doi.org/10.3390/en15155604.

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Article

Solar-Driven Sorption System for Seasonal Heat Storage under Optimal Control: Study for Different Climatic Zones

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Abstract: Solar thermal energy coupled to a seasonal sorption storage system stands as an alternative to fossil fuels to supply residential thermal energy demand in climates where solar energy availability is high in summer and low in winter, matching with a high space heating demand. Sorption storage systems usually have a high dependency on weather conditions (ambient temperature and solar irradiation). Therefore, in this study, the technical performance of a solar-driven seasonal sorption storage system, using an innovative composite sorbent and water as working fluid, was studied under three European climates, represented by: Paris, Munich, and Stockholm. All scenarios analyses were simulation-based under optimal system control, which allowed to maximize the system competitiveness by minimizing the system operational costs. The optimal scenarios profit from just 91, 82 and 76% of the total sorption system capacity, for Paris, Munich, and Stockholm, respectively. That means that an optimal control can identify the optimal sorption storage size for each location and avoid oversizing in future systems, which furthermore involves higher investment costs. The best coefficient of performance was obtained for Stockholm (0.31), despite having the coldest climate. The sorption system was able to work at minimum temperatures of −15 °C, showing independence from ambient temperature during its discharge. In conclusion, a seasonal sorption system based on selective water materials is suitable to be integrated into a single-family house in climates of central and northern Europe as long as an optimal control based on weather conditions, thermal demand, and system state is considered.

Keywords: water-based sorption storage; seasonal storage; simulations; control optimization; climatic zones

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Citation: Crespo, A.; Fernández, C.; de Gracia, A.; Frazzica, A. Solar-Driven Sorption System for Seasonal Heat Storage under Optimal Control: Study for Different Climatic Zones. *Energies* **2022**, *15*, 5604. https://doi.org/10.3390/en15155604

Chapter IX

9 Global discussion of results

With the objective of achieving a zero emissions buildings (ZEB) scenario by 2050, a seasonal sorption TES composed by a composite material and driven by solar thermal collectors was proposed in this PhD thesis (see Figure 20). The nature of that system implies highly dependency on ambient temperature and solar irradiation. The sizing and operation of a seasonal sorption system is not a straightforward task as to maximize the system efficiency, all the energy stored in summer, must be usefully discharged in winter in spite of the unfavourable weather conditions. This fact calls for the need for a detailed optimal control that adapts to the variability of annual weather conditions and thermal loads. Nevertheless, according to the state of the art, no author studied a seasonal sorption system under detailed optimal control. Among the different specific objectives of this PhD thesis, the main goal consisted of analysing and enhancing the performance of a SDSSTES system by means of different optimized control strategies and system designs.

Optimizing the control or system parameters of an energy system with several components requires a significant computational effort. Hence, the simulation time of each component plays a relevant role. In the first study of this thesis, two 2D numerical models (one explicit and one implicit) of the PCM tank (used as the LTHS by the seasonal energy storage system) were developed, validated, and compared. The results indicated that the explicit approach allowed to obtain good results accuracy with computational time 4 to 10 times less (depending on the number of nodes). Therefore, for further studies, there is no need to develop a numerical model with an implicit scheme as long as the explicit one has a suitable ratio between model nodes and the simulation time step for the model to converge. Indeed, the 1D numerical model used to simulate the thermal performance of the stratified water tank in papers two to five was implemented using an explicit approach. Furthermore, paper three analysed the impact of the number of nodes (33 vs 9) of the stratified water tank on the training process of the agent (DRL) and the operational costs of the system. The agent learnt a near-optimal control policy using only 9 nodes (which required muss less learning time) in the stratified water tank: the results showed a deviation of 1.9 % in the system operational costs, for the period of four months.

