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The Environmental Potential of Phase Change Materials in Building Applications. A Multiple Case Investigation Based on Life Cycle Assessment and Building Simulation

Roberta Di Bari ^{1,*} , Rafael Horn ¹ , Björn Nienborg ², Felix Klinker ³, Esther Kieseritzky ⁴ and Felix Pawelz ⁴

¹ Institute for Acoustics and Building Physics, University of Stuttgart, 70569 Stuttgart, Germany; rafael.horn@iabp.uni-stuttgart.de

² Fraunhofer Institute for Solar Energy Systems (ISE), 79119 Freiburg, Germany; bjoern.nienborg@ise.fraunhofer.de

³ ZAE Bayern, 97074 Würzburg, Germany; felix.klinker@zae-bayern.de

⁴ Rubitherm GmbH, 12307 Berlin, Germany; esther.kieseritzky@rubitherm.com (E.K.); felix.pawelz@rubitherm.com (F.P.)

* Correspondence: roberta.di-bari@iabp.uni-stuttgart.de

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Abstract: New materials and technologies have become the main drivers for reducing energy demand in the building sector in recent years. Energy efficiency can be reached by utilization of materials with thermal storage potential; among them, phase change materials (PCMs) seem to be promising. If they are used in combination with solar collectors in heating applications or with water chillers or in chilled ceilings in cooling applications, PCMs can provide ecological benefits through energy savings during the building's operational phase. However, their environmental value should be analyzed by taking into account their whole lifecycle. The purpose of this paper is the assessment of PCMs at the material level as well as at higher levels, namely the component and building levels. Life cycle assessment analyses are based on information from PCM manufacturers and building energy simulations. With the newly developed software "Storage LCA Tool" (Version 1.0, University of Stuttgart, IABP, Stuttgart, Germany), PCM storage systems can be compared with traditional systems that do not entail energy storage. Their benefits can be evaluated in order to support decision-making on energy concepts for buildings. The collection of several case studies shows that PCM energy concepts are not always advantageous. However, with conclusive concepts, suitable storage dimensioning and ecologically favorable PCMs, systems can be realized that have a lower environmental impact over the entire life cycle compared to traditional systems.

Keywords: phase change materials; PCM; thermal energy storage; life cycle assessment (LCA); Storage LCA Tool; Speicher LCA

1. Introduction

In a context calling for more affordable, sustainable and modern energy [1,2], the building sector is under particular attention as one of the main drivers of energy consumption. While most of the primary energy supply is delivered for energy production [3], heating and hot water in households alone account for 79% of the total final energy use. In addition, despite efforts made to improve energy efficiency, the final energy use for space conditioning grew from 118 million TJ in 2010 to around 128 million TJ in 2018 [4].

A strategy for energy saving is the combination of a source of renewable energy with thermal energy storage, which can be realized for heating and cooling systems not only through sensible heat storage materials but also through phase change materials (PCMs) and thermochemical materials (TCMs) [5,6]. Processes that enable thermal storage are reversible adsorption–desorption reactions, exothermic in adsorption and endothermic in regeneration [7]. Typically, water vapor is used in combination with thermally stable and inexpensive nanoporous materials belonging, for example, to the class of zeolites (Zeolite 13X) or composite sorbents [8,9]. Composite materials, such as multiwalled carbon nanotubes/lithium chloride (MWCN-LiCl) especially, have proven to be advantageous due to their heat storage density with both water and methanol as working fluid [10]. For PCMs, latent heat storage can be achieved through state of matter changes (solid → liquid and liquid → solid). While PCMs also allow for sensible heat storage (i.e., they store heat by raising the temperature of a liquid or solid and they release it with the decrease of temperature if required), they can absorb large amounts of heat at their melting point with constant temperature until all the material is melted [11]. Solidification of PCM occurs when the ambient temperature around the liquid material falls below the crystallization temperature, which leads to the release of the stored latent heat [12]. PCMs, which are mainly hydrated salts or paraffins, are available in any required typology; they can be organic or inorganic and suit any temperature in a range from -50 to 100 °C [13,14].

The advantages of innovative storage systems that incorporate PCMs in the building sector have already been investigated: in comparison with a traditional storage concept, containment volumes are reduced, allowing more storage capacity. The energy input/output occurs longer with almost constant temperatures. As a consequence, insulation of latent storage systems may be less sophisticated and expensive [15]. Together with energy storage systems, they can be directly attached to building components, e.g., walls or chilled ceilings, or included into cooling devices. In such cases, a reduction of direct greenhouse gas emissions during a building's operational stage can be achieved through energy savings [12,16,17]. However, these savings may be overcompensated by additional impacts caused by storage material production or other activities not necessary in conventional systems. As a consequence, innovative storage systems can contribute to tackling climate change if the overall environmental impact during the life cycle can be reduced. This requirement is also indirectly requested by 7th sustainable development goals (SDG7), which calls a reduction in environmental impacts that drive climate change [18].

The environmental impacts can be evaluated through life cycle assessment (LCA), a technique comprised of a set of procedures for compiling and examining the inputs and outputs of materials and energy and the associated environmental impacts directly attributable to the functioning of a product or service system throughout its life cycle. International Standard ISO 14040 establishes LCA principles and framework [19], while ISO 14044 defines requirements and guidelines [20].

With regard to PCMs, only a few LCA studies and investigations are available so far. However, existing studies are often very limited in detail or focus only on a specific application [21]. Existing studies consider only cost aspects or energetic evaluation in operation [22] without a link to the environmental impact evaluation over the entire life cycle of the storage material. When available, the environmental evaluation is oftentimes only carried out at the laboratory scale ($1\text{ m} \times 1\text{ m} \times 1\text{ m}$ cube) without reference to real application scenarios. Other works carry out analyses on a large scale and neglect a life cycle perspective [23].

In an effort to bridge the gap between the environmental promise of innovative storage materials and their actual environmental impact while considering system complexity and modularity, the "Storage LCA" (German "Speicher LCA") project was conducted, with funding from the German Federal Ministry of Economics and Technology (BMWi) and in collaboration with Fraunhofer ISE, ZAE Bayern and University Stuttgart. Some of the project results are presented in this paper [24]. The research focuses on a wide range of organic paraffins and salt hydrates with melting points between 10 – 15 °C for cooling systems and 58 – 62 °C for heating systems. Central heating systems combine the advantage of renewable energy supply through solar collectors with PCM thermal storage. With respect

to centralized cooling systems, cooling devices are accompanied by PCM cold storage that allows for a cooling load shift from day to night, increasing the efficiency of cold production. Furthermore, room-integrated chilled PCM ceilings or PCM ventilation systems are considered. The consideration of sensible, latent and thermochemical storage concepts, as well as their energetic performances evaluated through energy simulation, enables comprehensive environmental assessments of the materials and systems used for thermal energy storage in buildings. Furthermore, the data collection for LCA is based on up-to-date information coming from manufacturers and material developers [13,14]. Previous works related to the project provided results at the material and component levels and already demonstrated the benefits of PCM configurations with high storage density in comparison with, for example, water storage [15].

In the present study, the created “Storage LCA Tool” is presented [25]. Based on the obtained LCA and energy simulation data platform, both practitioners and experts in energy and storage can carry out analyses on different levels. With the help of graphs and numerical results, users are able to decide whether innovative storage systems are advantageous in comparison with conventional systems. This paper analyses the overall environmental assessment of PCMs applied in buildings and provides insight into the general effectiveness and environmental benefits of PCM storage systems.

2. Materials and Methods

For the analysis, a three-level approach was established. Terms used in this work and their respective definitions are given below [6].

- Storage material: In this case, the pure PCM storage material.
- Storage component: All auxiliary equipment such as containment, insulation and heat exchangers required to unlock the storage capacity of the material.
- Storage system concept: All components required for the building supply and for the provision of heat and/or cold. Storage materials, storage components and conventional building service systems for energy provision are included. The main function of the storage system concept is to supply a defined building (building type, energetic standard and climate location) over a defined heating or cooling period. Examples of the possible benefits of PCM systems are the increased use of environmental heat and cold or the reduction of heating or cooling load peaks, which enables lower installed heating or cooling capacities.

Environmental database and energy simulation results were combined in a common data platform, on which the final building LCA was provided consistently with the selected analyzed case study. The environmental database contained results coming from LCA analyses carried out in Gabi software (Version 8.0, Thinkstep, a sphaera company, Stuttgart, Germany) [26] (updated in 2019), according to the ISO 14040 and 14044 standards [19,20] and following specifications and suggestions for buildings [27–32]. Building energy simulations were carried out in TRNSYS (Version 18, Thermal Energy System Specialists LLC, Madison, WI, USA) [33].

2.1. LCA Specifications

In this work, LCAs were carried out at the material, component and energy concept levels (see Table 1). For the cradle-to-grave analyses, the considered life cycle modules were production stage (A1–A3, including raw material supply, transport and manufacturing) and end-of life (C3, C4 and D modules, including waste processing, disposal and eventual benefits due to recycling) [27]. For storage concept analyses, the operational building energy use was included (B6 module according to EN 15804 [27]). At the building level, a 20-year lifespan was considered, with reference to a nominal service life of the installation system without component replacement (module B4 according to EN 15804 [27]). Functional units are related to each level and specified in the following subsections.

Table 1. Life cycle assessment (LCA) specification according to [24,25,28].

Goal and Scope	Analyses of PCMs, Storage Components and Energy Storage Systems
System Boundaries	Cradle to grave analyses. Lifecycle modules [22]: Production (A1–A3) Use phase, including operational building energy demand (B6)—storage concept system only End-of-Life (C + D), including waste + credits due to recycling
Functional Unit (f.u.)	Defined for each level
Lifespan	20 years
Impact Categories	Global warming potential (GWP) (kg CO ₂ eq./f.u.) Primary energy demand total (PE _{tot}) (MJ/f.u.) Primary energy renewable total (PERT) (MJ/f.u.) Primary energy nonrenewable total (PENRT) (MJ/f.u.)

The investigated impact categories were selected in the project due to the goal and scope defined therein, including expectations of energy storage experts in regard to the tool content. For the evaluation of overall energy savings, the primary energy demand total (PE_{tot}) indicator was chosen; this can be divided into primary energy renewable total (PERT) and primary energy nonrenewable total (PENRT). The global warming potential (GWP) expresses the emission of greenhouse gases in kg CO₂ equivalent. The life cycle impact assessment (LCIA) characterization method suggested for buildings in EN15084-Annex 2 [27] was used.

2.2. Analysis at the Material Level

For the PCM analysis, a wide range of commercially available materials were investigated with the support of Rubitherm Technologies GmbH, a PCM producing company. The investigated materials were mainly organic paraffins (RTXX) [13] and inorganic salt hydrates (SPXX) [14] with different melting points in both encapsulated and non-encapsulated variants (Table 2).

