Modelling and simulation of a thermal storage system based on phase change materials integrated in a tertiary building.

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Abstract. Decarbonization of the building sector is one of the key challenges to achieve the ambitious goal of carbon neutrality by 2050, established in the European Green Deal. In this sense, current trends focus on the promotion of onsite renewable energy sources, as well as on the electrification of heating and cooling demands and sector coupling approaches through Power-to-heat strategies. This minimizes energy transportation losses while creating an increased need for storage systems. In this scenario, Thermal Energy Storage (TES) systems gain importance and provide the required flexibility, although the experience with high storage periods and volumes, fast response capacity, easy integration into building facilities and cost-effective and environmentally friendly solutions is still scarce. This paper focuses on a TRNSYS (Transient System Simulation Program) modelling and simulation analysis of different integration strategies of a TES system based on Phase Change Materials (PCM) into a real-scale tertiary building. The target building (CARTIF III) is located in Valladolid, Spain, within a Mediterranean climatic area, and incorporates different energy systems including a local photovoltaic (PV) field and a geothermal heat pump (HP). The combination of the PCM storage with the PV and the geothermal HP is studied for the cooling season (in summer) aiming at maximizing the overall system energy efficiency and minimizing the energy import from the grid, thus pursuing a Smart Island concept. Results from this study will feed the solution design for the actual integration project that will be addressed within the framework of a upcoming EU research project.

1 Background and objectives

Renewable energy sources (RES) are key to the decarbonization of the building sector, which is one of the highest energy consumers within the current EU energy context, accounting for up to 51% of total energy consumption. However, increasing RES shares

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present relevant challenges, such as the need to overcome their stochastic availability. Energy storage solutions are required for this purpose, so their development has recently been accelerated [1,2]. In particular, Thermal Energy Storage (TES) systems supporting Power-to-heat (PtH) strategies, which untaps energy flexibility potentials, offer an interesting alternative to enhance RES integration in buildings [3]. Phase Change Materials (PCM) take advantage of latent energy to offer high energy storage densities and represent one of the most promising TES technologies for building applications [4-8].

The present work aims to study the integration of a PCM-based cold storage tank into an existing tertiary building (CARTIF III), located in Valladolid (Spain) and designed under nearly-Zero Energy Buildings (nZEB) standards. This will be addressed through the development of a simulation model into the TRNSYS software, together with the definition and evaluation of different control and operation strategies. Results will help to propose an integration design that meets the needs of the target building during the summer period and allows for improved efficiency and flexibility in its energy use.

2 Description of the target building: CARTIF III

The PCM-based cold storage tank is to be integrated in an existing tertiary building, which is part of the offices and research facilities owned by CARTIF Technology Center, in the municipality of Boecillo, Valladolid (Spain): CARTIF III. The building (see Fig. 1) is composed by different office areas and six large warehouse spaces hosting energy and environmental research infrastructure. Its architectural concept (orientation, passive energy elements) and its energy equipment was designed and selected according to nZEB standards, aiming at less than' 60 kW h m^{-2} a^{-1} primary energy use.

Weather conditions at the building site are characterized by Mediterranean-continental climate with relatively cold winters and dry, hot summer periods. Temperature oscillations between daytime and night-time are high throughout the year.

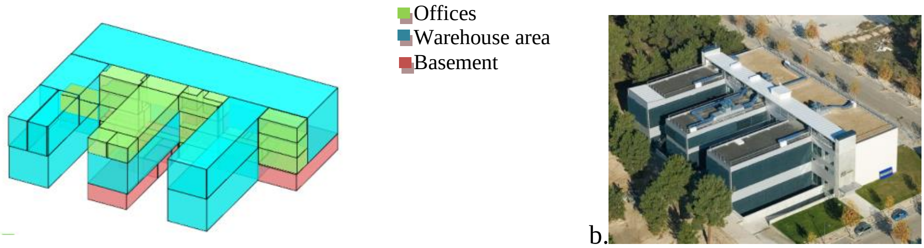
a. 