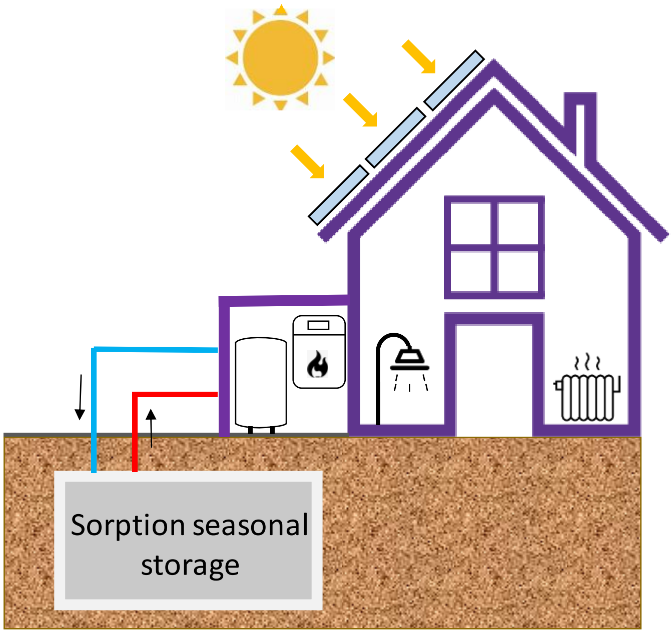

Figure 20: System under study integrated into a building.

The second study, consisted of analysing the performance of a SDSSTES system under a detailed optimized RBC strategy. The optimal scenario minimized the annual operational costs using nearly 10% less storage capacity, which translates to less storage size in future designs, and in consequence less investment cost and higher energy densities. This means that, the control strategy of a seasonal sorption system is a key factor to define the optimal system size.

With regard to smart control strategies, paper three analysed for first the time in the literature the impact of DRL on the performance of a SDSSTES system. The results showed robustly that DRL is the best control strategy to operate a SDSSTES system during winter. Bearing in mind that the system model contained some complexities, such as, iterative process, other smart control strategies such as MPC cannot be applied to this case study. Moreover, even though the sorption system on paper two was only studied for the winter period, the results suggested that the optimal size of the system based on operational costs may vary depending on the selected control strategy. In papers two, four, and five, the minimum operational costs were obtained with a lower volume of the sorption TES. The RBC strategy, although optimized, was not able to operate the system in an optimal global scenario. On the other hand, the control strategy based on DRL operated the system under un near-optimal global scenario, which could entail (under a scenario, in which the whole year is analysed) that a bigger sorption TES may be profitable.

The forth study, concluded that the performance of the seasonal sorption TES was highly impacted by the type and availability of LTHS. Indeed, the use of an ideal infinite LTHS, such as nearby industrial waste heat or geothermal energy, would allow reaching energy densities of the seasonal sorption TES of 139 kWh/m^3: 23% higher compared to the optimal scenario (discharge temperature set-point: constant, LTHS: water tank) submitted to an intermittent LTHS availability. These results indicated that the performance of a sorption TES system prototype measured under constant heat sources (usually in a laboratory) could not be fairly compared against studies that analysed the system submitted to transient weather conditions and thermal demands. Indeed, the comparison between seasonal sorption systems is a complex task, since the boundary conditions may be different between studies.

In paper 5, the system was studied under three representative climates: Paris (Atlantic), Munich (Continental), and Stockholm (Boreal). In line with papers 2 and 4, the parameters of the RBC strategy were optimized for every scenario. As expected, the optimal control parameters identified the maximum required capacity at each location. The seasonal system composed by a solar field of 17.5 m^2 and 3.6 m^3 of LiCl/Silica-gel reduced 45, 41, and 27 % the required energy and CO_2 emissions, for Paris, Munich and Stockholm, respectively.

Even though, the low ambient temperatures during winter made it impossible to use environmental heat in Stockholm and Munich, the use of a LTHS charged by solar heat, allowed to operate the water-based sorption TES at minimum ambient temperatures of -15 and - 11^o C, respectively. On the other hand, the sorption system located in Paris reached the highest system energy density thanks to the dry heater and the relatively high temperatures during mild days. Paper five demonstrated that a water-based sorption TES can successfully operate in North Europe without the need of a geothermal installation, which would increase the investment costs of the system.

