



**HYSTORE**

Hybrid Services from Advanced  
Thermal Energy Storage Systems

# **D2.1 Report on the final selection of PCM materials for HYSTORE solutions I-III**

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## 4. Nomenclature

AHC	apparent heat capacity
AIT	Austrian Institute of technology, Austria
ATHT	Applied Thermodynamics and Heat Transfer
CCS	carbon capture and storage
CCUS	carbon capture, utilization and storage
CF	carbon footprint
CFD	computational fluid dynamics
CHP	combined heat and power production
CO <sub>2</sub>	carbon dioxide
DEL	Deliverable
DHW	domestic hot water
DSC	differential scanning calorimetry
EoL	end of life
HEX	heat exchanger
HTF	heat transfer fluid
IBC	intermediate bulk container
KTH	Royal Institute of Technology, Sweden
LCA	life cycle assessment
LCT	life cycle thinking
LHTES	latent heat thermal energy storage
MPE	Micro/Multi port extrusion
MS	milestone
PCM	phase change material
PFC	product carbon footprint
RUBI	Rubitherm Technologies GmbH, Germany
RPW	refrigerant-PCM-Water
sIPCMLib	solid/liquid phase change material library
SS	stainless steel
T	temperature
TEMP	temperature
TES	thermal energy storage
WP	work package

## 5. Executive Summary

The objective of this deliverable is to identify the most suitable solid and liquid Phase Change Materials (PCMs) for solutions I-III. This includes considering the materials used in the storage heat exchanger, techno-economic metrics, and environmental impacts, while also aligning with the findings from T1.1.

Different climate conditions at the demsites consider various TES solutions. This deliverable contains results from the final material selection for solutions:

**I: PCM ALL-IN-ONE** solution (developed by AIT, PINK, OCHS, RAAL and RUBI)

**II: PCM LOW-TEMP. HEATING&COOLING** solution (developed by RUBI)

**III: PCM HEATING** (developed by KTH),

an update to Del. 2.2 data, results from the implementation of a PCM database/library and a qualitative Life Cycle Assessment (LCA).

Deliverable 2.2 (M12) showed the various options of potential PCMs in different temperature ranges. They were intensively tested and for each solution two different PCMs were pre-selected. The final chosen PCMs and their thermophysical properties are summarized here. RT60HC (warm side) and RT8HC (cold side) were chosen for the ALL-IN-ONE solution I. SP31 (low temp. heating) and SP12sk (low temp. cooling) are the two PCMs for solution II. For solution III the RT60HC also fits all requirements.

KTH added the final revised bench-scale cycling results summary for both PCMs (RT57HC and RT60HC). The long-term bench-scale cycling stability of these is still confirmed. The sPCMLib database will contain the bench-scale LHTES performance calculations of the cycled PCMs RT57HC and RT60HC, which were mostly performed with Python scripts. The results are supported by the information presented in Del. 2.2 report. These match also the material modeling for Deliverable 2.1 from KTH.

The developed solid-liquid Phase Change Material library (sPCMLib) provides tabulated thermal properties data and graphical visualizations of 178 PCMs, computer code to calculate thermal properties for common simulation software and an interactive interface for generation of customized thermal material properties.

The last chapter deals with the topic of life cycle assessment. Herein the different steps from material extraction over usage up to end of life of the PCMs are presented in a qualitative way to get a rough overview about the carbon footprint of each chosen material.

## 6. Introduction

This section presents a short report summary, a relation to other activities, the contribution of partners to this deliverable 2.1 and it ends with an outline of the deliverable.

### 6.1. Summary

The use of thermal energy storages (TES) becomes more and more relevant as a key technology in reducing greenhouse emissions. In order to advance beyond the state-of-the-art, which primarily consists of sensible TES (e.g. water) with a significantly lower specific storage capacity, latent heat TES are important to improve. For phase change material (PCM) storage systems to be successful over the long run, reliable PCMs that meet the precise TES design parameters and keep them stable throughout long-term cycling must be used.

One aim of this deliverable (within T2.1 and T2.2) is to present the final selection of PCMs for HYSTORE solution I PCM ALL-IN-ONE, solution II PCM LOW-TEMP HEATING & COOLING and solution III PCM HEATING. These phase change materials were intensively tested for their thermal, mechanical and chemical properties in Task 2.2. AIT developed and provided an open source phase change material database with all necessary thermophysical data, computer code for the common programming languages, graphic visualization and an interactive interface for the user. KTH updated data for bench-scale testing of two PCMs for Del. 2.2 and provided information about the final steps in LCA.

### 6.2. Relation to other activities

The gained results from Del. 2.2 about the properties of the tested PCMs are shortly presented here. These data represent the final chosen PCMs and are important for further works, storage material selection and the design of the TES solutions. This report and its data are also relevant for the Milestones MS2 and MS3 because of their storage compatibility. It will affect the final TES system operation, therefore directly influencing the WP3 – storage system and low-level controller development, manufacturing and lab testing, as a whole.

### Contribution of Partners

RUBI (Rubitherm Technologies GmbH) is responsible and editor of D2.1 report. They selected and tested the material, storage and heat exchanger for "PCM LOW TEMP. HEATING&COOLING". AIT and KTH are key partners and contributors for this report. KTH tested the chosen PCMs in a small scale and in a bench-scale. They will develop the PCM HEATING solution and the integration of control methods for the storage solutions. AIT, and RUBI are responsible for the selection of materials for "PCM ALL-IN-ONE solution". Moreover, AIT develops the open source database siPCMLib with material properties, numerical models and programming code, which can be used to perform CFD and Modelica simulations of the storage systems. The qualitative LCA was done by RUBI, KTH and AIT.



### 6.3. Structure of the Deliverable

The deliverable D2.1 report is structured as follows:

- Section 7 presents the final chosen PCMs from **RUBI** for solution I-III. Therefore, the **thermophysical and material intrinsic properties** are shown in tables and diagrams for each solution. The setup and methods were described in Del. 2.2.
- Section 8 presents the work on the solid/liquid Phase Change Material library (**sIPCMLib**) done by **AIT**. This library contains data, correlations and models for the computation of so-called "effective" thermal material properties of PCMs. It also provides code for the calculation of thermal properties, which can be used for numerical modelling of heat transfer and the analysis of thermal performance of PCMs.
- Section 9 shows the qualitative **LCA** of the used phase change material at **KTH** and **AIT**. From material extraction, manufacture, package & transport, usage up to end of life of the product. This LCA should give a rough overview of the carbon footprint from beginning to the end.

## 7. Material finalization /selection RT8HC, RT60HC, SP31

This section presents the final selection of phase change material (PCM) used in each HYSTORE solution I-III. Table 1 presents the given requirements gained from the proposal. Going further, the specifications of RT60HC, RT8HC and SP31 are shortly presented in a few diagrams and tables (reference: Del. 2.2. (M12, HYSTORE))

The selection of PCMs is based on many criteria, measurement methodologies, and the material's environmental impact. Some topics and test methods were already included in D2.2. As a result, we can utilize both organic (paraffins, fatty acids, alcohols, etc.) and inorganic (salt hydrates, nitrate or nitrite salts).

Table 1. Specific operating conditions for each HYSTORE solution

<b>Solution I: PCM ALL-IN-ONE (AIT)</b>	<b>Solution II: LOW-TEMP. PCM HEATING &amp; COOLING (RUBI)</b>	<b>Solution III: PCM HEATING (KTH)</b>
<ul style="list-style-type: none"> <li>• Average storage temperature ~60 °C</li> <li>• Sharp peak during solidification for domestic hot water (DHW)</li> <li>• Heating with secondary loop stainless steel (SS) HEX to 50°C</li> <li>• Size of the thermal storage capacity about 186 l</li> <li>• Density ~800 kg/m<sup>3</sup></li> <li>• Non-corrosive against aluminum</li> <li>• organic PCM</li> <li>• Heat storage capacity &gt;200 kJ/kg (55.6Wh/kg)</li> </ul>	<ul style="list-style-type: none"> <li>• Low temperature cooling: average storage temperature ~8 °C</li> <li>• Plan: research activity inorganic PCM 40-45°C</li> <li>• Updated conditions project site: PCM ~30°C for low temperature heating (see 7.2)</li> <li>• Long-term stable through separation inhibitors</li> <li>• Non-corrosive against polymeric materials</li> <li>• Non-flammable</li> </ul>	<ul style="list-style-type: none"> <li>• 5-10 K temperature difference with heat transfer fluid (HTF)</li> <li>• Freezing ≥ 40-45 °C</li> <li>• Melting ≤ 55-60 °C</li> <li>• Average ~50 °C</li> <li>• Approximate PCM volume: 750 l</li> <li>• On HTF side approximately:</li> <li>• @PCM freezing: inlet ~25-35 °C (outdoor@10°C)</li> <li>• @PCM melting: inlet ~65 °C (outdoor@10°C)</li> </ul>

### 7.1. Solution I: PCM ALL-IN-ONE

#### RT60HC

The chosen PCM RT60HC is a biobased, organic PCM with a high heat storage capacity of over 200 kJ/kg. It has a density of ~0.8 kg/l and has no corrosive effects on metals. RT60HC is easy to handle, though its form are small plates or pellets. Figure 1 shows the sharp enthalpy peaks for melting and solidification in the temperature range 60-61°C. For this, all given requirements are fulfilled by RT60HC and it is chosen as the final phase change material for the warm side of solution I: ALL-IN-ONE.

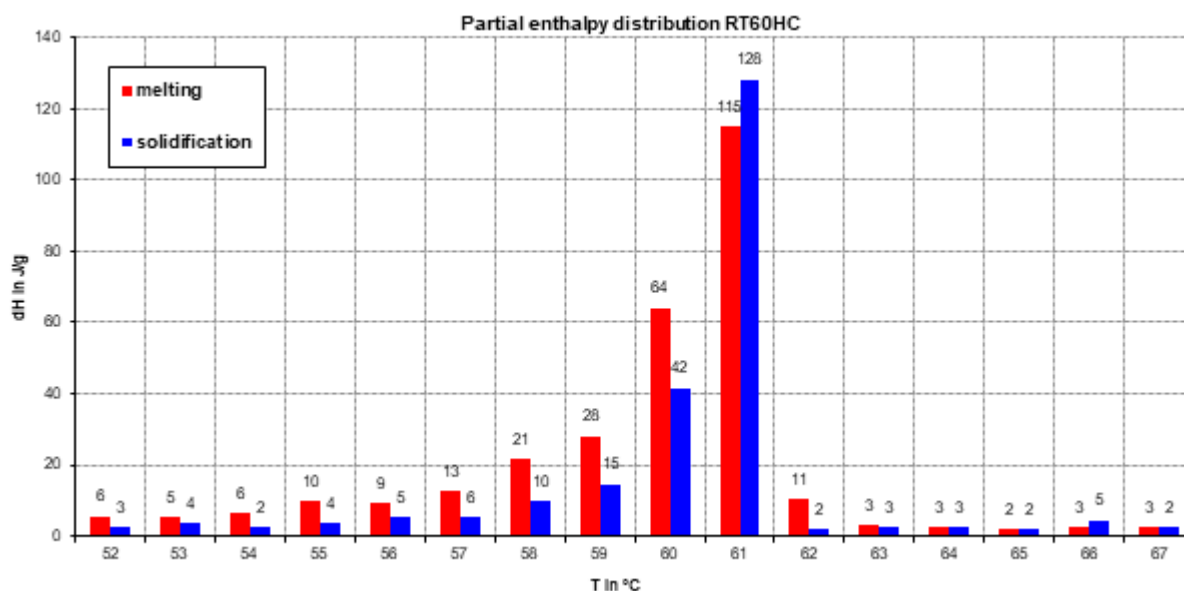


Figure 1. partial enthalpy distribution of RT60HC

Table 2. main thermophysical properties of RT60HC

The most important data	Typical values
Melting area	58-61 [°C] (main peak: 60°C)
Congeeing area	50-58 [°C] (main peak: 60°C)
Heat storage capacity $\pm 7.5\%$ (combination of latent and sensible heat in a temperature range of 52°C to 67°C)	210 [kJ/kg] 58 [Wh/kg]
Specific heat capacity	2 [kJ/kg*K]
Density solid (at 25°C)	0.85 [kg/l]
Density liquid (at 70°C)	0.75 [kg/l]
Heat conductivity (both phases)	0.2 [W/(m*K)]
Volume expansion	12 [%]
Flash point	175 [°C]
Max. operation temperature	90 [°C]

## RT8HC

The chosen PCM RT8HC is an organic PCM with a high heat storage capacity of 190 kJ/kg. It has a density of  $\sim 0.8$  kg/l and has no corrosive effects on metals. RT8HC is liquid at room temperature and for this easy to handle. Figure 2 Figure 1 shows the sharp enthalpy peaks for melting and solidification in the temperature range 7-8°C. RT8HC also fulfils all necessary requirements, though AIT might test this in the future, depending on the available resources. Rubitherm manufactured a small storage for solution II and RT8HC was tested for several cycles with an aluminum heat exchanger with very good results as seen in Figure 3.