Fig. 1. General view of the target building: a) building zones by use; b) CARTIF III aerial view

2.1 Energy generation and distribution systems at CARTIF III

The heating and cooling (H&C) demand at the target building is met by a biomass boiler and a ground-coupled heat pump (HP). The biomass boiler has a nominal heat output of 220 kW and a rated efficiency of 90%. The geothermal system feeding the HP is composed by 15 vertical boreholes (each 100m deep). The reversible HP delivers nominal heating and cooling capacities of 101.5 kW and 77 kW respectively, with a nominal COP (Coefficient of Performance) / EER (Energy Efficiency Ratio) of 4.35/3.81 according to the manufacturer's data. It should be noted that the HP operation is based on an on-off control, not being prepared for compressor modulation. A 44-kW heat exchanger (HX) installed in parallel to the heat pump allows for water-based free-cooling when the ground temperatures are favourable to provide direct cooling to the distribution systems.

The thermal energy distribution systems are composed by several rooftop air handling units (AHUs) and a radiant floor system. The AHUs cover the ventilation demands as well as part of the H&C needs at the warehouse areas. Air-based free-cooling strategies are incorporated in their operation. Moreover, a radiant floor system delivers both heating and cooling to the office areas. The system allows a low-temperature operation with a large thermal capacity, which is particularly interesting to be coupled with the geothermal system. In those building areas where both AHUs and radiant floor systems coexist, the utilization ratio is 20% and 80%, respectively. As a form of thermal storage and to absorb flow variations between primary and secondary circuits, three water tanks are installed (overall capacity of 1.5 m^3).

For what concerns electricity demands, CARTIF III is connected to the grid, but also equipped with 45-kW_p photovoltaic (PV) field located on the building roof. The current energy management of the PV field feeds the excess electricity production to the grid at each point in time, applying a cost compensation tariff for the energy injected into the grid.

During the summer season, the PV production coincides with daily periods in which the cooling energy needs are high. However, production and demand tend to be decoupled at some time of the day (particularly during early working hours) and thanks to the PV installed capacity, most of the days there is an excess energy production even in the central hours of the day. In such context, this work aims to analyse the potential for a PCM-based TES system to contribute to efficiently manage this excess energy production to increase the self-sufficiency of the target building.

3 Description of the PCM-based TES system

The proposed PCM-based TES system analysed in this study corresponds to an existing 9.15 m^3 PCM cold storage tank based on a coil heat exchanger immersed into a PCM with 11.4-12.4 ºC melting range and 183 kJ/kg specific latent heat capacity (see Fig. 2). It is based on a proprietary material development by the PCM tank manufacturer, which is especially selected for cooling applications. The system is equipped with 2 ports (1 inlet, 1 outlet) not allowing for simultaneous charging/discharging operation. Switching from one mode to another is facilitated by a connection layout and the proper control strategy for the position of the valves.

Fig. 2. Real view of the PCM-based TES system with connection pipes and valves

4 Description of the energy simulation model

A 3D model of CARTIF III geometry and main building components was created in Google SkectchUP and imported into TRNSYS environment for further definition of the constructive and operational characteristics. The building model (managed through TRNSYS Multi-zone building Type 56) was implemented into an overall energy simulation setup representing the existing energy equipment together with the proposed PCM-based TES system. The existing layout of the facilities and control strategies were integrated in the model and the TES system was placed in parallel to the current water-based storage tanks. TRNSYS Types from the standard and TESS libraries were used for the existing components, while a specific user-created Type based on [9] was used to model the PCM cold storage tank.

5 Definition of scenarios

The analysis of possible integration strategies was based on the definition of 6 case studies in which the operating conditions of the PCM in combination with the existing energy systems at the target building are varied. Assessment indicators are also provided to select the most interesting operating strategy according to different criteria.

5.1 Specification of the different case studies

The six different scenarios are described next:

'Base case' scenario: It represents the current system existing in CARTIF III without the PCM tank. Simulation results from this base case are compared with real measurements from the Building Energy Management System (BEMS) for validation purposes.

'In.PCM' scenario: It incorporates the PCM cold storage to the existing system modelled in the base case. The PCM charge (cooling input to the PCM) will be activated either when the PV production is higher than the heat pump electricity consumption, or when, having effective PV production, the previously existing water tank (water storage tank with a capacity of 1.5 m^3) is charged and there is no cooling demand. The discharge mode (cooling output from the PCM) will be activated when a cooling demand needs to be satisfied, the PV field cannot supply the heat pump electricity input (then, charge is not enabled) and the water tank is not available. This case presents the disadvantage that the energy produced by the heat pump can only be directed to one of the two storage systems (namely, the PCM and the existing water tank).