Table 10 presents the solar fraction (SF), COP, discharging efficiency ($\eta_{DIS,STES}$), and energy density achieved in the different papers that composed this PhD thesis. Starting from an energy density of 90 kWh/m^3 (considering the original sorption TES size), the sorption TES achieved a maximum energy density of 106 kWh/m^3 thanks to the proposed enhancements. Besides, if the optimal size were considered, the energy density of the sorption TES could reach average values of 117 kWh/m^3, which represents 65 % of the energy density reported at material level [23]. Some authors also reported the performance of seasonal sorption TES systems submitted to transient and discontinuous heat sources and sinks throughout the year (simulated-based). For example, Engel et al. [17] reported the energy densities of a seasonal sorption system located in Stockholm, the values ranged from 156 to 177 kWh/m^3 using 6 m^3 of zeolite and 36 m^2 of solar collectors. Indeed, it has to be pointed out that the system presented by [17] was based on zeolite 13X, using a much higher regeneration temperature (i.e. above 150 °C), requiring either concentrated solar thermal collectors or power-to-heat process to be efficiently charged. Moreover, starting from similar energy densities, temperature effectiveness plays a fundamental role to analyse the competitiveness of sorption TES systems. The temperature effectiveness of a sorption TES system with regeneration temperatures above 150 ºC is lower, which means that a higher temperature difference between the reaction and the condenser is required to charge the system. Jiang et al. [95] presented reasonable results of a hybrid compression-assisted sorption TES operated in severe cold regions (ambient temperature up to 30 ºC). However, the sorbate material of that study was ammonia, which may be avoided in residential applications. Other studies reported full demand coverage [44,45] or higher solar fractions [47]. However, those values may be overestimated or obtained with a larger surface of solar collectors or larger sorbent material. The energy densities reported throughout this PhD thesis were obtained using the volume of the material. If the energy densities would have been calculated in a volumetric basis (considering the volume of the adsorber), the values would have resulted lower. Comparing the results with a water stratified tank, the latter has an energy density of 93 kWh/m^3 assuming a temperature lift of 80 ºK (95-15 ºC). Moreover, this energy density would be reduced because of the thermal losses especially during the long-term seasonal storage period. This fact proves the benefits of sorption TES versus sensible storage systems.

The results obtained in this PhD thesis indicated that a seasonal sorption TES filled by LiCl/Silica gel and driven by solar energy is a suitable energy system to supply the thermal needs of a single-family house from a technical and operational costs point of view, as long as it optimally operated and contains the suitable LTHS. Nevertheless, further research must be carried out to push the technology at commercial level. The increase of penalties for emitting greenhouse emissions can favour the development of the technology.

Table 10: Evolution of some KPIs along papers 2 to 5

Paper	Location	LTHS	Control	SF [%]	COP [-]	e_d [kWh/m^3]	e_d* [kWh/m^3]	$\eta_{DIS,STES}$ [%]
2	Nuremberg	PCM tank	RBC	35	0.26	90	101	61
3	Nuremberg	WT	DRL	-	-	-	-	76
4	Nuremberg	WT	RBC	37	0.3	106	114	68
5	Paris	WT + dry heater	RBC	45	0.28	106	117	69
5	Munich	WT	RBC	41	0.27	97	118	70
5	Stockholm	WT	RBC	27	0.31	89	116	69

*: optimal sorption storage size. WT: water buffer tank

Finally, throughout the five simulation studies included in this PhD thesis, crucial knowledge has been provided on the optimal operation and performance analysis of a SDSSTES system integrated into a NZEB heating system. The main contributions of this PhD thesis are:

- The assessment of different approaches for solving 2D numerical models to reach a trade-off between results accuracy and computational time.
- The potential analysis of a seasonal sorption system driven by solar collectors operated under optimized RBC strategies and submitted to different weather conditions and thermal demands, and different European climates.
- The design and testing of a DRL tool implemented to optimize the control of a seasonal TES driven by solar collectors. The smart control policy was compared against an optimized RBC strategy.
- A detailed assessment of the influence of different factors on the discharge efficiency of a sorption TES system.