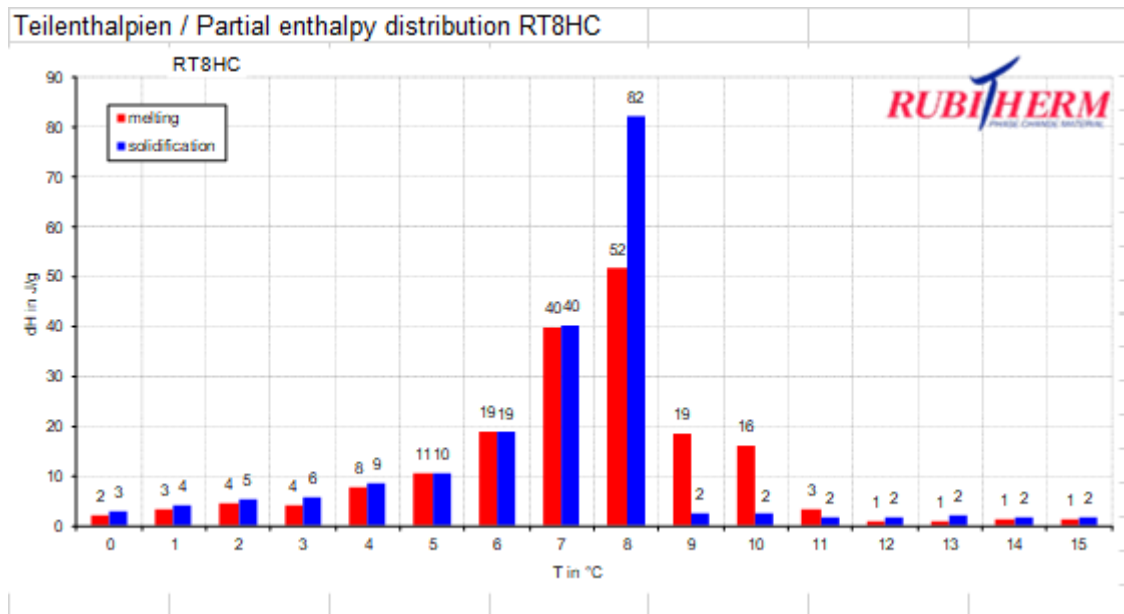


Figure 2. partial enthalpy of RT8HC

Table 3. main thermophysical properties of RT8HC

The most important data	Typical values
Melting area	7-9 [°C] (main peak: 8°C)
Congeealing area	8-7 [°C] (main peak: 8°C)
Heat storage capacity $\pm 7.5\%$ (combination of latent and sensible heat in a temperature range of 52°C to 67°C)	190 [kJ/kg] 53 [Wh/kg]
Specific heat capacity	2 [kJ/kg*K]
Density solid (at 25°C)	0.88 [kg/l]
Density liquid (at 70°C)	0.77 [kg/l]
Heat conductivity (both phases)	0.2 [W/(m*K)]
Volume expansion	12.5 [%]
Flash point	120 [°C]
Max. operation temperature	40 [°C]

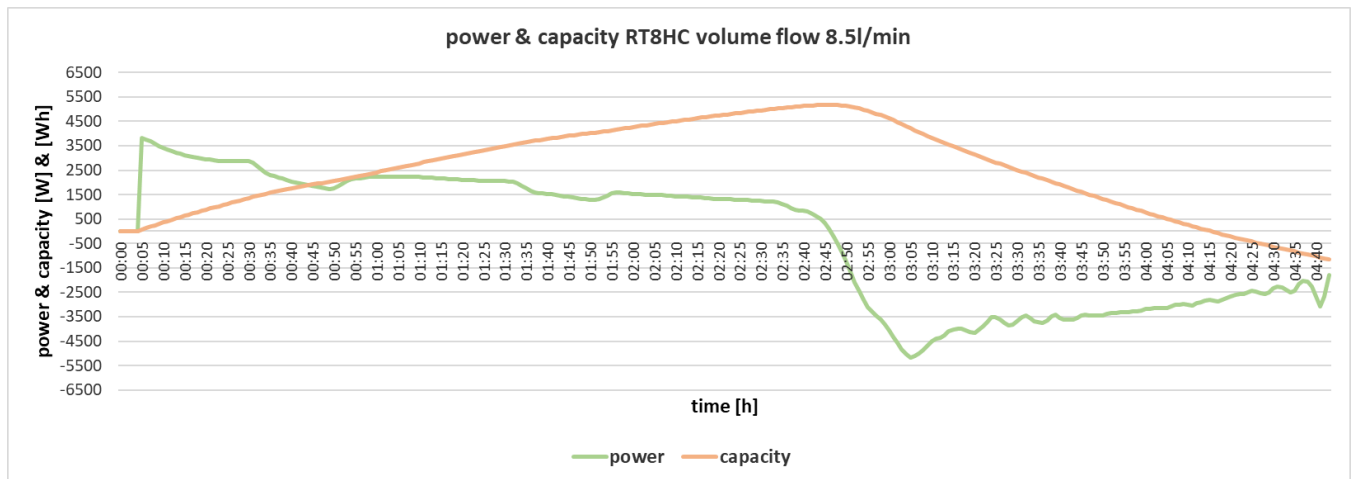


Figure 3. power and capacity of the TES with aluminum HEX; RT8HC

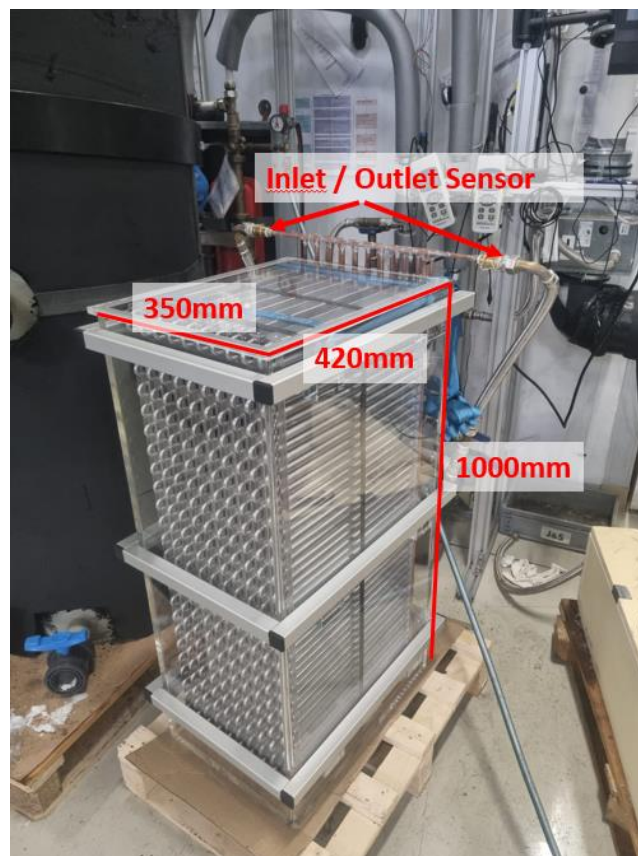


Figure 4. thermal energy storage with aluminum heat exchanger

Figure 4 pictures the TES unit for solution II LOW TEMP COOLING at RUBI. The dimensions of the storage are 350x420x1000 mm. The storage material consists of plexiglass and a metal bracing for additional stability. An aluminum heat exchanger is located on the inside. For testing of power and capacity of the storage, it was filled with RT8HC. There are also water connections for easy installation on the top of the storage. Figure 3 shows a diagram of the measured power and capacity of RT8HC with a flow rate of 8.5l per minute. The capacity rises over time upto its maximum peak at 2h45min. After this

point the capacity decreases to its minimum after 4h40 min. The power of the storage decreases quite constantly over time with a fast drop-off at the capacity peak at 2h45min.

## 7.2. Solution II: LOW-TEMP. HEATING & COOLING

### SP31

The chosen PCM SP31 is an inorganic PCM with a high heat storage capacity of over 200 kJ/kg. It has a density of ~1.3 kg/l and has a corrosive effect on metals. For this the use of a polymer storage and HEX is recommended. SP31 is solid at room temperature and has to be melted before filling in. Figure 5 shows the sharp enthalpy peaks for melting and solidification in the temperature range 30-33°C. The used separation inhibitors make it a long-term stable PCM. It fulfils all given requirements as is chosen as the final material for the low temperature heating PCM. Rubitherm manufactured a small storage for solution II and SP31 was tested for some cycles inside together with a polymeric HEX. The power of the storage can be seen in Figure 6.