'Sim.feed' scenario: This proposes a simultaneous feeding of the two storage systems. Feeding of the water tank will be prioritized, but since the heat pump cannot be modulated, the PCM can also be charged using the excess energy between heat pump thermal output and the actual cooling needs. The operating strategy aims to widen the operating range in charging mode, with the expectation of a greater use of the instantaneously produced PV energy and less energy wasted by being dumped to the grid.

'No.PV' scenario: This case analyses the effect of changing the PCM discharge condition, establishing the activation of the discharge mode only when there is no PV production. Its objective is to narrow the operating range in discharge mode to ensure that the stored energy is used only in moments of greatest need (when there is no PV production).

'Glob.ex' scenario: This case considers the existence of excess energy production when the PV output exceeds the global electricity power use of the building (including lighting, appliances, etc. in addition to the heat pump energy use). The discharge condition is also modified to enable the PCM discharge when the opposite condition is met (PV output lower than the global building electricity use). This strategy prioritizes the local use of PV to meet any electric load of the building and aims to study how the integration of the PCM could be affected by considering all the activities in the building within its global energy balance.

'P.min' scenario: This case considers the existence of excess energy production when the PV output is greater than the equivalent heat pump electricity input (electrical energy required to meet the building's thermal demand, calculated using the EER of the HP). This enables to store the excess of photovoltaic energy output over the electrical energy needed to satisfy the electrical demand of the chiller. In such condition, the PCM charging is activated, so the charging criterion is less strict than in the previous cases where the PV output needed to be higher than the total heat pump input or even the total building electricity load. Thus, this operating strategy aims to widen the operating range in charging mode, guaranteeing the supply with 100% renewable energy.

5.2 Assessment indicators

Table 1 lists the assessment indicators used to guide the selection of the best scenarios. Different aspects are accounted for by different indicator categories. The maximization of I3 will be prioritized to identify the most interesting cases.

Table 1. Assessment indicators used to guide the selection of best cases

Category	ID	Description
Energy	I1	Renewable electric energy consumed by the heat pump
	I2	Non-renewable electric energy consumed by the heat pump
	I3	Ratio between renewable and non-renewable heat pump energy use
Environmental	I4	CO_2 emissions linked to the non-renewable energy use*
Economic	I5	Economic cost linked to the non-renewable energy use†
Operation	I6	Ratio between time in discharge mode and the overall simulation period
	I7	Number of cycles (PCM melting/freezing) during operation

6 Results and discussion

A rough comparison between actual monitored data from two summer seasons at the target building and the simulation of the base case was conducted to ensure that the overall simulation model was appropriate for the analysis. Results are shown in Table 2.

Table 2. Comparison between monitored and simulated performance under the base case

Performance variables	Monitored	Simulated
PV energy production (GWh_e)	50.65	53.87
Heat pump energy output to the water tank (GWh_t)	47.74	51.56
Heat pump electricity use (GWh_e)	9.65	10.10

Results for the assessment indicators obtained from the simulation of each of the proposed scenarios are summarized in Table 3, while the evolution of some relevant variables for the most relevant cases are shown in Fig. 3 and Fig. 4.

Table 3. Comparison of the proposed scenarios in terms of the predefined indicators

ID.	Unit	Base case	In.PCM	Sim.feed	No.FV	Glob.ex	P.min
I1	GWh	5.88	8.98	9.59	7.44	8.67	9.53
I2	GWh	3.77	0.99	0.42	2.53	1.11	0.47
I3	%	60,90	90	95,84	74,66	88,65	95,30
I4	$kgCO_2$	782	207	87	524	230	97,45
I5	€	905	239	100	607	267	112,90
I6	%	-	20	63	2	60	51
I7	Nr.cycles	-	36	35	5	38	35

* Emissions and costs associated with grid electricity consumption were estimated according to the energy mix and intraday fluctuations (average value of 0.26 kg kW^{-1} h^{-1} and 0.3 € kW^{-1} h^{-1}, respectively)

a.

b.