Table 2. Analyzed phase change materials (PCMs), listed as organic materials and salt hydrates.

Paraffins	Salt Hydrates
RT10HC	SP15
RT11HC	SP21
RT18HC	SP58
RT24	
RT62HC	

For storage material analyses, impacts were given by the functional unit (impact/kWh material storage capacity). These were obtained through the unit transformation as shown by Equations (1) and (2):

$$\text{GWP} \left(\frac{\text{kg CO}_2 \text{ eq.}}{\text{kWh}} \right) = \text{GWP} \left(\frac{\text{kg CO}_2 \text{ eq.}}{\text{kg}} \right) \cdot \frac{1}{E_d \left(\frac{\text{kWh}}{\text{kg}} \right)}, \quad (1)$$

$$\text{PE}_{\text{tot}} \left(\frac{\text{MJ}}{\text{kWh}} \right) = \text{PE}_{\text{tot}} \left(\frac{\text{MJ}}{\text{kg}} \right) \cdot \frac{1}{E_d \left(\frac{\text{kWh}}{\text{kg}} \right)}, \quad (2)$$

where E_d is the PCM energy density, calculated by taking into account the PCM's physical properties and the working temperatures of the distribution system. The material properties were based on our own experimental testing supported by technical datasheets of PCM producers as well as the collection of information about manufacturing.

The material analysis was supported by the theoretical cycle-based payback time, namely the ratio between impacts due to PCM lifecycle and conventional reference systems (Equation (3)).

$$\text{Payback}_{\text{GWP}}\left(\frac{\text{kg CO}_2 \text{ eq.}}{\text{kWh}}\right) = \text{GWP}_{\text{PCM}}\left(\frac{\text{kg CO}_2 \text{ eq.}}{\text{kWh}}\right) \cdot \frac{1}{\text{GWP}_{\text{ref}}\left(\frac{\text{kg CO}_2 \text{ eq.}}{\text{kWh}}\right)}, \quad (3)$$

The energetic payback-cycles indicate the theoretical minimum number of full charge and discharge cycles the material must endure to have environmental benefits compared to conventional systems (without storage). At the material level, this number does not consider any capacity losses or other use-phase-related impacts. It thus provides a theoretical minimum value that systems have to achieve from an environmental perspective to provide an advantage compared to the chosen reference. The selected reference systems were the following:

- Gas heating with 0.24 kg CO₂ eq./kWh and PENRT = 3.85 MJ/kWh [13];
- Split cooling (SEER = 3.5) with 0.18 kg CO₂ eq./kWh and PENRT = 2.21 MJ/kWh [13];
- Water chiller (SEER = 4.7) with 0.13 kg CO₂ eq./kWh and PENRT = 1.65 MJ/kWh [13].

2.3. Analysis at the Component Level

At the component level, functional units were established singularly. By considering, for instance, a storage containment, the storage volume (m³) could be recommended as functional unit. In order to expand the data basis for LCA, several materials were selected at the component level based on implemented systems or recommendations from experts and users. Together, the components formed the storage system (see Table 3), which, in addition to the actual storage, also included other building installations such as the piping. For most components, an LCA on constructive aspects was sufficient, and production (A1–A3) and end-of-life (C + D) were considered. Since the focus of this work is on PCM storage systems, it does not show water-based energy storage systems and their respective components.

Table 3. Storage component list with their respective available materials.

Storage Component	Available Materials
Storage material	Water ⁴ or PCM (Table 2)
Storage containment	HDPE ¹ , steel ⁴ , stainless steel ^{1,4}
Insulation storage	Mineral foam, EPDM ² foam ⁴ ; XPS ³
PCM containment/capsules	Aluminum, steel, HDPE ¹

¹ High-density polyethylene. ² Ethylene propylene diene monomer rubber. ³ Extruded polystyrene. ⁴ Only for sensible water storage.

2.4. Analysis at the System Level

Analysis at the whole system level considered the building components and the operational stage. Environmental impacts were calculated by multiplying material impacts by their quantities. These were scaled by the established functional unit, namely the yearly impact per net surface unit (kg CO₂ eq./m² net surface year).

In order to determine the energy demand of all investigated systems, they were examined in several building types in a building simulation using TRNSYS 17 or TRNSYS 18 (Table 4) [32]. Each building type was considered in different climate zones (Athens, Strasbourg and Helsinki) and with different insulation levels. The insulation levels refer to insulation standards in the three different climate zones around the year 1990, where “no insulation”, “little” and “moderate” refer the insulation standards of Greece, Central Europe and Northern Europe, respectively. Buildings of this age are particularly interesting for system-level analyses, as the existing heating and cooling systems of these buildings are at the end of their life cycle and therefore need to be replaced. Simulations of energy-efficient buildings

are included as well. Together with the system provided with thermal storage, the reference system without thermal storage is simulated for comparison (Table 4).

Table 4. Energy concept systems list.

Category	Energy Supply and Storage	Distribution System
Central heating	(1) Gas boiler ¹	Radiators
	(2) Hot water storage + solar collector	Underfloor heating
	(3) PCM storage + solar collector	
Central cooling	(1) Water chiller ¹	Surface cooling
	(2) Split device ¹	Fan coil
	(3) Water chiller + cold water storage	
	(4) Water chiller + PCM storage	
Room-integrated	(1) Air cooling ¹	Natural ventilation ¹
	(2) PCM surface cooling + Water chiller	Surface cooling
	(3) PCM ventilation system	Air cooling

¹ Reference system.

2.5. Storage LCA Tool

“Storage LCA Tool” is available online for free [22]. The tool supports storage experts and practitioners by providing scientific support in the selection of environmentally suitable thermal storage materials and concepts for building applications. Comprehensive environmental assessments based on the LCA software Gabi ts [26] allow environmental assessments and comparisons at the material, component and system levels. In addition to the environmental database, simulation results have been included under the previously mentioned different boundary conditions.

All relevant components have been identified through expert surveys among the participating institutions and participants of the IEA Task 58—“Materials & components for thermal energy storage of the solar Heating and cooling” program of the International Energy Agency [33]. Based on the surveys, standard component and system setups have been derived and their parts have been modeled for LCA [15,22]. The models were based on ÖKOBAUDAT datasets [34] and our own models and were complemented by a material database to create and assess specific components that were not natively considered.

The tool is a useful instrument for all expert and nonexpert users. For this reason, two different tool usage modes are available (Figure 1).

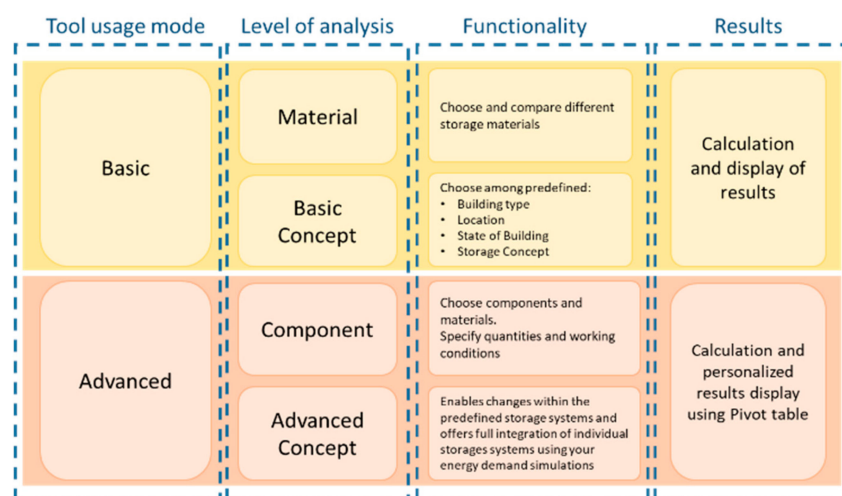


Figure 1. Storage LCA Tool functionality: advanced and basic modes.

The Basic Mode enables the user to perform comparisons of storage materials at predefined working temperatures. Minimum and maximum temperatures are defined according to the melting

temperature range of the selected PCM and operating temperature of the selected distribution system. At the system level, a simplified analysis of innovative storage system layouts at the building level can be conducted and compared with a reference system. User enters information about (1) building type, (2) location, (3) insulation level, (4) energy storage and supply concept. Depending on such specifications, a drop-down list of available storage system layouts is generated and the chosen one analyzed. The final analysis is based on default storage components/combinations as well as default energetic TRNSYS simulations. Analogously, reference systems layouts are automatically generated and analyzed based on LCIA and energy simulation results. Results can be visualized in numerical or graphical simplified form easy to understand.

Within the Advanced Mode, default storage components and systems can be customized individually and analyzed. Moreover, individual energy demand simulations may be integrated and a more detailed analysis performed. To ensure consistent results, advanced mode analyses are suggested for expert users and only if comprehensive information about storage system and building installations are available. Results visualization can be personalized as well through Pivot tables and diagrams according to the scope of the analysis.

3. Results

In this section, with the support of “Storage LCA Tool”, significant innovative storage materials as well as storage system concepts are selected and compared to their respective reference systems as demonstrative examples.

The chosen examples of storage system concepts for heating and cooling using innovative centralized PCM storage all use salt hydrates as storage materials. In the selected innovative cooling system, the relevance of the location for the selection of suitable and effective storage systems was emphasized. A heating concept has been selected in order to prove the great advantages of coupling PCM storage systems and solar collectors.

Generalized results for all energy concepts are presented in Section 4.

3.1. Material Level

To provide a broad spectrum of materials, the LCA makes use of a generic modeling approach, assuming similar production processes and routes wherever possible. This not only allows for comparison of materials with different technology readiness levels (TRLs), but also focuses on the impacts of the underlying raw materials. Detailed information at the material level is provided in the tool documentation [25]. As an example, a comparison between paraffin RT10HC, the salt hydrate SP15 and water is presented (Tables 5 and 6). Physical properties are derived from producers’ technical documentation (Table 5), while the environmental assessment is carried out by Storage LCA Tool (Table 6), which is able to compare up to three materials [25]. Both PCMs are assumed to be operated in the range of 10–16 °C. As already noticed by previous works, paraffins show higher GWP impacts and PENRT [6,15]. The required raw materials strongly influence the material’s global warming potential. For instance, the paraffin model only considers the petroleum-based route as a refinery by-product. In comparison with salt hydrates, paraffins consequently have higher environmental impacts (GWP of RT10HC is almost 50% higher in comparison with SP15, and the PENRT is 5 times higher) [35]. The selected system conditions result in long payback times for RT10HC (Figure 2). Therefore, from the environmental perspective, the salt hydrate is preferable in this case. Results analysis for all PCMs are available in Appendix A.