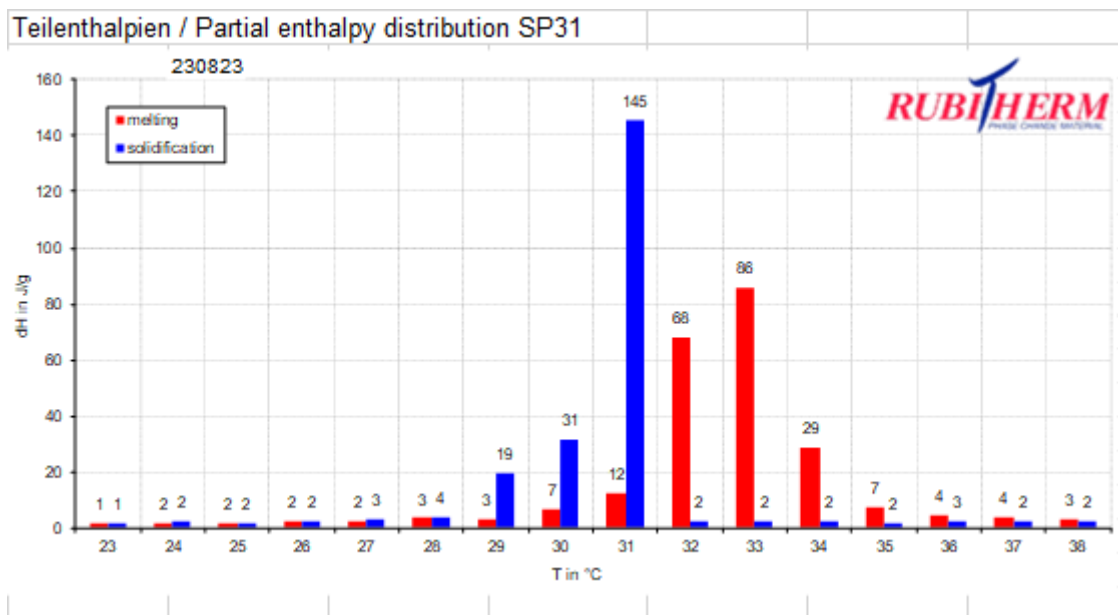


Figure 5. partial enthalpy of SP31

Table 4. main thermophysical properties of SP31

The most important data	Typical values
Melting area	31-33 [°C] (main peak: 32°C)
Congeaing area	28-30 [°C] (main peak: 30°C)
Heat storage capacity $\pm 7.5\%$ (combination of latent and sensible heat in a temperature range of 52°C to 67°C)	210 [kJ/kg] 58 [Wh/kg]
Specific heat capacity	2 [kJ/kg*K]
Density solid (at 25°C)	$\sim 1.35$ [kg/l]
Density liquid (at 70°C)	$\sim 1.25$ [kg/l]
Heat conductivity (both phases)	$\sim 0.5$ [W/(m*K)]
Volume expansion	$\sim 5$ [%]
Max. operation temperature	50 [°C]
Corrosion	Corrosive effects on metals

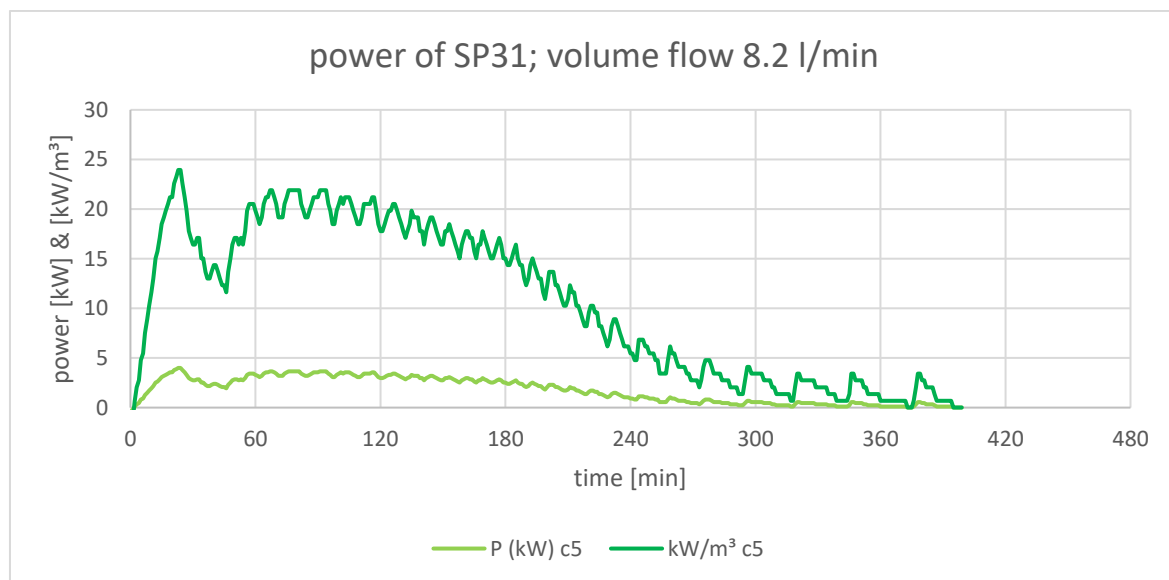


Figure 6. diagram of power of the SP31



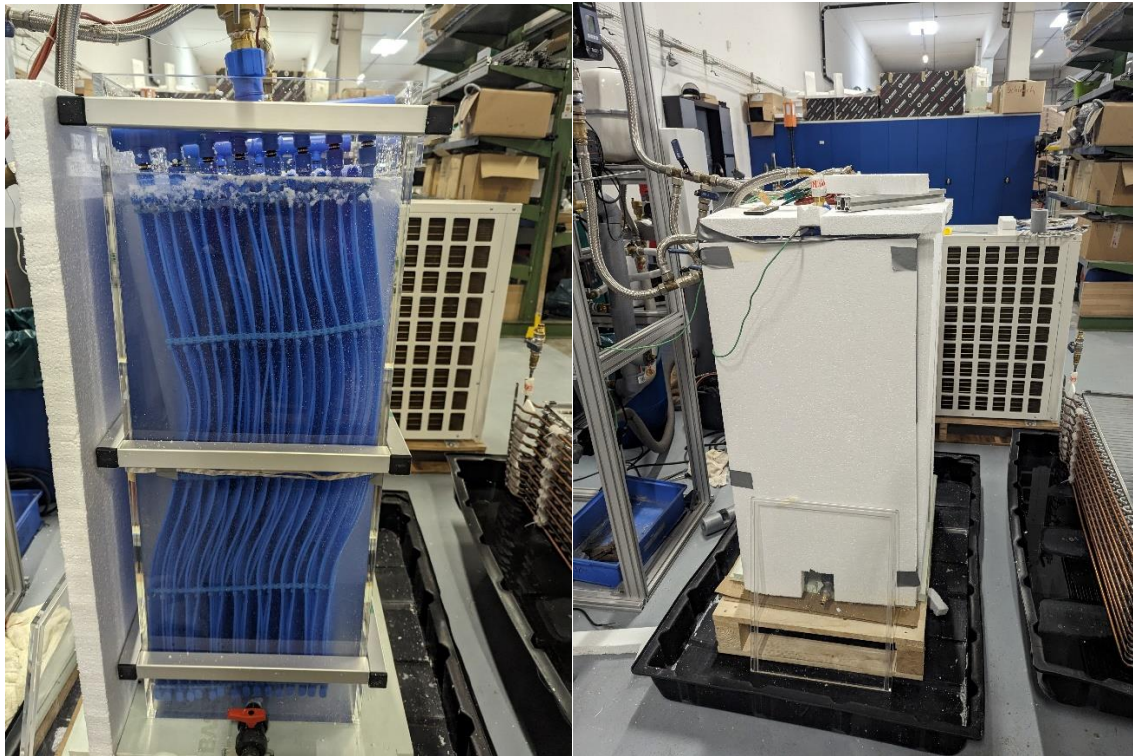


Figure 7. thermal energy storage with polymer heat exchanger and insulation

Figure 7 pictures the TES unit for solution II LOW TEMP HEATING at RUBI. The dimensions of the storage are 350x420x1000 mm. The storage material consists of plexiglass and a metal bracing for additional stability. A polymer heat exchanger is located on the inside. For testing of power and capacity of the storage, it was filled with SP31 and insulated. There are also water connections for easy installation on the top of the storage. Figure 6 shows a diagram of the measured power of SP31 with a flow rate of 8.2l per minute. The real data of the storage starts after 60 min, the maximum power of the storage is  $\sim 21$  kW/m<sup>3</sup> and it decreases over time as the storage is discharged. This is a prototype and the SP31 will be part of the demosite in Montserrat.

The initial idea of the Montserrat PCM system was to use a low-temperature PCM in parallel to the sorption system as added inertia to the cooling system. However, based on the pre-analysis of Montserrat's demand profiles and the detailed analysis of its thermal heating and cooling network, it is imperative to change its final application from low temperature cooling to low waste heat temperature application (temperature of phase change around 31°C). This need arises firstly from the inertia already existing in the district cooling network that would dilute the role of PCM storage at low temperature, and secondly from the operating characteristics of the thermochemical sorption system, where heat rejection occurs at a peak temperature of 35°C. Ideally, the return temperature should be targeted at 30°C. The heat thus rejected will be harnessed to preheat the high demand of domestic hot water of the building, which is introduced into the system at a temperature range of 8°C to 15°C. Consequently, to optimize the system's efficiency and facilitate this process, the phase change temperature of the PCM must be set at 31°C.



This adjustment is pivotal in our project's strategy to transition from utilizing a low-temperature PCM (spanning 7°C to 12°C) to one operating around 30°C. This strategic shift is not merely a technical preference, but a calculated decision aimed at augmenting the efficiency of preheating DHW (the DHW demand does not overlap with the cooling demand of the installation, hence the benefits of TES), especially when compared to the limited benefits of employing a low-temperature PCM in parallel with the sorption process within a district cooling network framework. The proposed approach leverages higher temperature PCM to more effectively capture and utilize waste heat, thereby enhancing overall system performance and contributing to significant energy savings.

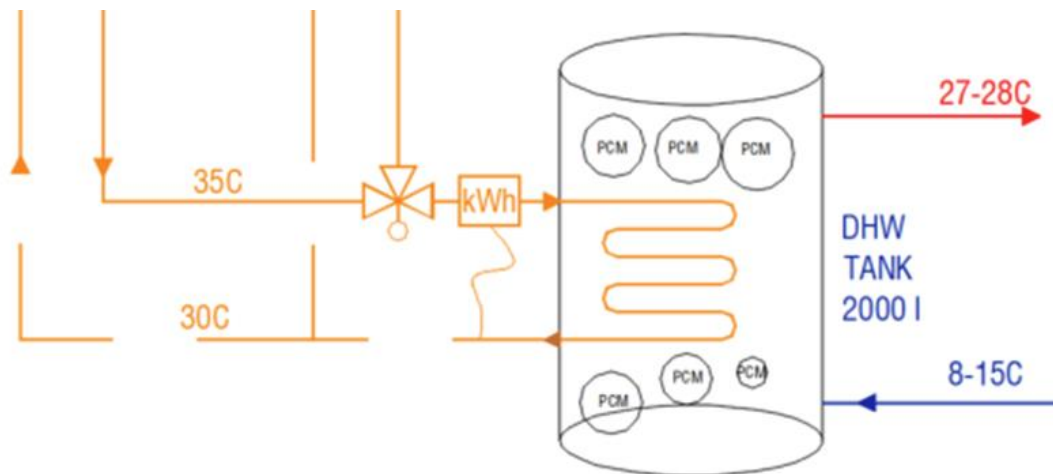


Figure 8. demosite for solution II in Montserrat

### 7.3. Solution III: PCM HEATING

#### RT60HC

The given requirements for solution III PCM HEATING (developed by KTH) are nearly the same as for solution I and for this the usage of the same PCM RT60HC is recommended. The PCM will be used in a stainless-steel tank and the volume should be ~750 I. In the next months it has to be clarified whether the PCM is encapsulated or not. This requires the use of a heat transfer fluid or a copper coil.

### 7.4. Updated data from Deliverable 2.2

Upon final calculations and adjustments on the RT57HC and RT60HC bench-scale testing performed at KTH, as reported in Deliverable 2.2 report, the final data on the cycling tests are summarized in Table 5, Table 6, Table 7 and Table 8. These have some minor refinements as compared to Deliverable 2.2 report (Tables 25-28) on heat loss.