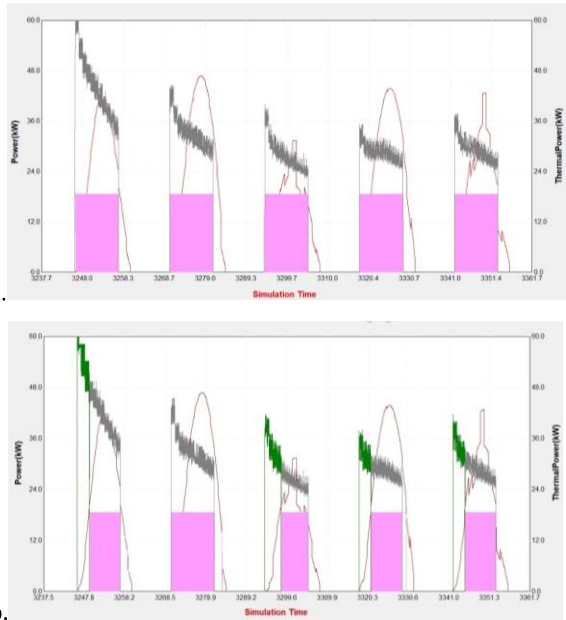


Fig. 3. Simulation results for: a) 'base case'; b) 'In.PCM'. PV production (in red), thermal energy demand (in grey) and heat pump electricity consumption (in pink) are shown.

Fig. 3 shows how daily peaks in the cooling demand are satisfied by the PCM system in the '*In.PCM*' scenario, avoiding the (non-renewable) energy use from the grid for the HP operation at the beginning of workdays. This behavior is also extended to the rest of simulated scenarios and reflects a desired impact of the PCM integration.

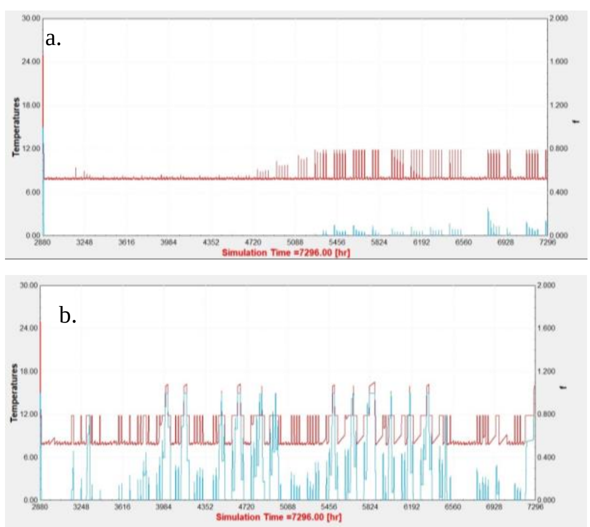


Fig. 4. PCM temperature (in red) and State of Charge (SoC) (in blue) along the simulated period for different scenarios: a) 'No.PV'; b) 'P.min'.

Fig. 4 reveals different intensities in the use of the PCM tank for different scenarios. Some (e.g. '*No.PV'*) never reach States-of-Charge (SoC) lower than 0.5 (melted fraction higher than 0.5) indicating possible oversizing or a very low discharge capacity, which negatively impacts all the other performance indicators. On the contrary, '*P.min'* presents a greater discharge depth, which would be desirable, utilizing the full energy potential of the PCM. However, there are long operation periods in which the PCM is not used.

Finally, according to the overall view of the assessment indicators, the most promising case is '*Sim.feed*', reporting an increase from 60% to 95.8% on the renewable energy fraction (in comparison with the base case) and being the case with the lowest costs and emissions. Based on these results, further optimization could be pursued.

7 Conclusions and future work

This study presents the simulation-based evaluation of different operating strategies defined for the integration of an existing PCM-based TES tank into a tertiary building. A complete simulation model of the building and its complex energy facilities has been obtained with accurate enough results to the purpose of evaluating PCM integration strategies. The inclusion of the PCM system improves the use of PV energy in all the proposed scenarios. Best results for the assessment indicators are obtained for the simplest control strategy allowing simultaneous feed of the PCM and the existing water tank ('*Sim.feed'*). This case reported 95.8% solar energy fraction while leading to a reduction of costs and emissions of 89%.

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