Table 5. Material properties of RT10HC (paraffin) and SP15 (salt hydrate) in comparison with water. Reproduced from [13,14], Rubitherm: 2019.

Name	Melting Enthalpy (Wh/kg)	Melting Range (°C)	Specific Heat Capacity (kJ/kg K)	Melting Point (°C)	Density (kg/m ³)
RT10HC	57.22	10–12	1.7	10	770
SP15	52.22	15–17	2.0	15	1350
Water	92.64		4.2	0	1000

Table 6. LCA analyses for RT10HC (paraffin) and SP15 (salt hydrate) in comparison with water. Reproduced from [25], IABP: 2019.

Name	GWP (kg CO ₂ eq./kWh ¹)	PENRT (MJ/kWh ¹)	Payback Cycles GWP	Payback Cycles PENRT
RT10HC	18.30	880.85	82.7	226
SP15	12.02	180.95	49.5	47
Water	0.0	0.02	0.0	0.012

¹ kWh material storage capacity.

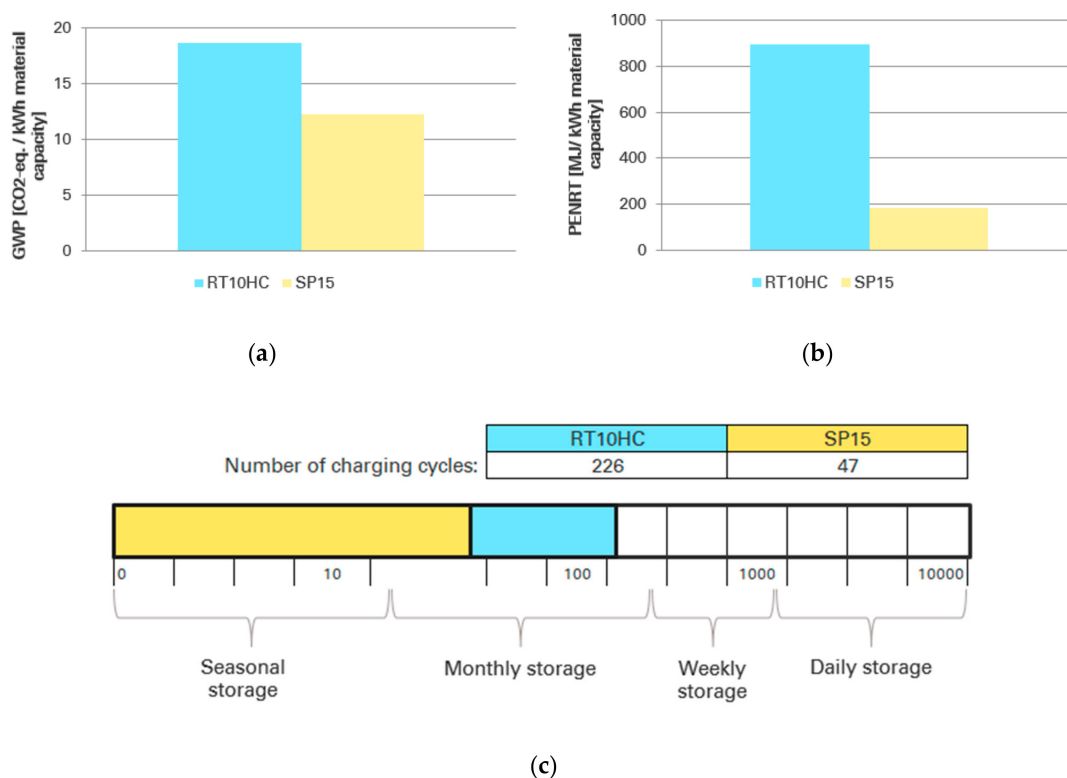


Figure 2. Environmental assessment through “Storage LCA Tool” of RT10HC and SP15: (a) global warming potential (GWP); (b) primary energy nonrenewable total (PENRT); (c) PENRT payback cycles. Reproduced from [25], IABP: 2019.

3.2. Component and System Levels

3.2.1. Helsinki—North European Insulation Standard

A cooling system with PCM storage in an office block located in Helsinki with moderate insulation level (North European insulation level) serves as an example. Together with the storage components (see Table 4), further elements constitute the overall storage energy concept, as shown in Figure 3a. The PCM storage is connected through valves and pipework to the building where the cold is distributed via chilled ceilings. In Figure 3b, the associated reference system for the comparison is represented. Unlike the innovative one, it does not entail any thermal storage. The water chiller and the distribution

system have the same features [24]. For the selected location, with a mean temperature of 6.05 °C, the annual cooling demand is 4.08 kWh/m² a (see Appendix B).

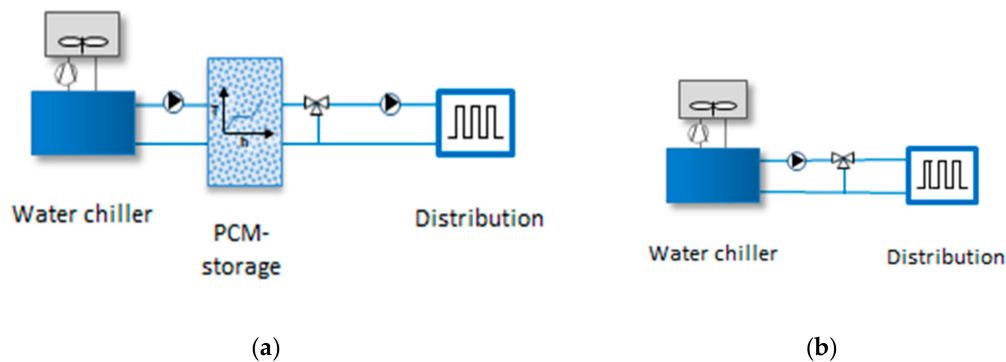


Figure 3. System layouts of (a) PCM storage for a cooling system and (b) a reference system. Reproduced from [24], Fraunhofer ISE 2019.

Table 7 reports comprehensive system information concerning materials and quantities. On this basis, LCIA is carried out, with the results reported in Table 8. Here, impacts are grouped according to their respective system (storage, cooling, distribution) and shown in both absolute and relative form.

Table 7. System information, including storage components. Reproduced from [25], IABP: 2019.

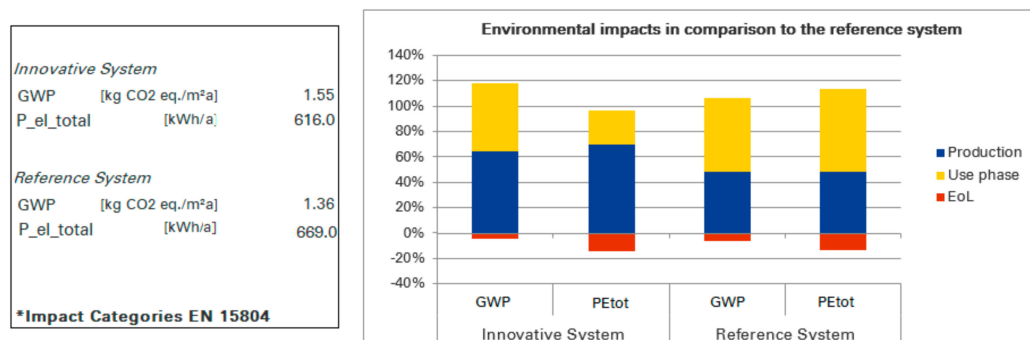
Storage component	Material	Amount	Unit	
Storage material	SP15	1755	kg	20% recycling rate
Containment	HDPE	85	kg	
Insulation (storage)	XPS	11.3	kg	
Heat exchanger	PP capillary tube	35	kg	
System component	Material	Amount	Unit	
Pipework	Steel	1755	kg	
Pipework insulation	XPS	2.97	kg	
Heat exchanger	PP capillary tube	45.5	kg	
Valves	Stainless steel	32	kg	
Circulation pump	Standard	250–1000	W	
Heat transfer fluid	Propylene glycol/water	30.85	kg	
Water chiller		11	kW	
Cooling surface	Copper (200 mm distance)	516	m ²	
Use Phase	Process	Amount	Unit	
Electricity	Electricity mix DE	616.0	kWh/a	

Table 8. Environmental assessment of system, including storage components Reproduced from [25], IABP: 2019.

Storage Component	A1–A3			C+D		
	GWP	PENRT	PERT	GWP	PENRT	PERT
Storage material	1125.5	169,937	1042.7	26.9	358.6	27.0
Containment	165.9	6224	286.6	96.5	−1902.8	−289.7
Insulation (storage)	959.7	29,376.7	538.4	18.5	−278.5	−54.8
Heat exchanger	98	2845	304.2	44.8	−160.4	−160.4
System component	GWP	PENRT	PERT	GWP	PENRT	PERT
Pipework	97	893.1	58.1	−54.6	−490.0	32.6
Pipework insulation	251.3	7683	141.0	4.8	−72.9	−14.4
Heat exchanger	127.4	3699.2	395.4	58.3	−1056.8	−208.5
Valves	33	394	61.6	−14.4	−129.8	8.2
Circulation pump	117.8	1588	254.4	−17.8	−254.9	−26.0
Water chiller	421.3	5731	987.8	−213.2	−2991.6	−336.5
Cooling surface	5627	98,806	12,733.5	−567.4	−26,682	−4409.2
Use Phase	GWP	B6 yearly PENRT	PERT	B6 Total (20 years)		
Electricity mix	376.42	4935.8	2062.1	GWP	PENRT	PERT
				7528.30	95,695.05	41,241.86

LCIA results (Table 8) show that the storage system is the main factor responsible for the evaluated impacts. Among storage components, the PCM (SP15) and its insulation (XPS) present the highest global warming potential (GWP) and primary energy nonrenewable demand (PENRT), respectively.

Finally, the system is compared with its respective reference system. As demonstrated by the results (see Figure 4), compared with the reference system, the inclusion of a PCM storage system entails greater impact due to production. Energy savings during the operational stage due to the increased efficiency in cold production enabled by the inclusion of thermal energy storage do not compensate for this initial impact over a 20-year analysis. As a result, the total GWP and PE_{tot} are slightly higher for the innovative system in the considered setup and climate zone.

**Figure 4.** PCM storage for a cooling system in comparison with the reference system. Reproduced from [25], IABP: 2019.

The high environmental impact may be due to the selected boundary conditions. The energy simulation results included in the tool show an electricity demand of 616 kWh per year (kWh/a) for cold production and distribution. The reference system in turn consumes 669 kWh/a. The electricity savings for the innovative system amount to only 8%. Hence, in this case, the investigated innovative cooling system in a building with standard insulation level may not be the most effective solution due to the selected rather cool Helsinki climate zone.