In summary, these PCMs were cycled between around 35 °C and 85 °C, while the data analysis was done between 35 °C to 79 °C (filtering out the isothermal parts). Each heating and cooling cycle accounted for around 16 hours. Heat storage and thus heat loss calculations were also

considered for the corresponding time points between the 35 °C to 79 °C temperature ranges. This corresponded up to ~9 hours in heating, ~11 hours in cooling for RT57HC and up to ~7 hours in heating and ~9 hours in cooling for RT60HC. The heat stored in the SS HEX parts were calculated without considering the time factor, only as the sensible heat stored between 35 °C-79 °C. The heat loss was calculated by deducting the heat stored from the heat supplied. This corresponds to the heat from the HTF deducted by the total absorbed by the PCM and the SS HEX parts during heating cycles, and the heat from the PCM deducted by the sum of that absorbed by the HTF and SS HEX parts during cooling cycles. Further details of this methodology are found in Deliverable 2.2 report. Although these heat loss data are only relevant to this bench-scale system, the methodology is relevant even to the HYSTORE solutions and hence (while serving as an addendum to the values in Deliverable 2.2 (Tables 25-28)), this is presented here.

It is important to note here that due to the quite raw specific heat capacity values from the calorimetric method employed in the material analysis (c.f. Deliverable 2.2, section 6.1.2), the PCM heat storage capacities here appear to be over-estimated. This is more evident in the heating cycles. In addition, the weight of the stainless steel LHTES container and HEX parts (referred to as SS-HEX as a whole) altogether which is considered as 150 kg is also an approximate value given by these units' manufacturer. These uncertainties on specific heat capacities and approximation on the SS-HEX mass affect the estimation of the heat stored in these SS parts, considered as 3300 kJ. When comparing the TES capacity from the PCM (latent and sensible heats combined) versus the heat provided (in heating) and absorbed (in cooling) by the heat transfer fluid (HTF) and heat absorbed by the SS-HEX (in the considered temperature range), it seems that the heat loss in fact is a heat gain. This is however merely an artifact due to these uncertainties in specific heat capacities as well as the SS-HEX weight.

Nevertheless, this aspect does not affect the obtained PCM-TES capacity data for cycling performance, which are very comparable and consistent throughout all the tested cycles, 27 for RT57HC and 53 for RT60HC. These verify very satisfactory cycling stability of both these PCMs RT57HC and RT60HC for this type of long-term cycling.

Table 5. RT57HC LHTES capacity, energy delivered by HTF and heat losses for 27 heating cycles

No. Cycle	TES capacity from PCM [kJ]	%difference of each cycle Vs. average	HTF [kJ]	%difference of each cycle Vs. average	Heat stored in the Stainless Steel (kJ)	Heat losses (kJ)	Real % of energy loss
Cycle 1	19135	0.51%	-15516	0.1%	3300	6919	-45%
Cycle 2	19289	0.30%	-15015	2.7%	3300	7574	-50%
Cycle 3	19215	0.09%	-15695	0.8%	3300	6820	-43%
Cycle 4	19321	0.46%	-15884	1.8%	3300	6737	-42%
Cycle 5	19296	0.33%	-15941	2.1%	3300	6654	-42%
Cycle 6	19284	0.27%	-15679	0.8%	3300	6906	-44%
Cycle 7	19219	0.07%	-15757	1.2%	3300	6763	-43%
Cycle 8	19261	0.15%	-15392	0.7%	3300	7169	-47%

Cycle 9	19197	0.18%	-15444	0.5%	3300	7054	-46%
Cycle 10	19212	0.11%	-15428	0.6%	3300	7084	-46%
Cycle 11	19202	0.16%	-15407	0.7%	3300	7095	-46%
Cycle 12	19268	0.19%	-15778	1.3%	3300	6790	-43%
Cycle 13	19199	0.17%	-15364	0.9%	3300	7135	-46%
Cycle 14	19272	0.21%	-15041	2.6%	3300	7531	-50%
Cycle 15	19297	0.34%	-15731	1.0%	3300	6866	-44%
Cycle 16	19223	0.05%	-15664	0.7%	3300	6859	-44%
Cycle 17	19249	0.09%	-15659	0.7%	3300	6890	-44%
Cycle 18	19276	0.22%	-15748	1.1%	3300	6828	-43%
Cycle 19	19286	0.28%	-15341	1.0%	3300	7245	-47%
Cycle 20	19314	0.42%	-15136	2.1%	3300	7478	-49%
Cycle 21	19281	0.25%	-15735	1.0%	3300	6846	-44%
Cycle 22	19290	0.30%	-15613	0.4%	3300	6977	-45%
Cycle 23	19233	0.00%	-15523	0.1%	3300	7010	-45%
Cycle 24	19279	0.24%	-15510	0.1%	3300	7069	-46%
Cycle 25	19301	0.35%	-15631	0.5%	3300	6970	-45%
Cycle 26	19298	0.34%	-15230	1.6%	3300	7368	-48%
Cycle 27	18574	3.42%	-15551	0.1%	3300	6323	-41%
<b>Average [kJ]</b>	<b>19232</b>		<b>-15534</b>		<b>3300</b>	<b>6998</b>	<b>-45%</b>
<b>Average [kWh]</b>	<b>5.2</b>						

Table 6. RT57HC LHTES capacity, energy delivered by HTF and heat losses for 27 cooling cycles

No. Cycle	TES capacity from PCM [kJ]	%difference of each cycle Vs. average	HTF [kJ]	%difference of each cycle Vs. average	Heat stored in the Stainless Steel (kJ)	Heat losses (kJ)	Real % of energy loss
Cycle 1	-15767	0.49%	11630	0.80%	3300	-837	5%
Cycle 2	-15881	0.11%	11880	2.10%	3300	-702	4%
Cycle 3	-15876	0.08%	11545	0.35%	3300	-1032	6%
Cycle 4	-15838	0.12%	11697	1.15%	3300	-841	5%
Cycle 5	-15865	0.02%	11391	0.44%	3300	-1174	7%
Cycle 6	-15890	0.15%	11202	1.43%	3300	-1388	9%
Cycle 7	-15855	0.03%	11476	0.00%	3300	-1079	7%
Cycle 8	-15867	0.03%	11413	0.33%	3300	-1154	7%
Cycle 9	-15874	0.07%	11502	0.13%	3300	-1072	7%
Cycle 10	-15851	0.05%	11574	0.51%	3300	-977	6%
Cycle 11	-15857	0.02%	11437	0.21%	3300	-1120	7%
Cycle 12	-15865	0.02%	11379	0.51%	3300	-1186	7%
Cycle 13	-15857	0.02%	11467	0.05%	3300	-1090	7%

Cycle 14	-15868	0.04%	11426	0.26%	3300	-1142	7%
Cycle 15	-15861	0.00%	11357	0.62%	3300	-1204	8%
Cycle 16	-15857	0.02%	11325	0.78%	3300	-1232	8%
Cycle 17	-15865	0.02%	11248	1.19%	3300	-1317	8%
Cycle 18	-15870	0.05%	11289	0.97%	3300	-1282	8%
Cycle 19	-15862	0.01%	11316	0.83%	3300	-1246	8%
Cycle 20	-15865	0.02%	11278	1.03%	3300	-1287	8%
Cycle 21	-15864	0.02%	11265	1.10%	3300	-1300	8%
Cycle 22	-15862	0.00%	11229	1.29%	3300	-1333	8%
Cycle 23	-15878	0.09%	11587	0.57%	3300	-991	6%
Cycle 24	-15882	0.11%	11871	2.05%	3300	-711	4%
Cycle 25	-15859	0.01%	11739	1.36%	3300	-820	5%
Cycle 26	-15853	0.04%	11671	1.01%	3300	-882	6%
Cycle 27	-15852	0.04%	11669	1.00%	3300	-883	6%
<b>Average [kJ]</b>	<b>-15861</b>		<b>11476</b>		<b>3300</b>	<b>-1085</b>	<b>7%</b>
<b>Average [kWh]</b>	<b>4.4</b>						

Table 7. RT60HC LHTES capacity, energy delivered by HTF and heat losses for 53 heating cycles

No. Cycle	TES capacity from PCM [kJ]	%difference of each cycle Vs. average	HTF [kJ]	%difference of each cycle Vs. average	Heat losses (kJ)	Heat stored in the Stainless Steel (kJ)	% heat loss
Cycle 1	14959	1.77%	-14288	3.40%	3971	3300	-28%
Cycle 2	15257	0.20%	-14743	0.32%	3814	3300	-26%
Cycle 3	15178	0.31%	-14612	1.21%	3866	3300	-26%
Cycle 4	15228	0.01%	-14298	3.33%	4230	3300	-30%
Cycle 5	15225	0.00%	-14511	1.89%	4014	3300	-28%
Cycle 6	15209	0.12%	-14528	1.78%	3981	3300	-27%
Cycle 7	15223	0.02%	-14521	1.82%	4002	3300	-28%
Cycle 8	15218	0.06%	-14278	3.46%	4240	3300	-30%
Cycle 9	15343	0.76%	-13266	10.31%	5377	3300	-41%
Cycle 10	15216	0.07%	-14312	3.24%	4204	3300	-29%
Cycle 11	15232	0.04%	-14546	1.65%	3986	3300	-27%
Cycle 12	15231	0.03%	-14553	1.61%	3978	3300	-27%
Cycle 13	15238	0.08%	-14676	0.77%	3862	3300	-26%
Cycle 14	15229	0.02%	-14795	0.03%	3734	3300	-25%
Cycle 15	15219	0.05%	-14542	1.68%	3977	3300	-27%
Cycle 16	15225	0.01%	-14348	3.00%	4177	3300	-29%
Cycle 17	15237	0.07%	-14424	2.48%	4113	3300	-29%
Cycle 18	15213	0.09%	-14347	3.00%	4166	3300	-29%

Cycle 19	15228	0.01%	-14076	4.84%	4452	3300	-32%
Cycle 20	15233	0.04%	-14187	4.09%	4346	3300	-31%
Cycle 21	15240	0.09%	-14448	2.31%	4092	3300	-28%
Cycle 22	15229	0.02%	-14542	1.68%	3987	3300	-27%
Cycle 23	15200	0.17%	-14680	0.75%	3820	3300	-26%
Cycle 24	15211	0.10%	-14446	2.33%	4065	3300	-28%
Cycle 25	15235	0.06%	-14455	2.27%	4080	3300	-28%
Cycle 26	15264	0.25%	-14704	0.59%	3860	3300	-26%
Cycle 27	15203	0.15%	-14793	0.01%	3710	3300	-25%
Cycle 28	15231	0.03%	-14567	1.51%	3964	3300	-27%
Cycle 29	15240	0.09%	-14655	0.92%	3885	3300	-27%
Cycle 30	15242	0.10%	-14758	0.22%	3784	3300	-26%
Cycle 31	15232	0.04%	-14618	1.17%	3914	3300	-27%
Cycle 32	15248	0.14%	-14678	0.76%	3870	3300	-26%
Cycle 33	15245	0.12%	-14872	0.55%	3673	3300	-25%
Cycle 34	15203	0.15%	-14842	0.34%	3661	3300	-25%
Cycle 35	15223	0.02%	-15038	1.67%	3485	3300	-23%
Cycle 36	15242	0.10%	-15372	3.93%	3170	3300	-21%
Cycle 37	15222	0.03%	-15379	3.98%	3143	3300	-20%
Cycle 38	15225	0.01%	-15368	3.90%	3157	3300	-21%
Cycle 39	15210	0.11%	-15025	1.59%	3485	3300	-23%
Cycle 40	15250	0.15%	-15162	2.51%	3388	3300	-22%
Cycle 41	15230	0.03%	-15124	2.25%	3406	3300	-23%
Cycle 42	15209	0.11%	-15431	4.33%	3078	3300	-20%
Cycle 43	15230	0.03%	-15380	3.98%	3150	3300	-20%
Cycle 44	15246	0.13%	-15260	3.17%	3286	3300	-22%
Cycle 45	15224	0.02%	-15198	2.75%	3326	3300	-22%
Cycle 46	15246	0.13%	-15190	2.70%	3356	3300	-22%
Cycle 47	15250	0.15%	-15320	3.58%	3230	3300	-21%
Cycle 48	15228	0.01%	-15110	2.16%	3418	3300	-23%
Cycle 49	15231	0.03%	-15137	2.34%	3394	3300	-22%
Cycle 50	15258	0.21%	-15279	3.30%	3279	3300	-21%
Cycle 51	15237	0.07%	-15340	3.72%	3197	3300	-21%
Cycle 52	15232	0.04%	-15642	5.75%	2890	3300	-18%
Cycle 53	15240	0.09%	-15748	6.47%	2792	3300	-18%
<b>Average [kJ]</b>	<b>15226</b>		<b>-14791</b>		<b>3736</b>	3300	<b>-25%</b>
<b>Average [kWh]</b>	<b>4.23</b>						