Chapter 10

10 Final conclusions and future work

10.1 Conclusions

The main objective of this PhD thesis is to analyse and increase the performance of a solar-driven seasonal sorption TES system submitted to transient weather conditions through optimal operation and system design, to reach a competitive level of the sorption technology based on a composite sorbent material. For this purpose, numerical models of the different system components were developed and validated. Moreover, different optimal control strategies were implemented, explored, and compared. The system was analysed under different designs and climatic conditions. The specific findings of this PhD thesis are the following:

- Explicit 2D models of the analysed PCM storage tank were accurate enough and computationally lighter compared to implicit ones as long as the right time step was selected.
- To maximize the efficiency of a seasonal sorption TES system coupled to solar thermal collectors, the control parameters must be optimized for each climatic location based on climatic conditions, thermal demand and system state.
- The weather conditions and the type of LTHS highly impact on the thermal performance of a seasonal sorption TES and must be analysed in detail. Indeed, the COP of the sorption TES system could be increased by 24 % using a continuous LTHS.
- An optimized RBC strategy allowed to minimize the operational costs with a lower volume of the sorption TES, which would reduce the capital costs.
- DRL demonstrated to be a better control strategy to manage seasonal sorption TES systems compared to an optimized RBC strategy. Nevertheless, it required extensive knowledge in programming and long training phase (computational effort).
- The optimal size of the sorption TES submitted to transient weather conditions may vary based on the selected control strategy in terms of operational costs.

Increasing the size of the sorption TES based on operational costs calls for the need to analyse the capital costs of the system.

- A seasonal system composed of 17.5 m^2 of evacuated tube collectors and 3.6 m^3 of LiCl/Silicagel reduced 41% the natural gas consumption and CO_2 emissions of a NZEB single-family house in Central Europe (Munich), in an optimal scenario. The implementation of a seasonal water-based sorption TES filled by LiCl/Silicagel and driven by solar collectors is technically feasible in Atlantic, Continental, and Boreal climates in spite of the low winter ambient temperatures.
- The optimally sized seasonal sorption TES operated with an optimized RBC strategy under real transient weather conditions could reach an energy density of 117 kWh/m^3, which corresponds to 65% of the value reported at material level (180 kWh/m^3).
- Even though, the findings of this PhD thesis have contributed to improve the performance of a seasonal sorption TES, they have not positioned yet the technology to a commercial level. Further studies must keep going at material, system, and operational level.

10.2 Future work

Regardless of the detailed analysis performance of the seasonal system under study, further research tasks can be assessed. According to the simulation results, the energy density of the seasonal sorption TES could be increased up to 139 kWh/m^3 if a continuous LTHS was available. In a future study, the implementation in the system simulation of a geothermal heat source to work as LTHS for the evaporator in cold climates will be assessed.

Throughout this PhD thesis, a technical analysis of the seasonal system has been performed. A techno-economic analysis of the system has been ignored due to the initial research stage of sorption TES prototypes, which makes it difficult to obtain reliable and realistic costs, which can damage the spread of the technology. Some companies manufacture tailor-made sorption TES prototypes, so their costs are much higher compared to the final price once the technology would be in a more mature commercial stage. Once the manufacturing costs are at a reasonable stage, a techno-economic analysis of the technology must be carried out.

The competitiveness of DRL as a control strategy to optimally operate sorption TES systems has been proved. Nevertheless, the training strategy of the smart control was always focused in a short range (few days) horizon. This fact avoided the agent to learn long-term strategies throughout the year to optimally take decisions over the STES charge/discharge during a season. More effort can be done in this direction in order to employ neural network architectures able to cope with such a long range dependency, involving larger training times and computing resources.

Lastly, the system and its corresponding controller should be implemented at a prototype or real scale in a building.