3.2.2. Athens—North European Insulation Standard

A further analysis can be carried out for the same cooling system, water chiller + SP15 storage, in an office building with moderate insulation located in Athens. The new selected location has a mean temperature of 16.54 °C, and the annual cooling demand is 48.01 kWh/m²a (see Appendix B). The total primary energy demand of the innovative system is reduced compared to the reference, and there are slight reductions of the total GWP. According to the simulation results included in the tool, this system has an electrical energy demand of 7445 kWh/a due to water chiller and cooling distribution. The reference system in turn has a total demand of 9039 kWh/a. On one hand, the cooling demand is higher due to the selected location, but on the other hand, an innovative system can provide greater benefits, with an 18% reduction in electricity demand for the cooling system. As a result, despite the high GWP due to SP15 production, the impacts can be more than compensated for. For the whole lifecycle, the selected innovative system records a GWP reduction of almost 10% (Figure 5).

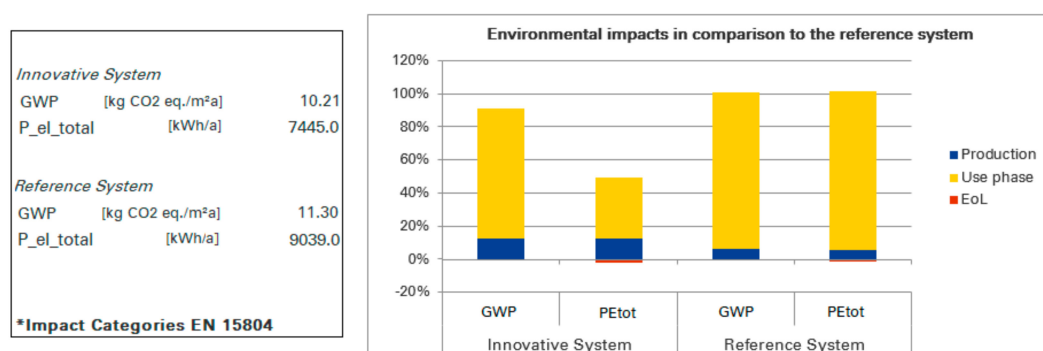


Figure 5. PCM storage for a cooling system in comparison with the reference system. Reproduced from [25], IABP: 2019.

3.2.3. Centralized Heating System with PCM Storage: Office Block in Helsinki

In contrast to the previous case study, the same building with an equal energy standard is now provided with a centralized heating system (see Figure 6a). A storage system using the salt hydrate SP58 is considered. The PCM storage with a volume of 16.49 m³ is combined with solar collectors (with an area of 149.40 m²). The reference system consists of a gas boiler with domestic hot water storage and underfloor heating (see Figure 6b) [24]. For the selected location with a mean temperature of 6.05 °C, the annual heating demand is 137.39 kWh/m²a (see Appendix B).

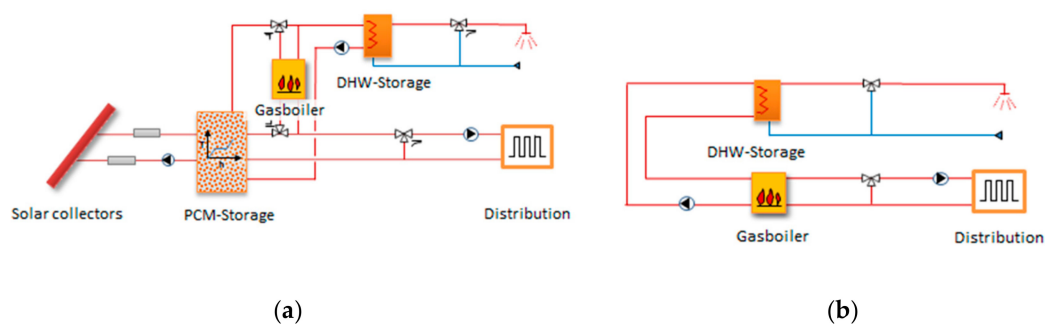


Figure 6. System layouts of (a) PCM storage for a heating system and (b) a reference system. Reproduced from [24], Fraunhofer ISE 2019.

The results of the analysis demonstrate the effectiveness of this choice. In terms of both GWP and PEtot, high savings are recorded. This is in the first place due to the solar collectors, which increase the total energy savings. The simulation results included in the tool show an electricity demand related to pumps and the collector circuit of 881.8 kWh/a and an energy demand of 52.74 kWh/a for heating

provided by the gas boiler. Cooling demand is not included. For the reference system, the lack of solar collectors reduces electricity demand to 71.4 kWh but considerably increases the gas demand, which reaches 79.38 kWh/a (+44% in comparison with the innovative system). The gas demand strongly affects the final environmental assessment. The innovative system shows environmental advantages with a 46% reduction of the total GWP (Figure 7).

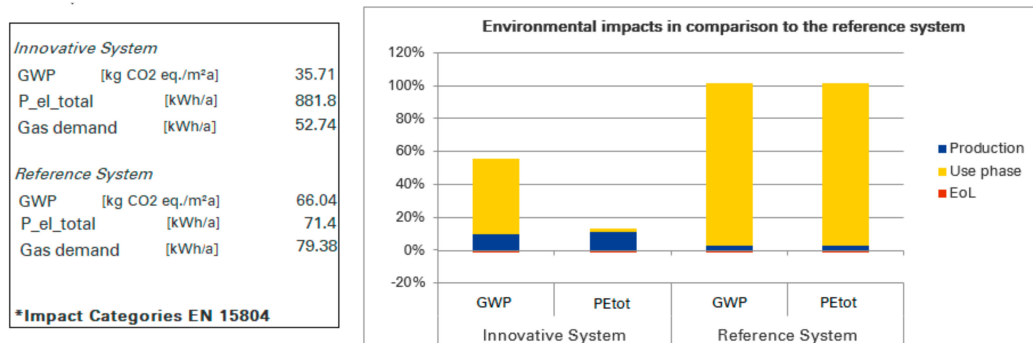


Figure 7. PCM storage for a heating system in comparison with the reference system. Reproduced from [25], IABP: 2019.

As the previous example, the storage material (SP15) is the main factor responsible for evaluated impacts. Storage thermal insulation (XPS) has only a minor influence on the overall evaluation (Table 9).

Table 9. Environmental assessment of the system, including storage components. Reproduced from [25], IABP: 2019.

Storage Component	A1–A3			C + D		
	GWP	PENRT	PERT	GWP	PENRT	PERT
Storage material	39,112.6	578,430	26,345.5	340.9	4548.3	342.5
Containment	121.0	4540	209.1	70.4	−1387.9	−211.3
Insulation (storage)	6011.1	183,994	3372.2	115.8	−1744.4	−343.2
Heat exchanger	98	394	304.2	44.8	−160.4	−160.4
System component	GWP	PENRT	PERT	GWP	PENRT	PERT
Pipework	543.3	4918.8	320.0	−300.8	−2698.9	179.3
Pipework insulation	35.1	1073.4	19.7	0.7	−10.2	−2.0
Heat exchanger	1616	46,922.3	5015.4	739.2	−13,404.8	−2644.4
Valves	33	1588.2	254.4	−17.8	−254.9	−26.0
Circulation pump	117.8	172,718.2	54,986.6	−8014.0	−111,185.4	−32,834.6
Gas boiler	526.6	6364.3	983.4	−137.0	−1622.8	−79.6
Underfloor heating	5627	98,805.6	12,733.5	−567.4	−26,681.8	−4409.2
Use Phase	B6 yearly			B6 Total (20y)		
	GWP	PENRT	PERT	GWP	PENRT	PERT
Electricity mix	538.8	6848.9	2951.7	10,776	136,979	59,034
Gas low temperature boiler	14,944	240,366	4576.5	298,881	4,807,327	91,530

4. Discussion

Since results typically vary from case to case, evaluations of the utility of a PCM application cannot be based on the results of a single case, such as those considered in the previous section. In order to derive generalizable conclusions and to identify eventual common characteristics from the combined energetic–environmental investigations, all results coming from “Storage LCA Tool” have been assessed in a meta-analysis, i.e., data from multiple case studies were combined.

Environmental impacts have been gathered and sorted by storage system, PCM storage material, building type, insulation level and location. For each case, impacts ($GWP_{inn\ sys}$ and $PENRT_{inn\ sys}$) of

the innovative system have been divided by the impacts of the associated reference system ($GWP_{ref\ sys}$ and $PENRT_{ref\ sys}$), according to Equations (4) and (5). Two ratios are thus calculated: (1) a GWP ratio over the whole lifecycle, which describes the environmental performance, and (2) a primary nonrenewable energy demand ratio over the building use phase (B6 module), which is used to analyze the efficiency of the storage system.

$$GWP\ ratio = \frac{GWP_{inn\ sys}(kg\ CO_2\ eq.)}{GWP_{ref\ sys}(kg\ CO_2\ eq.)} \quad (4)$$

$$PENRT\ ratio_{B6} = \frac{PENRT_{inn\ sys,B6}(MJ)}{PENRT_{ref\ sys,B6}(MJ)} \quad (5)$$

Results are visualized in an x–y diagram, where the GWP ratio is plotted on the y-axis and energy efficiency ratio is plotted on the x-axis (see Figure 8). If both ratios are less than 1, the system is deemed advantageous from both environmental and energy perspectives. If the PENRT ratio is less than 1, savings due to energy storage are recorded and the storage system can be deemed efficient. In the worst-case scenario, in which both ratios are greater than 1, the storage system is found to have very energy-intensive production processes and high nonrenewable energy demand. In such cases, storage systems are not advantageous.