Table 8. RT60HC LHTES capacity, energy delivered by HTF and heat losses for 53 cooling cycles

No. Cycle	TES capacity from PCM [kJ]	%difference of each cycle Vs. average	HTF [kJ]	%difference of each cycle Vs. average	Heat stored in the Stainless Steel (kJ)	Heat losses (kJ)	% heat loss
Cycle 1	-13217	2.28%	11524	3.50%	3300	1607	-12%
Cycle 2	-13527	0.02%	11621	4.21%	3300	1394	-10%
Cycle 3	-13515	0.08%	11766	5.29%	3300	1551	-11%
Cycle 4	-13484	0.30%	11576	3.88%	3300	1392	-10%
Cycle 5	-13564	0.29%	11130	0.58%	3300	866	-6%
Cycle 6	-13527	0.02%	11234	1.35%	3300	1007	-7%
Cycle 7	-13495	0.22%	11127	0.55%	3300	932	-7%
Cycle 8	-13562	0.27%	11196	1.07%	3300	934	-7%
Cycle 9	-13535	0.07%	11275	1.65%	3300	1040	-8%
Cycle 10	-13504	0.16%	11156	0.77%	3300	952	-7%
Cycle 11	-13539	0.10%	11122	0.52%	3300	883	-7%
Cycle 12	-13511	0.10%	11120	0.50%	3300	909	-7%
Cycle 13	-13507	0.13%	11015	0.28%	3300	808	-6%
Cycle 14	-13530	0.04%	10950	0.75%	3300	720	-5%
Cycle 15	-13548	0.17%	11147	0.70%	3300	899	-7%
Cycle 16	-13522	0.02%	11055	0.02%	3300	833	-6%
Cycle 17	-13546	0.15%	11030	0.16%	3300	784	-6%
Cycle 18	-13515	0.07%	11052	0.00%	3300	837	-6%
Cycle 19	-13541	0.12%	11051	0.00%	3300	810	-6%
Cycle 20	-13544	0.14%	11003	0.36%	3300	759	-6%
Cycle 21	-13504	0.16%	11020	0.24%	3300	816	-6%
Cycle 22	-13513	0.09%	10929	0.91%	3300	716	-5%
Cycle 23	-13529	0.03%	11287	1.74%	3300	1058	-8%
Cycle 24	-13521	0.03%	11308	1.89%	3300	1087	-8%
Cycle 25	-13526	0.00%	11187	1.00%	3300	961	-7%
Cycle 26	-13531	0.05%	11357	2.25%	3300	1126	-8%
Cycle 27	-13494	0.23%	11333	2.08%	3300	1139	-8%
Cycle 28	-13530	0.04%	11288	1.75%	3300	1058	-8%
Cycle 29	-13527	0.02%	11292	1.78%	3300	1065	-8%
Cycle 30	-13515	0.07%	11272	1.63%	3300	1057	-8%
Cycle 31	-13521	0.03%	11280	1.69%	3300	1059	-8%
Cycle 32	-13529	0.03%	11211	1.18%	3300	982	-7%
Cycle 33	-13505	0.15%	11148	0.71%	3300	943	-7%
Cycle 34	-13517	0.06%	11045	0.05%	3300	828	-6%
Cycle 35	-13533	0.06%	10997	0.41%	3300	764	-6%
Cycle 36	-13512	0.10%	11011	0.30%	3300	799	-6%
Cycle 37	-13511	0.10%	10873	1.33%	3300	662	-5%



Cycle 38	-13551	0.19%	10833	1.62%	3300	582	-4%
Cycle 39	-13522	0.02%	10910	1.05%	3300	688	-5%
Cycle 40	-13529	0.03%	10899	1.13%	3300	670	-5%
Cycle 41	-13534	0.07%	10813	1.77%	3300	579	-4%
Cycle 42	-13519	0.05%	10841	1.57%	3300	622	-5%
Cycle 43	-13528	0.03%	10727	2.41%	3300	499	-4%
Cycle 44	-13540	0.11%	10763	2.14%	3300	523	-4%
Cycle 45	-13524	0.01%	10775	2.05%	3300	551	-4%
Cycle 46	-13526	0.01%	10692	2.66%	3300	466	-3%
Cycle 47	-13527	0.01%	10697	2.63%	3300	470	-3%
Cycle 48	-13529	0.03%	10677	2.77%	3300	448	-3%
Cycle 49	-13532	0.05%	10573	3.54%	3300	341	-3%
Cycle 50	-13524	0.01%	10555	3.68%	3300	331	-2%
Cycle 51	-13526	0.01%	10721	2.45%	3300	495	-4%
Cycle 52	-13529	0.03%	10713	2.51%	3300	484	-4%
Cycle 53	-13525	0.00%	10612	3.26%	3300	387	-3%
<b>Average [kJ]</b>	<b>-13525</b>		<b>11044</b>		<b>3300</b>	<b>819</b>	<b>-6%</b>
<b>Average [kWh]</b>	<b>-3.8</b>						

## 8. Solid-liquid Phase Change Material library sPCMlib

### 8.1. Introduction and scope of the library

The solid-liquid Phase Change Material library sPCMlib provides computer code for the calculation of the so-called "effective" thermophysical properties of PCM for the following programming languages/CFD programs: Python, Matlab, Modelica/Dymola and Ansys Fluent. The PCM properties can be used for the numerical modeling of heat transfer in PCM and for the analysis of the thermal performance of PCM enhanced materials and components. The database contains data, correlations and models for the computation of a more realistic phase transition of PCM, therefore accounting for the following phenomena: non isothermal phase change, extended crystallization temperature range caused by hysteresis, multi-step phase transitions (Figure 9).

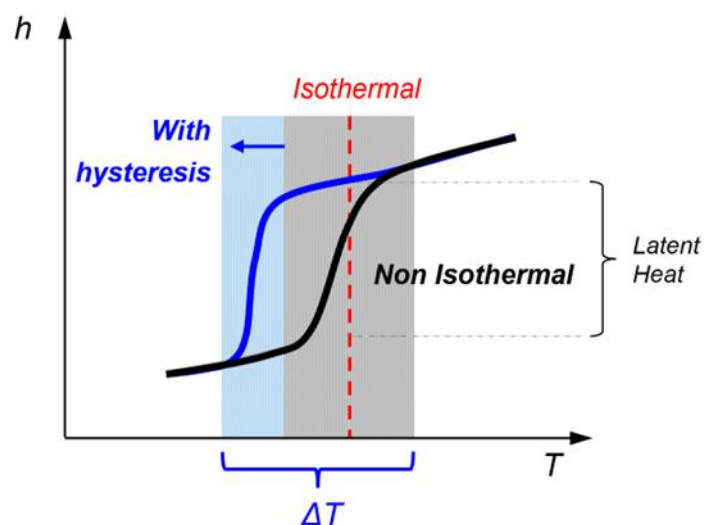


Figure 9. Ideal versus real phase change behavior of PCMs

To date, the library includes a total of 178 PCMs from 6 different manufacturing companies: Rubitherm GmbH, Pluss Advanced Technologies Pvt Ltd, Axiotherm GmbH, Croda International Plc, Climator Sweden AB and Knauf Gips KG. The materials included in sPCMlib differ from each others for: material class (wax, salt-hydrate, paraffin-based etc.), phase change temperature (from -63 to 115 °C), encapsulation method (macro- or micro-encapsulation), biobased classification. Moreover, different measurement procedures have been used to determine the heat capacities of the PCMs: 3-layer-calorimetry, heat-flux Differential Scanning Calorimetry (DSC) and T-history. An overview of the PCM currently included in sPCMlib is provided in Figure 10.



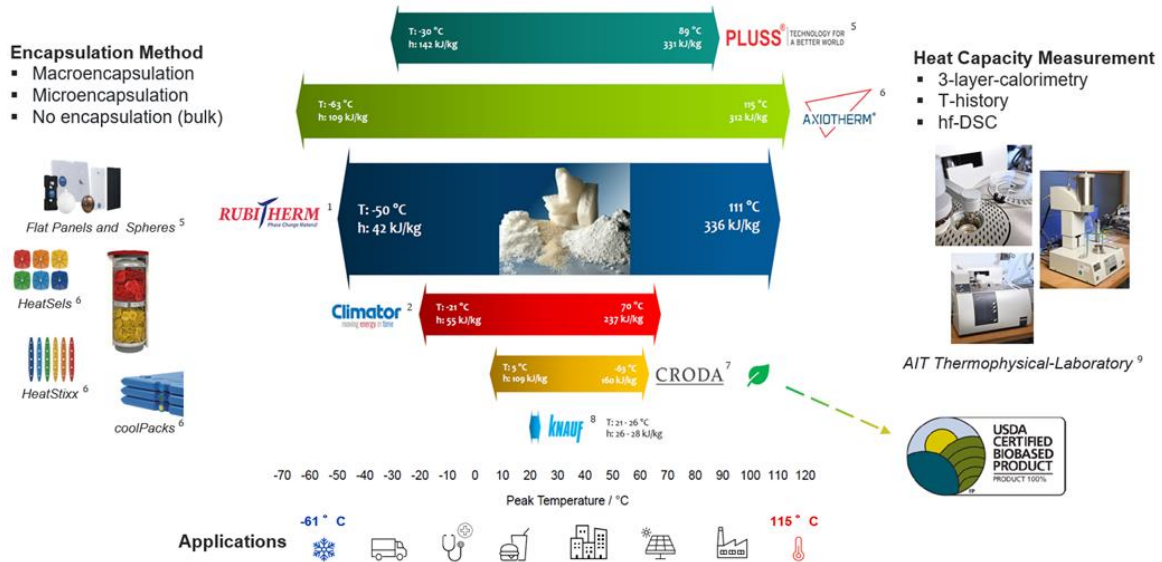


Figure 10. Overview of PCM included in the solid-liquid Phase Change Material library slPCMlib

The general workflow for the integration of new PCMs to the database is based on three major steps, as described in Figure 11. First, data are collected from the PCM manufacturers. In most of the cases, heat capacity data is usually provided in the company's datasheets in the form of partial enthalpy datasets, while the other thermophysical properties are given as single values for the solid and liquid phases. Once the data is collected, it is processed by the use of two-phase, temperature-dependent phase transition models, where the solid and liquid phases coexist as homogeneous mixture within a mushy zone, as further described in section 3. Post-processed data corresponds to continuous functions for all the relevant effective thermophysical properties of PCMs for heating and cooling, such as: apparent heat capacity, phase fraction, enthalpy, density and thermal conductivity. Therefore, a computer code including the full abovementioned datasets is available for the user for download.