Other research activities

Other journal publications

The PhD candidate carried out other scientific research besides the one presented in this thesis during the execution of his PhD. The resulting publications are listed below:

1. **A. Crespo**, I. Muñoz, W. Platzer, M. Ibarra, A, Integration enhancements of a solar parabolic trough system in a Chilean juice industry: Methodology and case study, Solar Energy 224 (2021), 593-606. https://doi.org/10.1016/j.solener.2021.03.041.
2. D. Vérez, E. Borri, **A. Crespo**, B.D. Mselle, A. de Gracia, G. Zsembinski, L.F. Cabeza**,** Experimental study on two pcm macro-encapsulation designs in a thermal energy storage tank, Applied Sciences (Switzerland) 11 (2021) 6171. https://doi.org/10.3390/app11136171.
3. D. Vérez, E. Borri, **A. Crespo**, G. Zsembinski, B. Dawoud, L.F. Cabeza**,** Experimental study of a small-size vacuum insulated water tank for building applications, Sustainability 13 (2021), p.5329-1-5329-11. https://doi.org/10.3390/su13105329.
4. A. de Gracia, J. Tarragona, **A. Crespo**, C. Fernández, Smart control of dynamic phase change material wall system, Applied Energy 279 (2020), 115807. https://doi.org/10.1016/j.apenergy.2020.115807.

Book chapter participation

- A. de Gracia**, A. Crespo,** D. Vérez, J. Tarragona, L.F. Cabeza, Encyclopedia of Energy Storage, Control Solutions for TES Applications, Elsevier 579-583 (2022), ISBN 9780128197301. https://doi.org/10.1016/B978-0-12-819723-3.00028-7.

Contributions to international conferences

The PhD candidate contributed to different international conferences:

1. **A. Crespo,** V. Palomba, M. Mikhaeil, B. Dawoud, A. de Gracia, L.F. Cabeza, A. Frazzica, Experimental study of a LiCl/Silica gel sorption thermal energy storage prototype. CNIT 2022 - XII National and III International Conference on Engineering Thermodynamics (Madrid -Spain). Oral presentation. Published in Proceedings Books. ISBN: 978-84-09-42477-1.
2. A. de Gracia, **A. Crespo**, C. Fernández, Comparison of strategies to control a movable wall with PCM. CNIT 2022 - XII National and III International Conference on Engineering Thermodynamics (Madrid -Spain). Poster presentation.
3. **A. Crespo,** A. de Gracia, D. Vérez, L.F. Cabeza, C. Fernández, Use of reinforcement learning to optimize the control of solar thermal collectors coupled to seasonal thermal energy storage, EnerSTOCK 2021, 15th International virtual conference on Energy Storage, Ljubljana (Slovenia), 2021. Poster presentation.
4. D. Vérez, E. Borri, **A. Crespo**, B.D. Mselle, A. de Gracia, G. Zsembinszki, L.F. Cabeza, Methods for the determination of the state-of-charge of a thermal energy storage device, EnerSTOCK 2021 - 15th International Virtual Conference on Energy Storage, University of Ljubljana, Ljubljana, Slovenia, 2021.
5. D. Vérez, E. Borri, **A. Crespo**, B.D. Mselle, A. de Gracia, G. Zsembinszki, L.F. Cabeza, Experimental study on the effect of flat and thin slab encapsulation design on a PCM tank, EnerSTOCK 2021 - 15th International Virtual Conference on Energy Storage, University of Ljubljana, Ljubljana, Slovenia, 2021.

Scientific reports

The PhD candidate also contributed to scientific reports in the framework of SWS-Heating H2020 European project:

1. Main contributors: C. Klearchos, N. Chalikakis, D. Chalikaki, E. Borri, D. Veréz, A. Crespo, A. de Gracia, C. Fernández, L.F. Cabeza. Additional contributors: A. Leontaritis, S.Varvagiannis. Deliverable 5.2 - Report on “Development and testing of a smart control environment”. May 2021. Project title: “Development and Validation

of an Innovative Solar Compact Selective-Water-Sorbent-Based Heating System". Project Acronym: SWS-Heating. Project of Horizon 2020.