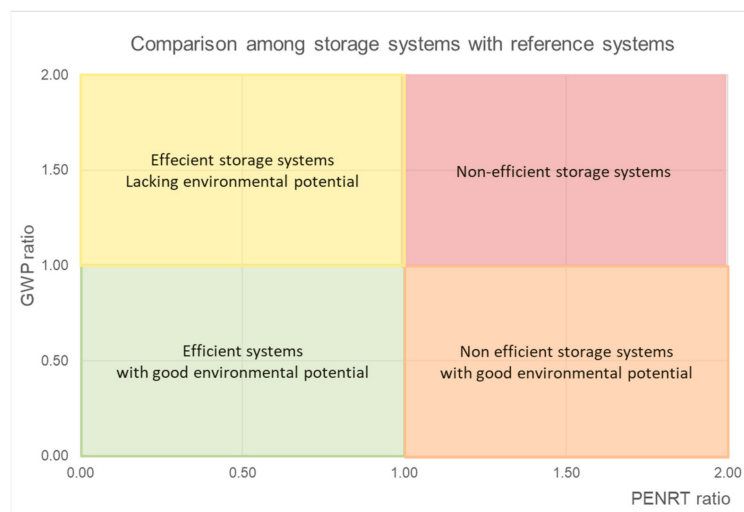
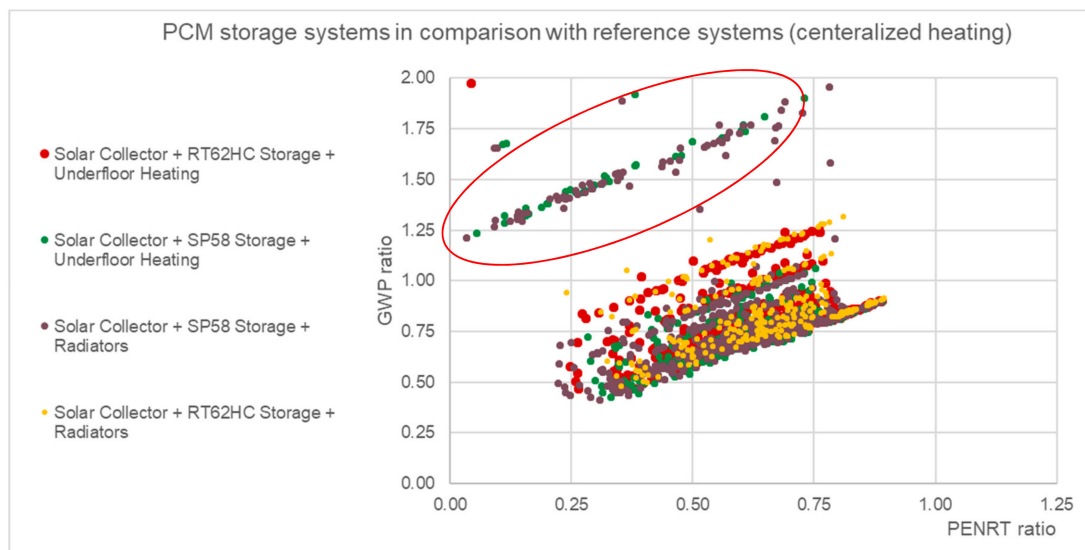


Figure 8. Interpretation of results for following figures (scheme).

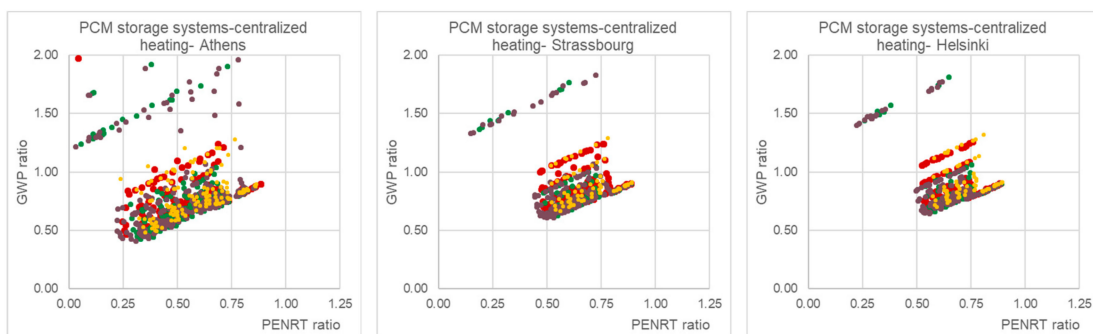
4.1. Centralized Heating Systems

In Figure 9a centralized heating systems with PCM storage are considered and compared to the corresponding reference systems and are differentiated by PCM type. In the Figure 9b–d, results are filtered by location. The evaluated innovative systems use two different storage materials, namely RT62HC (organic) and SP58 (salt hydrate), and two different distribution systems, namely radiators and underfloor heating. The following parameter variations were implemented:

- 6 collector sizes (1.03 to 228.8 m²);
- 12 storage sizes (daily to seasonal storage: 0.05 to 1181 m³);
- 3 building types (single-family house, multifamily house, office building);
- 4 building insulation standards (none, little, moderate, efficient);
- 3 locations (Athens, Strasburg, Helsinki);
- 2 PCMs (RT62HC, SP58).



(a)



(b)

(c)

(d)

Figure 9. Environmental assessment through “Storage LCA Tool” of centralized heating systems, showing (a) comparison with reference systems and (b–d) results filtered by location: (b) Athens; (c) Strasbourg; (d) Helsinki.

The combination of PCM storage tanks with solar collectors seems to be largely advantageous and enables energy savings and emission reductions in most cases, as indicated by the accumulation of points in the lower left quadrant in Figure 9a. Different distribution systems seem to be not relevant to the whole lifecycle. There are also results in the upper left quadrant (red circle in Figure 9a) which show high GWP ratios. These cases mainly belong to systems with SP58 and seasonal storage, which enable energy savings but lead to high GWP ratios above 1.3 due to the high amount of PCM and its infrequent use. They mostly occur in Athens (Figure 9b) and decrease in North European locations such as Helsinki (Figure 9d).

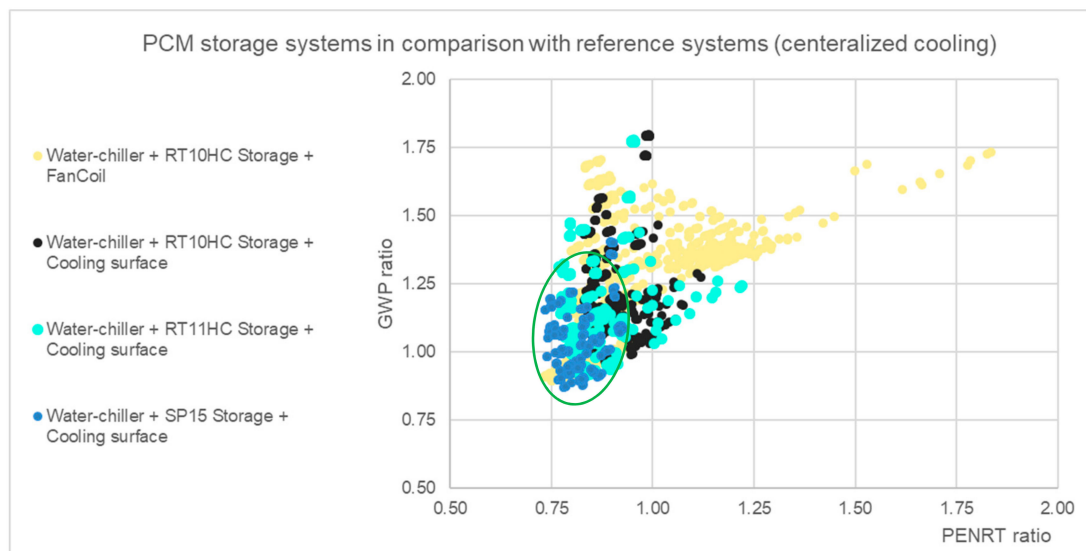
The combination of solar collector + RT62HC (with both distribution systems) presents less variation in terms of environmental potential and energy storage. The best savings are recorded by solar collector + SP58 storage + radiators for a single-family house located in Athens with little insulation (GWP ratio = 0.44; energy ratio = 0.32). The worst performance (GWP ratio 2.13; energy ratio = 0.77) is recorded for a solar collector + SP58 storage + underfloor heating system in an energy-efficient office block in Strasbourg with high storage volume (121.82 m³) and small collector surface (5.65 m²). A more detailed visualization of results can be found in Appendix C (Figure A1).

4.2. Centralized Cooling Systems

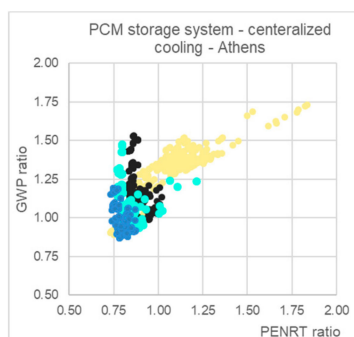
The following parameter variations were implemented:

- Three water chillers (2 to 31 kW capacity);
- Nine storage sizes (daily to seasonal storage: 0.25 to 19 m³);
- Three building types (single-family house, multifamily house, office building);
- Four building insulation standards (none, little, moderate, efficient);
- Three locations (Athens, Strasburg, Helsinki);
- Three different PCMs (RT10HC, RT11HC, SP15).

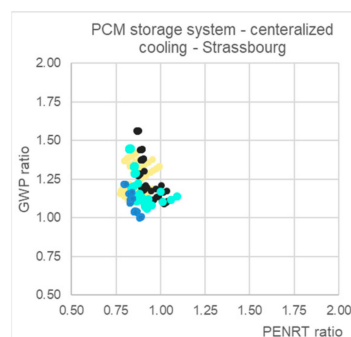
As already mentioned in Section 3.2.3, the achievable energy savings in central cooling systems are lower in comparison with those recorded for heating systems (Figure 10a). As in the example above, the results in Figure 10b–d are filtered by location. Compared with the reference systems, only a few innovative PCM storage concepts achieve positive environmental balances. In these cases, the energy savings due to the efficiency improvements in cold generation, which are achieved by shifting the cooling load into the night by integrating a PCM cold storage, more than compensate for the higher environmental impact due to the additional storage components.



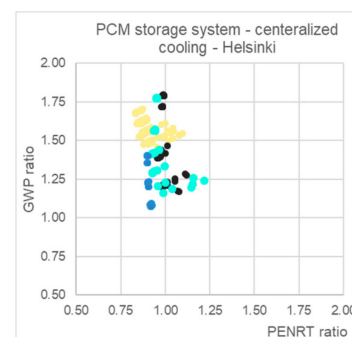
(a)



(b)



(c)



(d)

Figure 10. Environmental assessment through “Storage LCA Tool” of centralized cooling systems, showing (a) comparison with reference systems and (b–d) results filtered by location: (b) Athens; (c) Strasburg; (d) Helsinki.

Unlike heating systems, better performances are reached in Mediterranean area (Athens, see Figure 10b), while PCM systems in Helsinki lack good environmental performances overall (Figure 10d).

Water chiller + RT10HC + fan coil systems show high performance variability, especially in Athens, while the SP15 storage + cooling surface combination offers a better performance in more cases with lower variability (green circle in Figure 10a). An office block located in Athens (no insulation) provided with RT10HC storage + fan coil and a storage volume of 7.11 m³ has the best performance (GWP ratio = 0.89; energy ratio = 0.75). The worst performance (GWP ratio = 1.73; energy ratio = 1.84) is recorded by the same energy concept used in a single-family house in Athens, with low storage volume (0.34 m³) and little insulation [22]. More results details are available in Appendix C (Figure A2).