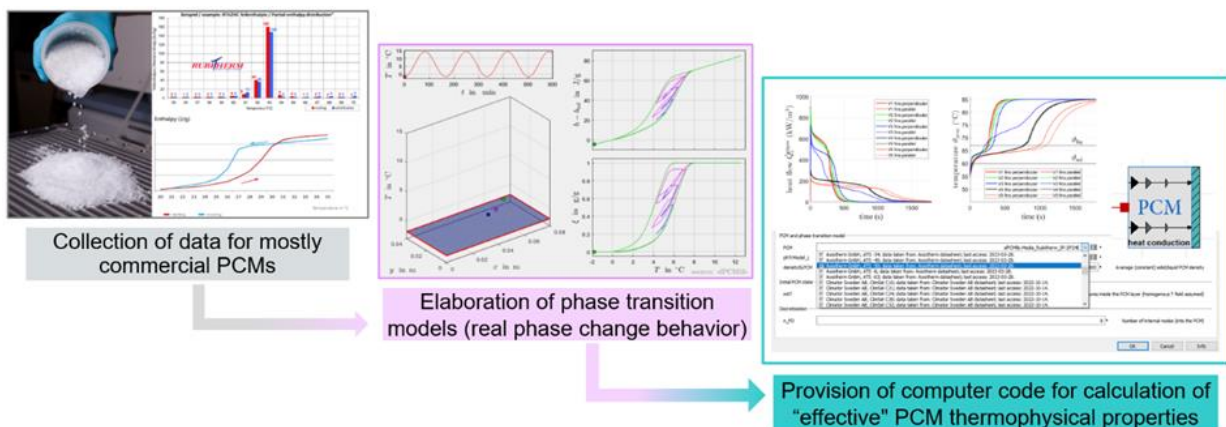


Figure 11. General workflow for slPCMlib

## 8.2. General features of sIPCMlib

### 8.2.1 Selection and screening of PCM using the database interface and interactive filters and graphs

The library provides the user with the possibility to select the PCM based on relevant material properties or product specifications, given in the form of filters and switches (red box in Figure 12). The user can select the PCM based on: manufacturing company, product family, material class, phase change temperature, encapsulation type, data source and heat capacity measurement method. Once the material is selected, the main interface presented in Figure 12 is filled out with relevant information about the PCM. An info-box on “material’s specification” summarizes in a small paragraph some of the general properties of the PCM according to the manufacturer’s website, among which, for instance, the application field in which the material is usually employed. The overview table for the selected PCMs shows in a concise format the main thermophysical properties of the PCMs at solid and liquid state, as well as the phase transition enthalpy and temperature ranges, and other relevant metadata. For biobased PCMs an additional green leaf symbol is added next to the “In/-Organic” field. Lastly, an info-box about measurement procedure and data processing includes specific information on the way data was generated by manufacturers and integrated in the library.

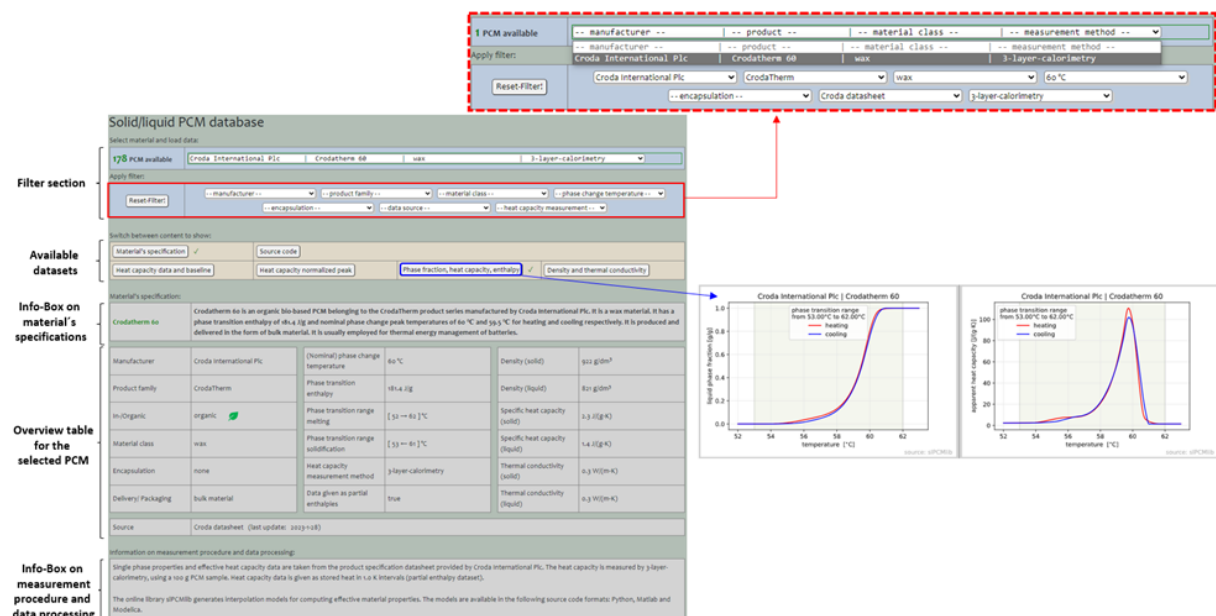


Figure 12. Main interface for selection of PCM in the sIPCMlib database

To visualize the full PCM property datasets, a switch between “heat capacity data and baseline”, “heat capacity normalized peak”, “phase fraction, heat capacity, enthalpy” and “density and thermal conductivity” allows the user to have online access to the continuous properties coming from the data processing (an example is given in the blue box in Figure 12).

### 8.2.2 Graphic visualization of effective thermal material properties

Most of the manufacturers provide PCM data for heating and cooling. These are treated in sIPCMlib as two different datasets. A special example is provided for the PCM Crodatherm 32 in Figure 13. Here, the heat capacity data is shown as histogram plot, with a net distinction between the baseline area (grey) corresponding to the sensible heat contribution, and the colored area (orange or blue for heating and cooling respectively), representing the latent heat contribution during the phase transition of the PCM.

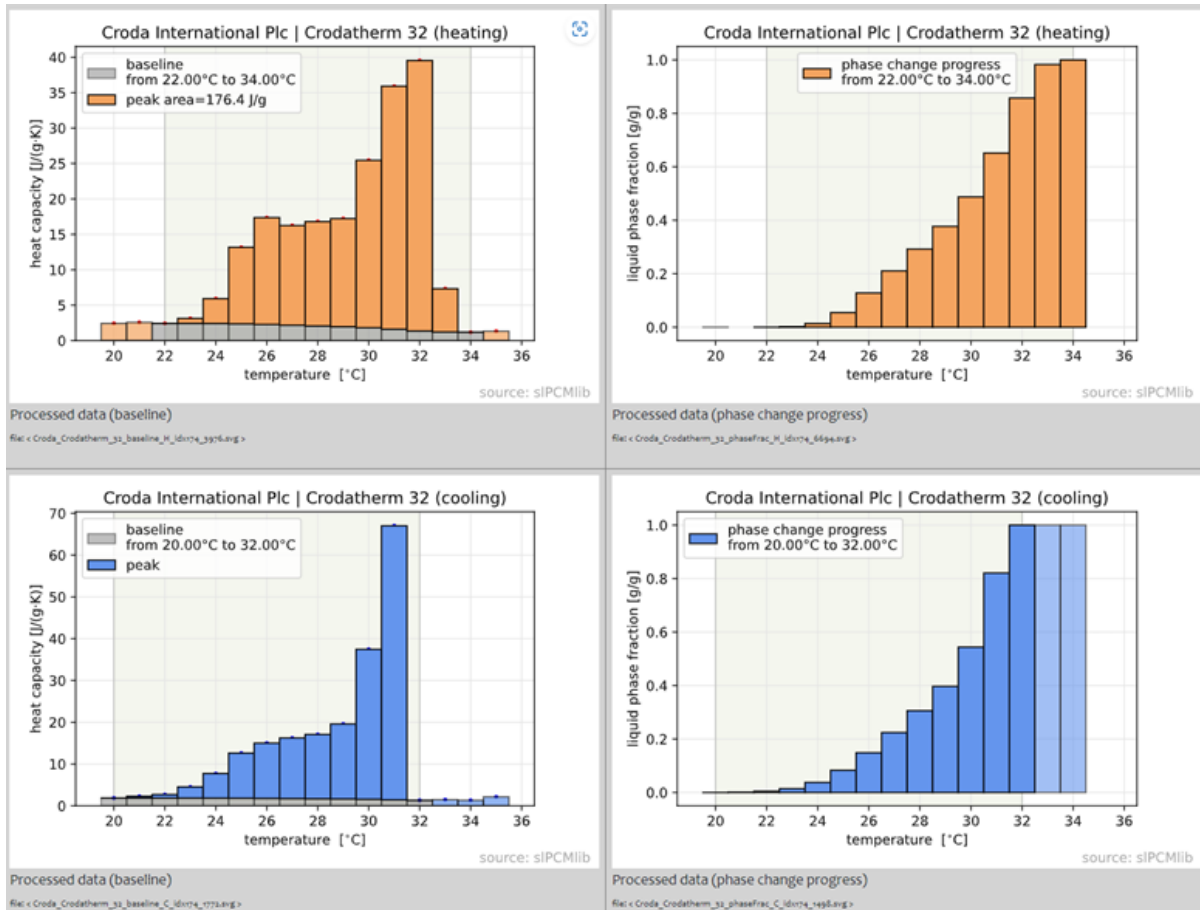


Figure 13. Heat capacity data for heating and cooling. Distinction between baseline and latent heat contributions

An example of continuous dataset for the same PCM is given in Figure 14. Here, the heating and cooling datasets are plotted together with a red (heating) and blue (cooling) curves respectively. Whenever data is processed and differs from the original manufacturer’s datasheet, i.e. interpolation and smoothing techniques are used to generate the continuous curves for a specific property, this is indicated in the figure description.