2. Main contributors: E. Borri, A. Crespo, J. Argelich, A.de Gracia, C. Fernández, L.F. Cabeza. Additional contributors: S. Karellas, A. Charalampidis, A. Frazzica, V. Palomba, M. Weitzer, L.Franke. Deliverable 3.2 – Report on "Optimised system control and strategies", April 2021. Project title: Solar-Biomass Reversible energy system for covering a large share of energy needs in buildings. Project acronym: SolBio-Rev. Project of Horizon 2020.

Contributions to seminars and workshops

1. European Researchers' Night 2021. Poster "Control inteligente en sistemas de almacenamiento térmico estacional" in the "La nostra recerca" section.
2. European Researchers' Night 2021. Workhsop "El viatge de l'energia, des del Sol fins a la teva dutxa".
3. RIbERA, Virtual seminar "I Webinar de la red iberoamericana de investigación de las energías renovables y cuidado del medio ambiente".
4. RedTES, Virtual seminar "El papel del almacenamiento de energía térmica en la transición energética en España".

Scientific foreign-exchange

The PhD candidate did one stay abroad during the development of this PhD thesis.

The research stay done by the candidate was carried out at the Italian National Research Council (CNR) - Instituto di Tecnologie Avanzate per l'Energia (ITAE). The exchange was sponsored by the FI-SDUR grant from the AGAUR and the Erasmus+ grant. During the research stay, the candidate performed experiments with a sorption module based on composite sorbents and employing water as working fluid. System variables such as the maximum and average thermal storage power (kW) of the module or its energy density (kWh / m^3) were measured. As a result of this stay, a conference paper was published (Proceedings).

Other activities

Projects participation

- Methodology for analysis of thermal energy storage technologies towards a circular economy (MATCE). Ministerio de Ciencia, Innovación y Universidades de España, RTI2018-093849-B-C31 - MCIU/AEI/FEDER, UE, 2019-2022.
- Red Española en Almacenamiento de Energía Térmica (RED-TES). Ministerio de Ciencia, Innovación y Universidades de España, RED2018-102431-T, 2020-2022.
- GREiA. Grup de Recerca en Energia i Intel·ligència Artificial (SGR). Generalitat de Catalunya, 2017 SGR 1537, 2017-2021.
- Innovative Microsolar Heat and Power Systems for Domestic and Small Business Buildings compact hybrid storage systems for low energy buildings (INNOVA MICROSOLAR). European Union's Horizon 2020 research and innovation programme under grant agreement n° 723596, 2016-2022.
- Development and Validation of an Innovative Solar Compact Selective-Water-Sorbent-Based Heating System (SWS-HEATING). European Union's Horizon 2020 research and innovation programme under grant agreement n° 764025, 2018-2023.
- Solar-Biomass Reversible energy system for covering a large share of energy needs in buildings (SolBio-Rev). European Union's Horizon 2020 research and innovation programme under grant agreement n° 814945, 2019-2023.

Teaching

- Fluid mechanics: 3 ECTS during the academic year 2021/2022.
- Energy storage: 0.5 ECTS during the academic year 2021/2022.
- Fluid mechanics: 3.5 ECTS during the academic year 2022/2023.

Organizing committee participation

- Researcher´s Night 2020, 15th edition 2020. Lleida, Spain.
- Researcher´s Night 2021, 16th edition 2021. Lleida, Spain.

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Ghemawat, G. Irving, M. Isard, M. Kudlur, J. Levenberg, R. Monga, S. Moore, D.G. Murray, B. Steiner, P. Tucker, V. Vasudevan, P. Warden, M. Wicke, Y. Yu, X. Zheng, TensorFlow: a system for large-scale machine learning, in: Proc. 12th USENIX Symp. Oper. Syst. Des. Implementation, OSDI 2016, Savannah; United States, 2016: pp. 265–283.

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