4.3. Decentralized Systems

Finally, decentralized PCM ventilation systems were analyzed. The two different systems are a water chiller with a chilled PCM ceiling (Figure 11a) and a water chiller with a PCM ventilation system (Figure 11b).

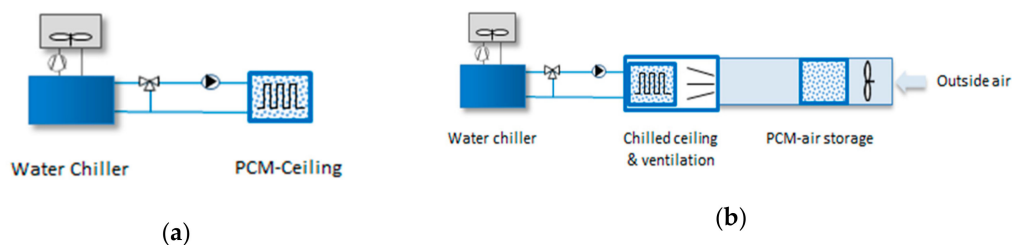


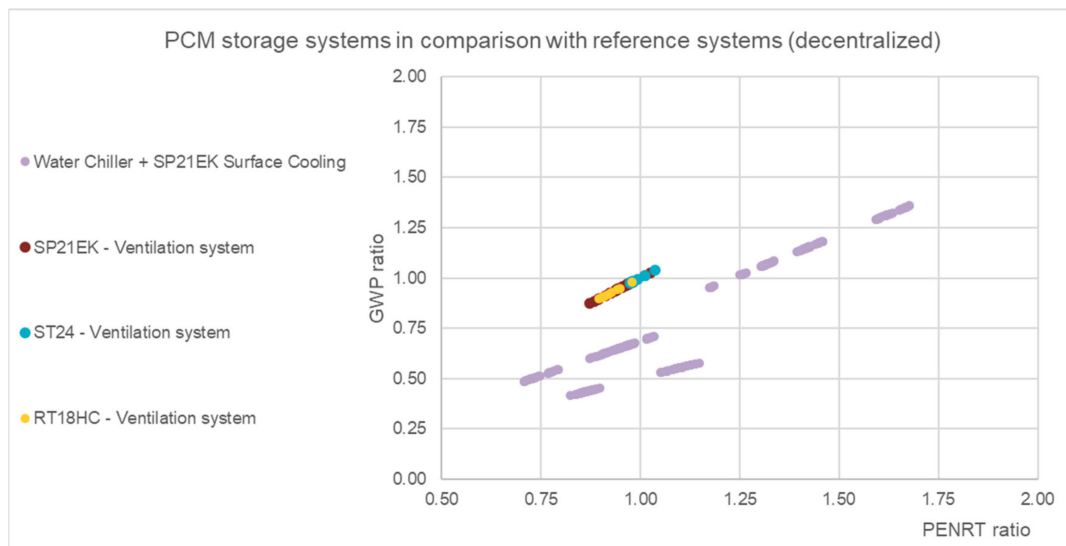
Figure 11. PCM storage for decentralized systems. System layouts of (a) water chiller + PCM cooling surface and (b) water chiller + PCM ventilation systems. Reproduced from [24], Fraunhofer ISE 2019.

The following parameter variations were implemented:

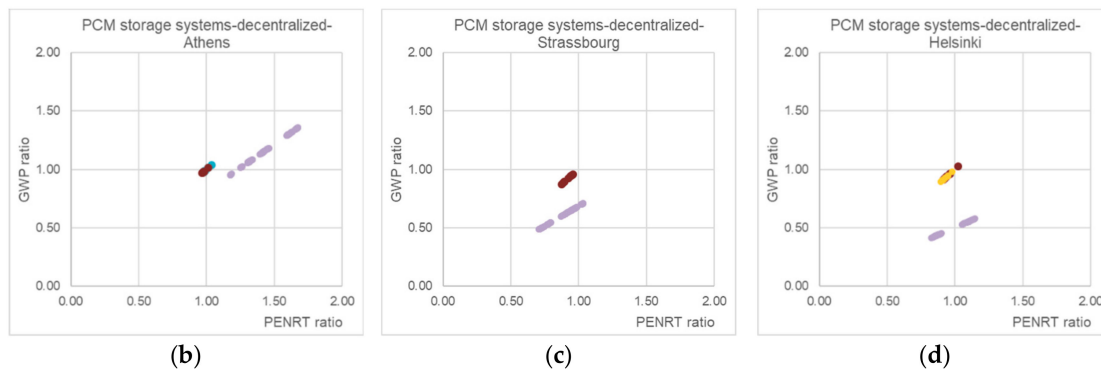
- Three water chiller powers (18 to 36 kW);
- Three water chiller temperatures (6, 10 or 14 °C);
- Three PCM mass distribution for chilled PCM ceilings (11, 16 or 22 kg/m²);
- Three storage volumes for PCM ventilation systems (1, 2 or 3 m³);
- Three volume flow rates for PCM ventilation systems (500, 1000 or 2000 m³/s);
- One building type (office building);
- Four building insulation standards for chilled PCM ceiling simulations (none, little, moderate, efficient);
- One building insulation standard for PCM ventilation systems (efficient);
- Three locations (Athens, Strasburg, Helsinki);
- Four different PCMs (RT18HC, SP21EK, RT24, SP24).

Results are shown in Figure 12a. Here, a linear relationship between environmental impacts and energy demand is found.

Among the simulated examples (only office buildings), most cases located in Strasbourg (Figure 12c) offer advantageous energy performances, and all are environmentally advantageous. In comparison, the applications located in Helsinki offer even greater environmental savings while showing higher variability in energetic performance (Figure 12d). The systems simulated for Athens did not provide relevant energetic or environmental advantages (Figure 12c).



(a)



(b)

(c)

(d)

Figure 12. Environmental assessment through “Storage LCA Tool” of decentralized systems, showing (a) comparison with reference systems and (b–d) results filtered by location: (b) Athens; (c) Strassbourg; (d) Helsinki.

Water chiller + SP21EK surface cooling systems show a wide range of performance variability depending on location (Figure 12b–d). The best performance (GWP ratio = 0.42; energy ratio = 0.82) is recorded by this energy concept, located in a highly insulated office block in Helsinki with a PCM mass distribution for surface cooling of 22.4 kg/m^2 . The worst result (GWP ratio = 1.02; energy ratio = 1.26) is recorded in an energy-efficient office block located in Athens (PCM mass distribution for surface cooling of 22.4 kg/m^2) [22]. A more detailed visualization is available in Appendix C (Figure A3).

5. Conclusions

Within this work, further LCA data were generated and provided by “Storage LCA Tool” for the support of decision-making in field of innovative storage materials, which are available or being researched for application in building services engineering. Through “Storage LCA Tool”, analyses were carried out at different levels.

At the pure PCM level, the integration of updated information coming from PCM producers proved to be relevant for the assessment of the environmental potential of storage systems. A wide range of capacity-specific environmental effects depending on materials and their applications in heating, cooling and ventilation systems was demonstrated. Outcomes of analyses at the material level demonstrate the advantages of paraffins in terms of thermal storage but also indicate their higher environmental impacts. Conversely, the consideration of these environmental impacts during material

production (e.g., when determining the synthesis route) offers the potential to minimize environmental impacts throughout the life cycle. This calls for more research on organic paraffins, which is actually ongoing, in order to minimize the primary energy (nonrenewable) demand for PCM production by replacing the raw materials by renewable sources and furthermore increase their recycling potential [6]. The environmental optimization of salt hydrate raw materials offers optimization potential as well.

At a higher level, two significant cooling and heating systems have been analyzed. Together with the amount of PCM in the thermal storage, the composition of the required auxiliary components (storage insulation, containment, heat exchanger, etc.) shows a great influence on the overall LCA. For this reason, it is necessary to evaluate each quantity carefully, in order to avoid excessively adverse environmental impacts and, at the same time, guarantee enough storage capacity.

By coupling such results with building energy simulation results, innovative PCM storage concepts seemed to be advantageous, especially if associated with a source of renewable energy such as solar collectors. In this case, PCM storage systems can represent an advantageous alternative to a traditional gas boiler in a heating system. Other factors that affect the benefits of PCM thermal energy storage are boundary conditions, i.e., building type, location and insulation level. These factors influence the yearly energy demand and the efficiency of the considered storage systems. Not surprisingly, by ensuring enough thermal insulation on the building envelope, advantageous PCM applications for cooling systems are recorded in warmer locations.

PCM thermal storage systems are, in some cases, advantageous alternatives to traditional water storage. To prove that, analog analyses have been carried out by assuming hot water tank storage (HWT) within heating systems and cold water tank storage (CWT) for cooling systems. In Figure 13, each water storage system is compared with all of the above-reported PCM storage systems. Systems have been distinguished as heating or cooling systems and divided by distribution system. With regard to heating systems, hot water storage (HWT) systems show greater advantages.

It is well known that solar thermal heating systems can save significant amounts of energy compared to conventional gas heating if they are correctly dimensioned. This is confirmed by this study. The impact is quantified and lies in the PENRT ratio range of 0.05 to 0.98, depending on the load and system size. In terms of GWP, the results are more ambiguous. Large PCM storage systems for long-term storage have a high impact due to production. Due to the low cycle number they are not used effectively, so the savings during use phase cannot always compensate for the footprint of production. Water storage systems, on the other hand, have a much lower impact during production and therefore yield better results here. The rather wide temperature range available for heat storage additionally results in a comparable volumetric energy density of water- and paraffin-based thermal storage. All case studies are located in the diagram area belonging to efficient systems with environmental potential.