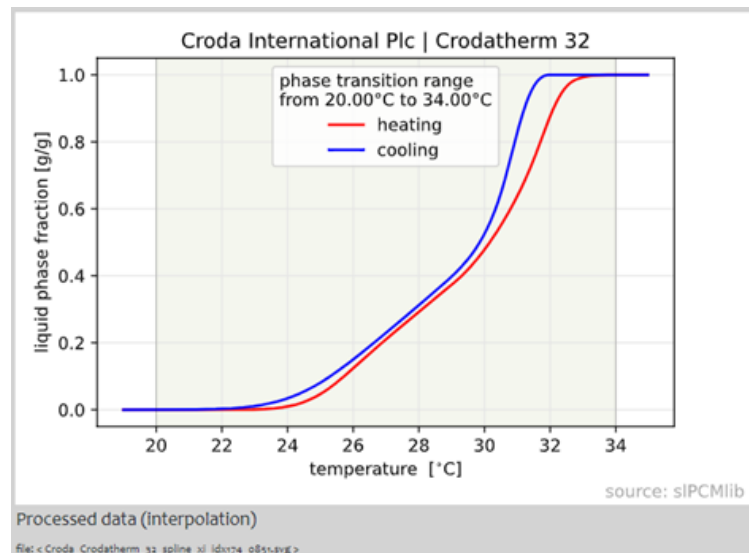


Figure 14. Liquid fraction for Crodatherm 32 during heating and cooling

### 8.2.3 Code export functions

Once a material is selected, a source code containing the continuous datasets of its thermophysical properties is available for the user to download for the following programming languages/simulation software: Python, Matlab, Modelica/Dymola and Ansys Fluent. This latter can be directly copied using the function "Copy to clipboard" or even downloaded in the correct format using the option "save to file", as presented in Figure 15.

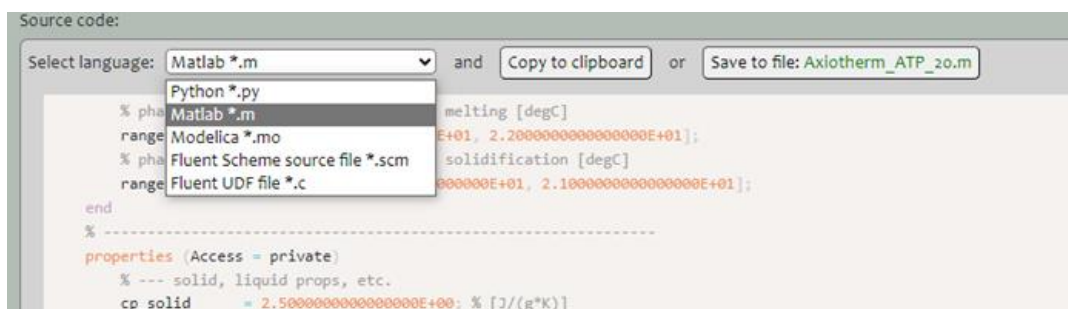


Figure 15. Code export functions in sIPCMLib

### 8.2.4 Interactive interface "Explore" to get a quick overview

The Explore interactive interface gives the user a quick overview of the materials included in sIPCMLib by plotting their phase change enthalpy over their phase change temperature. A switch function allows the selection of the phase change temperature per unit mass or per unit volume. The materials are sorted by manufacturer (color) and product family (symbol). The user can pick the PCMs of interest by deselecting the manufacturers/product families which are less relevant for him. The wideness of the temperature range could be selected by zooming in or out within the plot area. Finally, when the user places the mouse pointer directly on a specific PCM, its most important thermophysical properties are displayed in a box, e.g. its material class, phase change enthalpy and density in the liquid state, as visible in Figure 16.

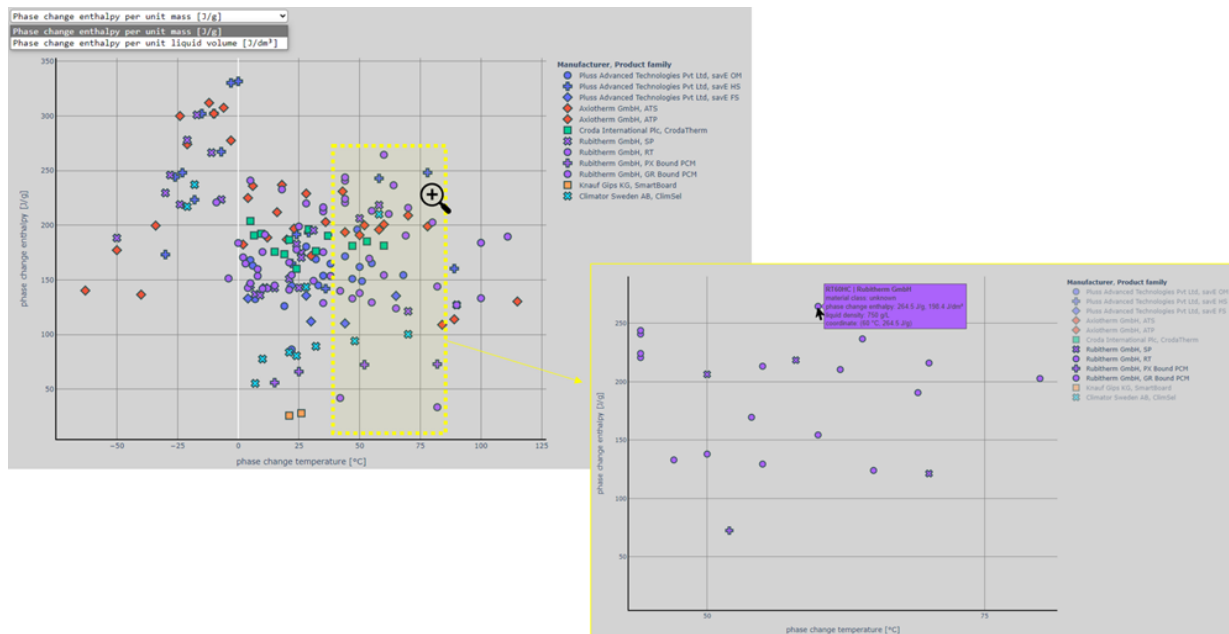


Figure 16. "Explore" interface in slPCMLib

### 8.2.5 Interactive interface "User-defined" for customized effective thermal materials properties

The interactive interface "User-defined" offers the possibility to customize the effective thermal properties of a PCM for which data is not yet available in the database. The user can set the phase transition range and the phase transition enthalpy, as well as the other relevant single phase change properties of the material at solid and liquid state, e.g. specific heat capacity, thermal conductivity, density, thermal expansion and dynamic viscosity. Moreover, a preferred peak shape function could be selected between: smooth step, sigmoid function, Gumbel minimum distribution and Log-Normal distribution. Therefore, the material properties are computed, and could be graphically visualized, with the possibility to switch between their plots (blue selection in Figure 17). Finally, the dataset source code could be exported, as explained in 7.2.3.

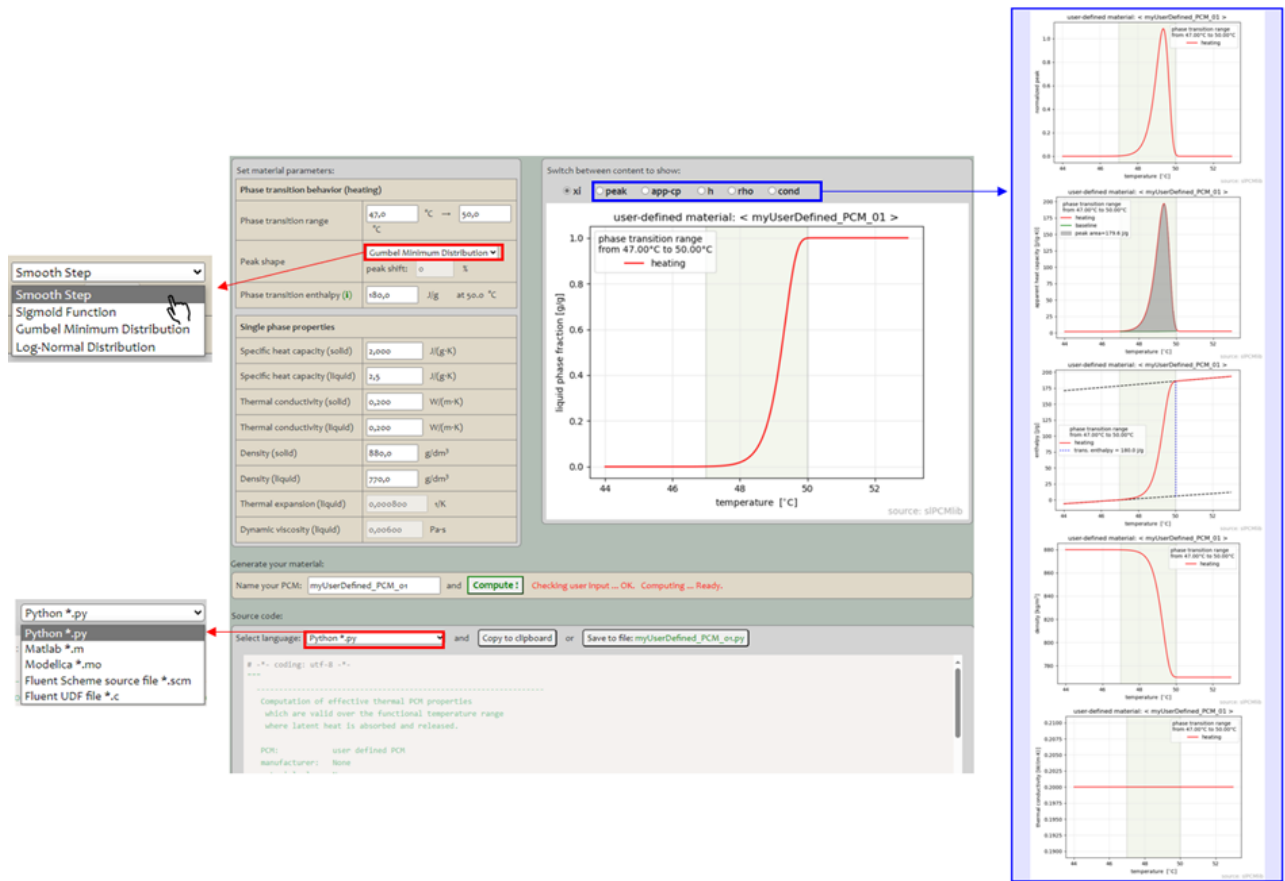


Figure 17. "User-defined" interface in sIPCMlib

### 8.2.6 Interface "Links & Network" to acknowledge external contributors

The interface "Links & Network" acknowledge the several external contributors which have collaborated with sIPCMlib to include a greater number of PCMs, as well as to extend the programming languages and simulation software supported by the library (Figure 18). The latter are divided in three main categories: "Companies and Accredited Laboratories", "Universities and Research Institutions" and "Databases and Libraries". The AIT accredited Laboratory for Thermophysics supports sIPCMlib providing valuable knowledge on material characterization methods. Companies in the field of PCM production and characterization, such as METTLER TOLEDO GmbH and Croda International Plc, have shared valuable information regarding thermophysical properties of PCMs, as well as their measurement methods. Moreover, the research group of Applied Thermodynamics and Heat Transfer (ATHT) at the University of Ghent has provided relevant inputs to the numerical modeling of heat transfer problems with phase change, solution methods and code development for Ansys Fluent. Finally, the cooperation with other relevant PCM databases and libraries is considered valuable for the further development of sIPCMlib. For example, ongoing discussions on material properties, standards and data processing are held with some members of IEA ECES Annex 29 and SHC Task 42, who have developed the thermalmaterials.org database.




## Links & network


We would like to thank our partners for their valuable contributions and support!

### Companies and Accredited Laboratories


[Mettler-Toledo GmbH](#)  
**Contact: Dr. Andreas Bach**  
 METTLER TOLEDO supports sIPCMlib by providing a large quantity of thermophysical measurements for pure PCM. Thanks to its contribution, we have received more than 50 organic and inorganic PCM. The data processing and its integration in sIPCMlib is currently ongoing. A large database of PCM properties is available for METTLER TOLEDO's customers, who purchase their calorimetry equipment, see [www.mt.com/ta-libraries](http://www.mt.com/ta-libraries).