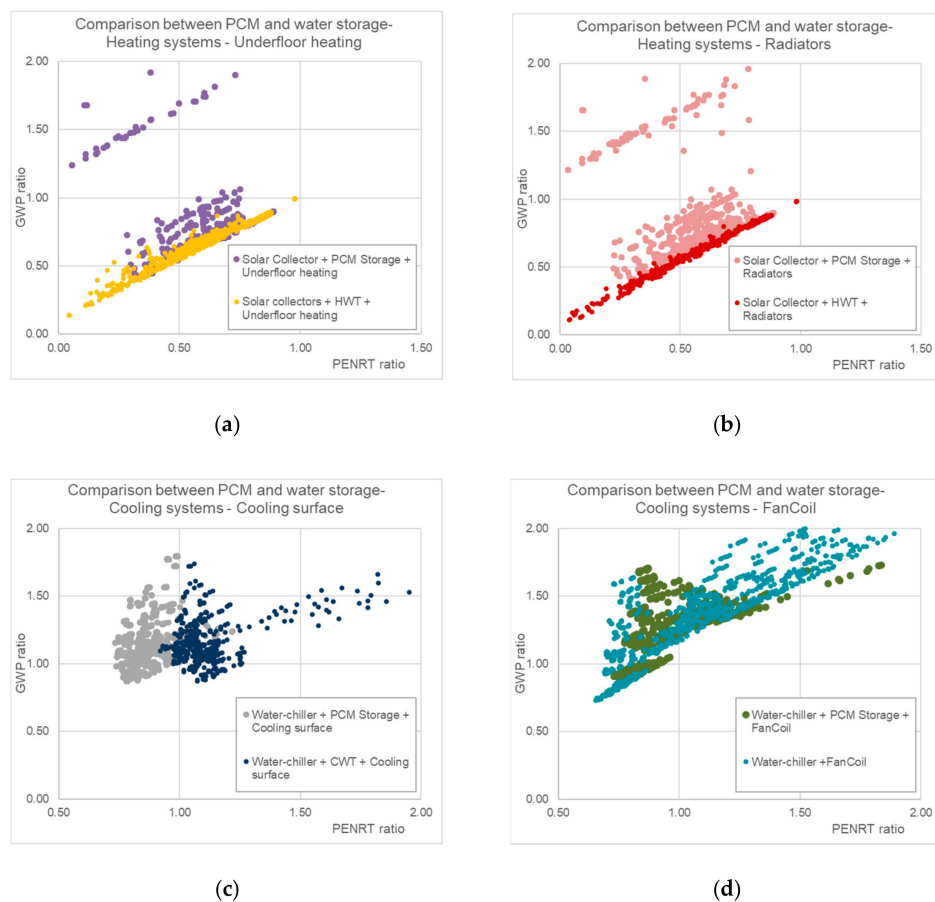


Figure 13. Environmental assessment through “Storage LCA Tool” of water storage systems for (a) centralized heating with underfloor heating; (b) centralized heating with radiators; (c) cooling systems with surface cooling; and (d) cooling systems with fan coil.

In contrast, PCM cooling systems are more likely to provide more efficient energy storage and have lower environmental impact compared to a cold water storage reference system. In cooling applications, the temperature interval usable for cold storage is significantly smaller than in heating applications. A PCM storage unit can fully exploit its advantages here due to its high heat storage capacity in a small temperature range. A PCM storage unit allows a significantly smaller storage volume and higher storage temperatures than a comparable water storage unit. On the one hand, this reduces the environmental impact caused by the production of the storage insulation material and the storage cylinder (especially since the PCM storage unit can be made of plastic, whereas the water storage unit is made of steel or stainless steel); on the other hand, the cold can be generated more efficiently due to a higher storage temperature, so that the environmental impact during the utilization phase is reduced.

This strongly affects the final environmental assessment of the innovative cooling systems (Figure 13c,d). Hence, in cooling systems, a PCM storage may be preferable to water tanks.

Despite the large number of energy concepts simulated, the data platform still needs to be improved and enriched. In this study, no degradation of the PCM’s thermal properties over thousands of cycles is considered, which would affect the LCA results. At the storage system concept level, in this work, PCM applications for decentralized energy systems showed benefits, although the results are restricted to only one building type. In general, further innovative PCM storage materials; energy concepts; or boundary conditions, including locations, building types and insulation standards, can be included and analyzed through the “Storage LCA Tool”. So far, this tool has been assessed (including validation of results) through beta tests, both internal (with help of project partners) and external,

with feedback coming from LCA experts and potential tool users. The tool is freely available on the website https://www.iabp.uni-stuttgart.de/new_downloadgallery/GaBi_Downloads/SpeicherLCA.zip for further testing.

Author Contributions: Conceptualization, R.D.B. and R.H.; methodology, R.H., B.N. and F.K.; software, R.D.B.; validation, B.N., F.K. and R.H.; investigation, R.D.B.; data curation, R.H., B.N., F.K., E.K. and F.P.; writing—original draft preparation, R.D.B.; writing—review and editing, R.H., B.N., F.K. and E.K.; visualization, R.D.B.; supervision, R.H.; project administration, B.N. All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest: The authors declare no conflict of interest.

Appendix A

In Table A1, material properties of the analyzed PCMs are reported according to [13,14]. In Table A2, results of LCA analysis of PCMs are presented. All PCMs are applied for use in a cooling surface with operating temperature range of 10–16 °C.

Table A1. Material properties of PCMs and water. Reproduced from [13,14], Rubitherm: 2019.

Name	Melting Enthalpy (Wh/kg)	Melting Range (°C)	Heat Capacity (kJ/kg K)	Melting Point (°C)	Density (kg/m ³)
RT10HC	0.055	10–12	2.0	10	770
RT10HC (Enc ¹)	0.041	10–12	1.7	10	1270
RT11HC	0.055	10–12	2.0	11	770
RT11HC (Enc ¹)	0.041	10–12	1.7	11	1270
RT18HC	0.072	16–20	2.0	18	825
RT18HC (Enc ¹)	0.053	16–20	1.7	18	1311
RT21	0.043	18–23	2.0	21	825
RT21 (Enc ¹)	0.032	18–23	1.7	21	1311
RT24	0.043	21–24	2.0	24	825
RT24 (Enc ¹)	0.032	21–24	1.7	21	1311
RT62HC	0.043	60–63	2.0	62	825
SP15	0.050	15–17	2.0	15	1350
SP15 (Enc ¹)	0.037	15–17	1.7	15	1700
SP21EK	0.047	21–23	2.0	21	1350
SP21EK (Enc ¹)	0.035	21–23	1.7	21	1551
SP58	0.069	56–59	2.0	58	1350
SP58 (Enc ¹)	0.051	56–59	1.7	58	1551
Water	2.000	0	4.2	0	1000

¹ Macroencapsulated.

Table A2. LCA analyses of PCMs and water applied on a cooling surface with operating temperatures 16–20 °C. Reproduced from [25], IABP: 2019.

Name	GWP (kg CO ₂ eq./kWh ¹)	PENRT (MJ/kWh ¹)	Payback Cycles GWP	Payback Cycles PENRT
RT10HC	18.3	880.9	82.8	226.0
RT10HC (Enc)	91.9	1877.9	372.8	476.4
RT11HC	18.1	877.01	81.9	225.0
RT11HC (Enc)	91.6	1873.8	371.9	475.3
RT18HC	316.4	15,348.6	1309.5	3981.9
RT18HC (Enc)	1398.9	28,602.2	5751.4	7414.2
RT21	314.6	15,325.5	1302.1	3975.9
RT21 (Enc)	1397.3	28,582.2	5745.0	7409.0
RT24	314.2	15,318.6	1300.4	3974.1
RT24 (Enc)	1396.9	28,576.1	5743.5	7407.4
RT62HC	314.2	15,318.6	1300.4	3974.1
SP15	12.0	180.95	49.6	47.0
SP15 (Enc)	88.9	1266.1	360.9	324.6
SP21EK	127.1	1794.2	523.0	465.8
SP21EK (Enc)	777.7	10,673.4	3195.7	2766.8
SP58	527.1	7795.0	2169.2	2023.7
SP58 (Enc)	1173.5	16,616.6	4824.2	4309.6
Water	0.0	0.01	0.009	0.0

¹ kWh material storage capacity.

Appendix B

In this Appendix, relevant information for building energy simulations is reported. Table A3 presents mean, maximal and minimal temperatures of each location. Table A4 gives an overview of the established insulation level. Lastly, in Table A5, specific heating and cooling demands are listed for simulation of the chosen office building [24].

Table A3. Overview of the climate data used to calculate the soil surface temperature. Reproduced from [24], Fraunhofer ISE 2019.

Location	Helsinki	Strasbourg	Athens
$\theta_{\text{Mean, year}}$ (°C)	6.05	11.22	16.54
$\theta_{\text{Monthly_min}}$ (°C)	−4.97	2.09	6.63
$\theta_{\text{Monthly_max}}$ (°C)	18.36	20.07	25.87
Amplitude (°C)	11.67	8.99	9.62

Table A4. U-values were used for energy simulation of office buildings at the different locations. The building efficiency is examined at all locations. Reproduced from [24], Fraunhofer ISE 2019.

Insulation Level	Office Building			
	None (Mediterranean)	Little (Central Europe)	Moderate (North Europe)	Efficient
U exterior wall W/(m ² K)	2.10	0.93	0.38	0.35
U roof W/(m ² K)	2.77	0.56	0.20	0.15
U floor W/(m ² K)	2.83	0.95	0.30	0.20
U window W/(m ² K)	2.83	2.83	1.40	0.70

Table A5. Specific heating and cooling energy demands for simulations of office buildings. Reproduced from [24], Fraunhofer ISE 2019.

Building Type	Insulation Level	Location	Heating Demand kWh/m ² /y	Cooling Demand kWh/m ² /y
Office Building	None	Athens	196.79	53.79
	Little	Athens	75.53	47.84
	Moderate	Athens	29.56	48.01
	Efficient	Athens	17.93	42.74
	Little	Strasbourg	160.20	8.02
	Moderate	Strasbourg	72.76	13.88
	Efficient	Strasbourg	48.53	13.87
	Moderate	Helsinki	137.39	4.08
	Efficient	Helsinki	93.32	4.95

Appendix C

In this Appendix, the overall environmental performances are reported for each single energy concept for better understanding. In Figure A1, results for centralized heating systems are presented.

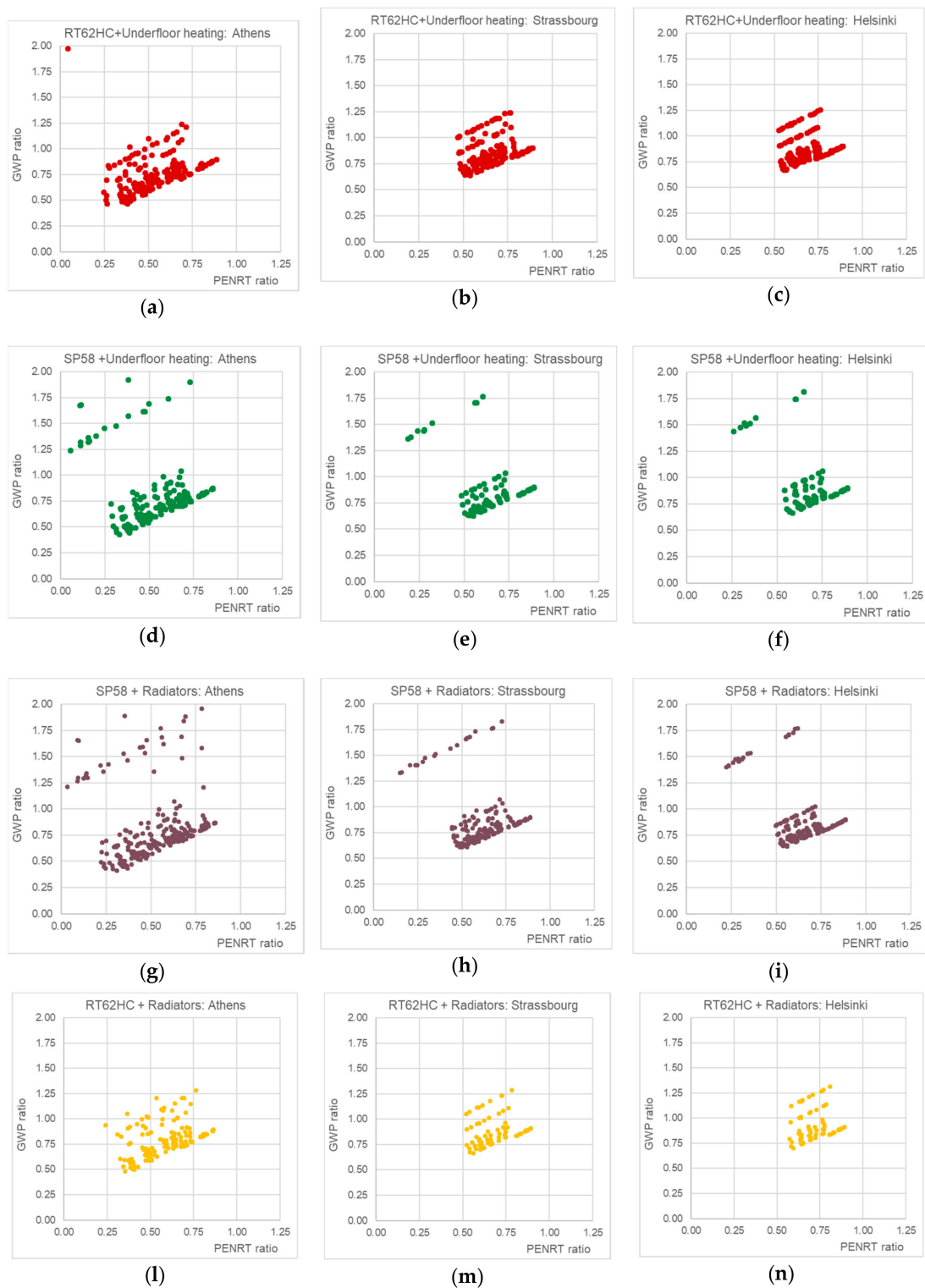


Figure A1. Environmental assessment through “Storage LCA Tool” of PCM storage systems applied for use in centralized heating systems, divided by location and energy concept.

For a better understanding, results for centralized heating systems are presented in Figure A2.

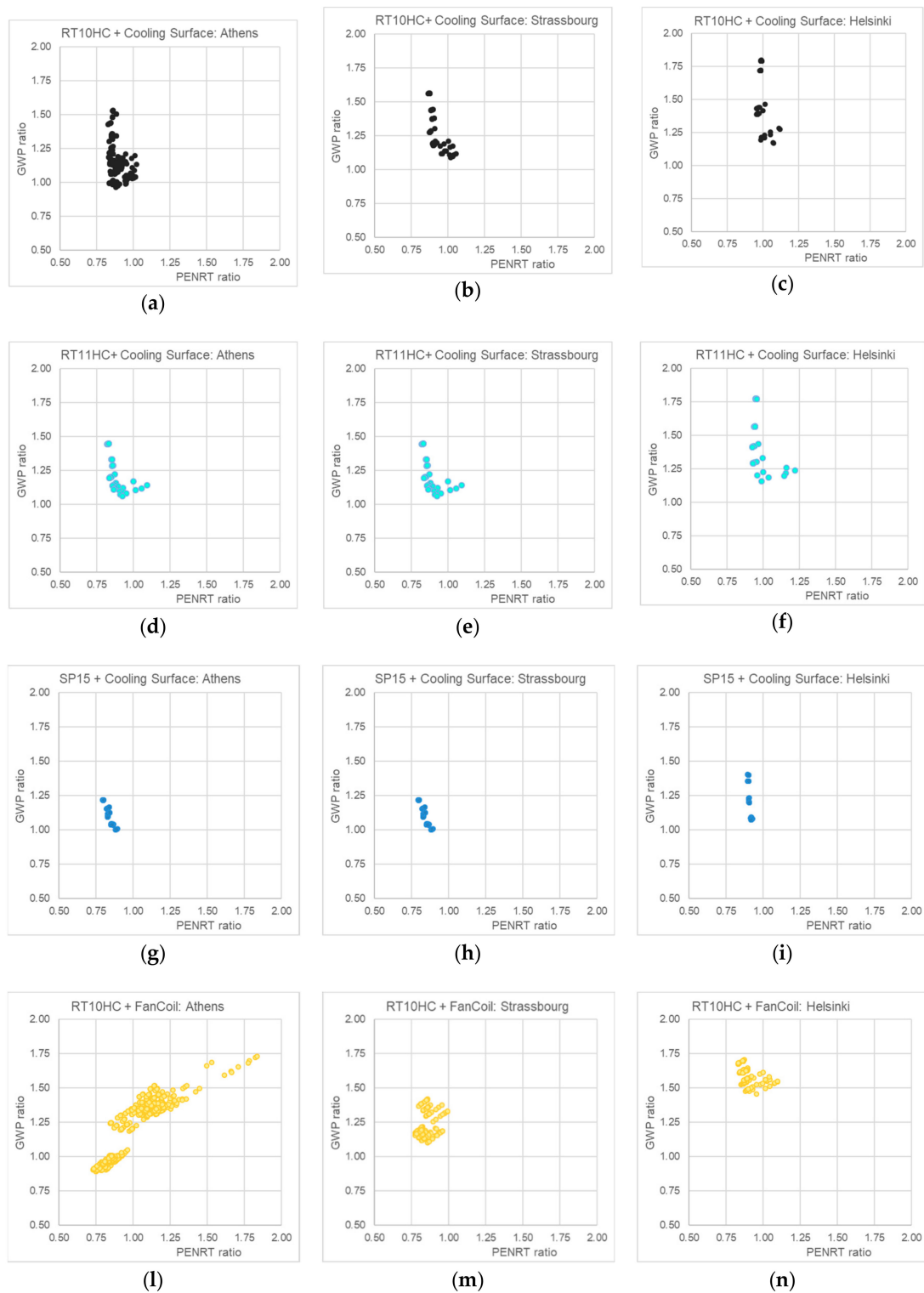


Figure A2. Environmental assessment through “Storage LCA Tool” of PCM storage systems applied for use in centralized cooling systems, divided by location and energy concept.

In Figure A3, results for decentralized systems are presented.

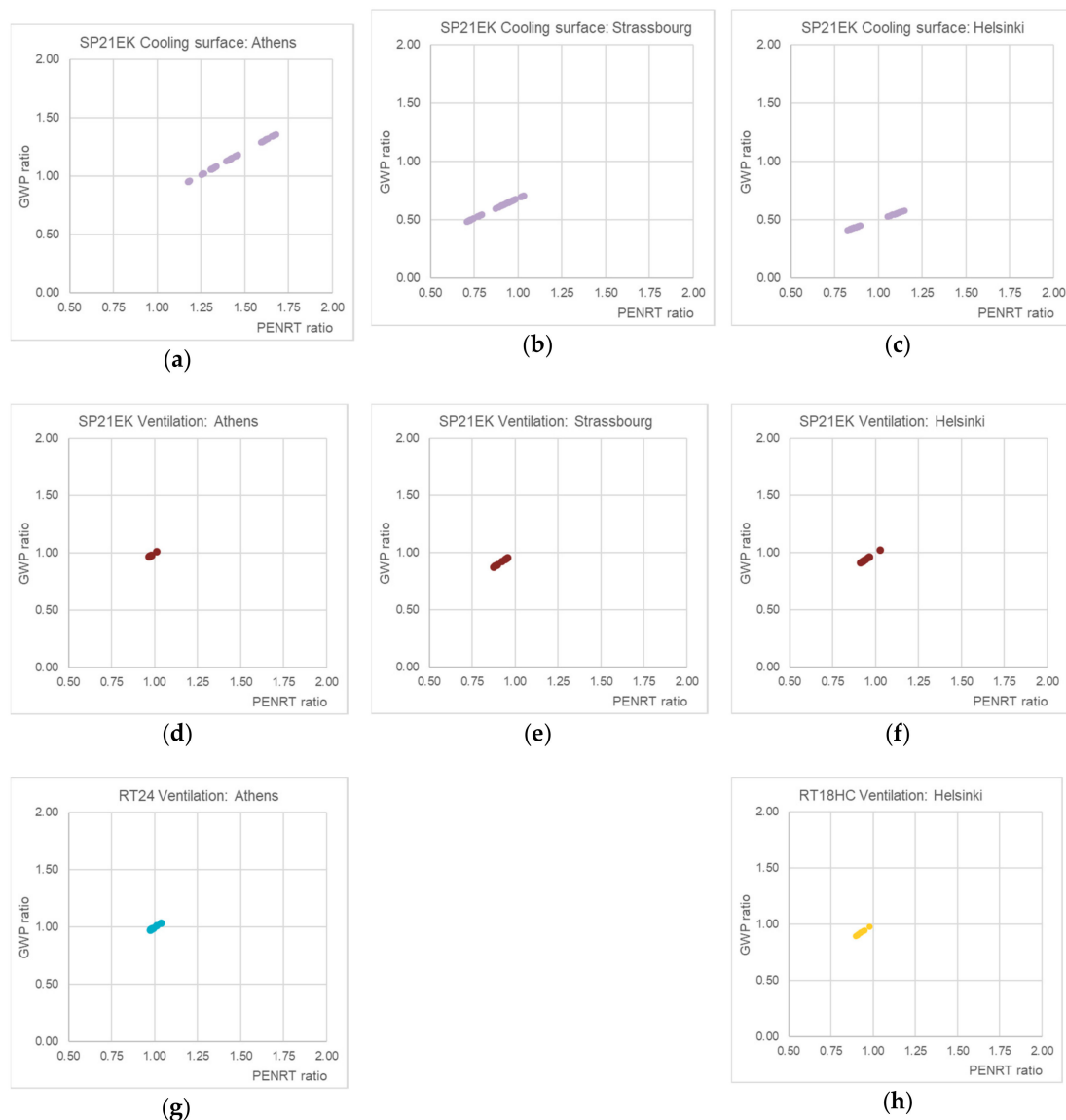


Figure A3. Environmental assessment through “Storage LCA Tool” of PCM storage systems applied for use in decentralized systems, divided by location and energy concept.

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