[Croda](#)  
**Branch office: Croda Ibérica SAU**  
**Contact: Dr. Jon Vilasau**  
 Croda supports sIPCMlib by providing thermophysical measurements of their biobased PCM waxes in micro- and macro-encapsulated form. Croda shares with sIPCMlib specific information and valuable inputs on their measurement methods which are developed according to the RAL standard.




[AIT Laboratory for Thermophysics](#)  
**Contact: Dr. Daniel Lager**  
 The AIT Laboratory for Thermophysics supports sIPCMlib as an accredited testing laboratory (EN ISO/IEC 17025) providing valuable knowledge on material characterization methods.



### Universities and Research Institutions

[Research group Applied Thermodynamics and Heat Transfer \(ATHT\)](#)  
**Contact: Prof. Michel De Paepe**  
 The Research group Applied Thermodynamics and Heat Transfer (ATHT) at the Faculty of Engineering and Architecture of Ghent University supports sIPCMlib with valuable inputs to the numerical modeling of heat transfer problems with phase change, solution methods and code development for Ansys Fluent. Our special thanks go to Dr. Wim Beyne and Maité Goderis!



### Databases and Libraries

[thermalmaterials.org](http://thermalmaterials.org)  
**Contact: Dipl.-Biol. Stefan Gschwander**  
 The open-source database [thermalmaterials.org](http://thermalmaterials.org) contains thermophysical measurements and properties of phase change materials (PCM), sorption and thermochemical materials (TCM), which has been generated according to measurement standards developed within the framework of the IEA ECES Annex 29 and SHC Task 42. The database is developed and maintained by the Fraunhofer Institute for Solar Energy Systems. We acknowledge the collaboration and many discussions on material properties, standards and data processing methods.




Figure 18. "Links & Network" interface in sIPCMlib

### 8.3. Data processing workflow and modeling of PCM effective properties

The following assumptions are taken for modeling effective PCM properties [1]:

- There are only two phases (two-phase model): a solid and a liquid phase
- Phase transitions are induced by temperature and are independent of pressure
- Phase transitions extend over a temperature range (non-isothermal phase transitions) and are continuous
- Within the phase transition temperature range the solid and liquid phases coexist as a homogenous mixture
- The material is in a semi-solid or semi-liquid state which produces a mushy zone in the PCM domain
- Properties of the mushy state are local effective (also apparent) mixture properties, which are defined by a weighting of contributions from solid and liquid phases. The

weighting is based on the phase change progress, i.e. the mass (or volume) phase fraction. As an example, the enthalpy could be calculated as follows:

$$h(T) = (1 - \xi(T)) h^s(T) + \xi(T) h^l(T) \tag{1}$$

Where  $\xi$  is the phase fraction of the material as a function of temperature, and  $h^s$  and  $h^l$  are the solid and liquid enthalpies of the PCM, whose difference is equal to the latent heat of the material.

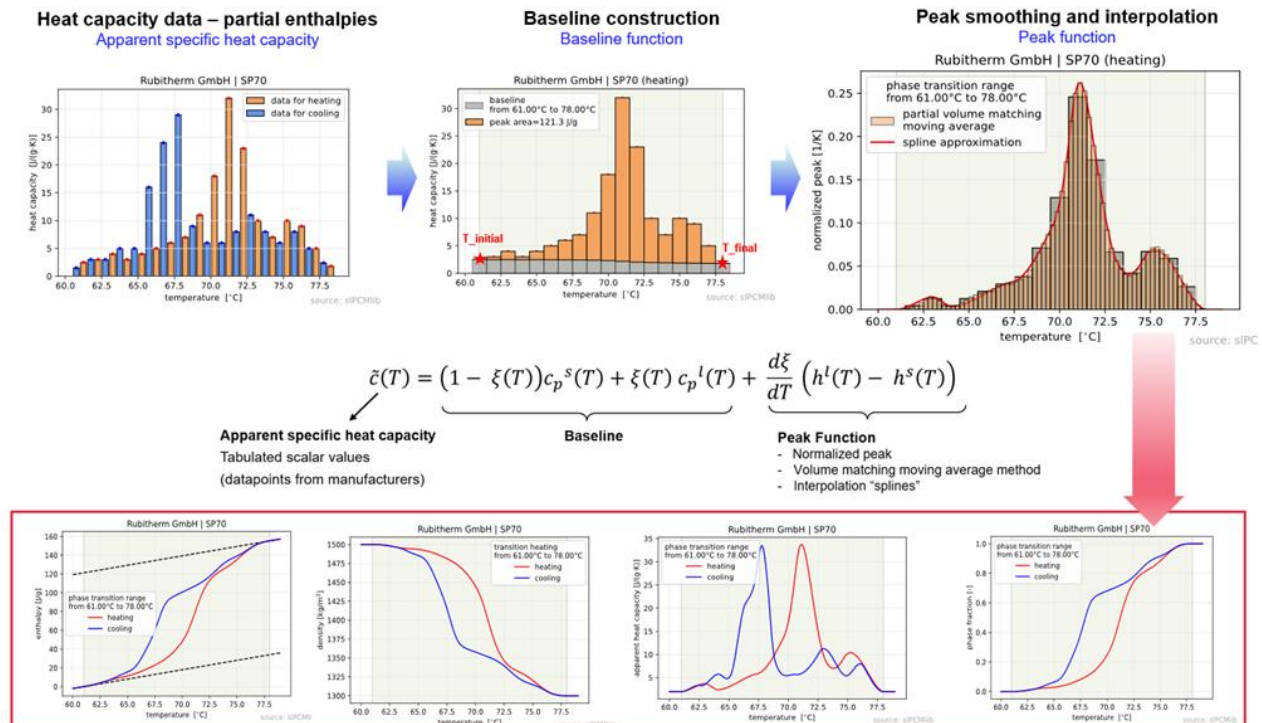


Figure 19. Data processing workflow

Based on the aforementioned assumptions, the following workflow is used to process the data from the manufacturers and provide continuous temperature-dependent curves for all the relevant thermophysical properties (Figure 19):

1. The heat capacity data is collected for a specific PCM produced by a manufacturer. This is usually provided in the form of partial enthalpy datasets for heating and cooling, and could be expressed as a function of the phase fraction of the PCM, which is varying within the mushy zone as a function of temperature and within 0 (PCM fully solid) and 1 (PCM fully liquid). The goal of the data processing is to transform this type of tabulated dataset in a continuous and smooth peak function
2. The baseline function is constructed by identifying two temperature limits at the lower and upper boundary of the phase transition region. The area below the baseline function (in grey in Figure 19) is accountable for the sensible heat exchanged during the process and must be subtracted from the total heat capacity to calculate the latent storage capacity of the PCM. The baseline function is obtained by summing the



contribution of the temperature-dependent specific heat capacities of the PCM at solid and liquid state, and averaged over the liquid fraction of the material

3. The phase fraction of the PCM corresponds to the integral of the normalized peak function. Moreover, peak smoothing techniques are used to obtain a continuous function over the temperature range of interest. Once the peak function is obtained, all the other thermophysical properties of the PCM are calculated as a function of it, i.e. apparent heat capacity, density, enthalpy and thermal conductivity

## 8.4. The role of sPCMLib in the HYSTORE project

### 8.4.1 KTH functions

As reported in Deliverable 2.2, bench-scale long-term cycling stability tests were performed at KTH for the short-listed PCM candidates RT57HC and RT60HC. Their material property calculations were performed using Python as explained in detail there, in section 7.1.3 for fundamental concepts and in Appendix B for the specific codes for several calculation steps. These Python codes will be made available within this sPCMLib, for other similar type of bulk-scale PCM-TES capacity analyses. Here, what is meant by bulk scale analyses are e.g. conducted at bench-scale (or pilot-scale) and in many cycles, thus generating a large database of data that benefits from this type of automated calculations. These correspond to the numerical modelling at material-scale provided from KTH, for this current report.

### 8.4.2 Ansys Fluent: Modeling of PCM melting behaviour in RPW-HEX

Modelling the solidification and melting behavior of PCMs can present several challenges, including non-isothermal phase change, multi-step transitions, complex enthalpy-temperature relations and convective heat transfer. To tackle these challenges, a novel numerical method based on information of effective properties and phase change behavior of commercial PCM included in sPCMLib has been developed for modelling their complex phase change behavior in Ansys Fluent CFD software. The case study is based on the heat exchanger fin geometry designed by RAAL for the "ALL-IN-ONE Solution".

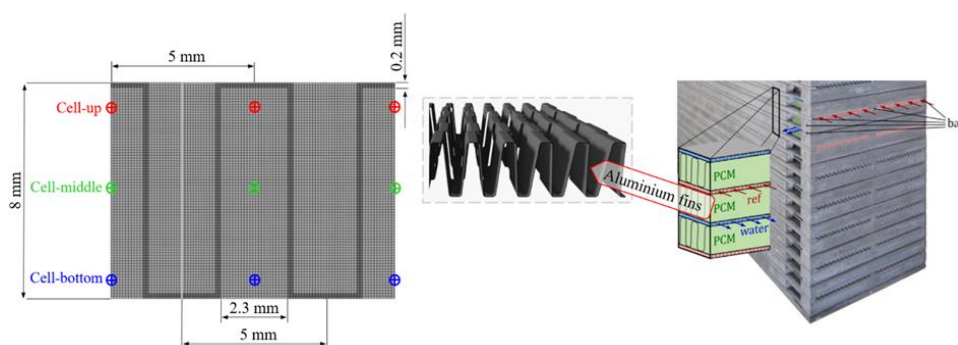


Figure 20. Simulation mesh and aluminium fin geometry

The air fins are made from 0.2 mm thick aluminium sheets folded in trapezoidal shape (Figure 20, center). The refrigerant flows in micro-multiport extrusion (MPE) aluminum tubes, directly in contact with the fins (Fig. 12 right, marked as bars). The investigation focuses on the heat transfer inside the cavities formed by the air fins filled with PCM, approximated by a

rectangular shape (Figure 20, left). The heat transfer contribution of the MPE tubes is modelled within the boundary conditions, e.g. a temperature ramp profile. The geometry considers a PCM and a fin domain, identified as "fluid" and "solid" bodies, respectively (Figure 20, left). Furthermore, symmetry constraints are applied to the outer vertical walls of the domain to mirror the geometry and obtain a continuous fin structure across the x-axis.

The melting process of the PCM is simulated by adopting the apparent heat capacity (AHC) method. The apparent specific heat capacity is calculated as the derivative of the specific enthalpy considering a temperature dependent phase change enthalpy:

$$c_{app}(T) = (1 - \beta(T))c_p^s + \beta(T)c_p^l + (d\beta(T)/dT) (h^l(T) - h^s(T)) \quad (2)$$

Where  $h^s(T)$  and  $h^l(T)$  are the extrapolated single phase solid and liquid specific enthalpies [7]. The temperature dependent liquid volume fraction  $\beta(T)$  equals the liquid mass fraction  $\xi(T)$  and represents the phase change progress. The AHC model differs from the standard Solidification and Melting (S&M) model implemented in Ansys Fluent, which is instead based on the enthalpy porosity method and does not consider the heat capacity as a continuous function of temperature, but as a stepwise function.

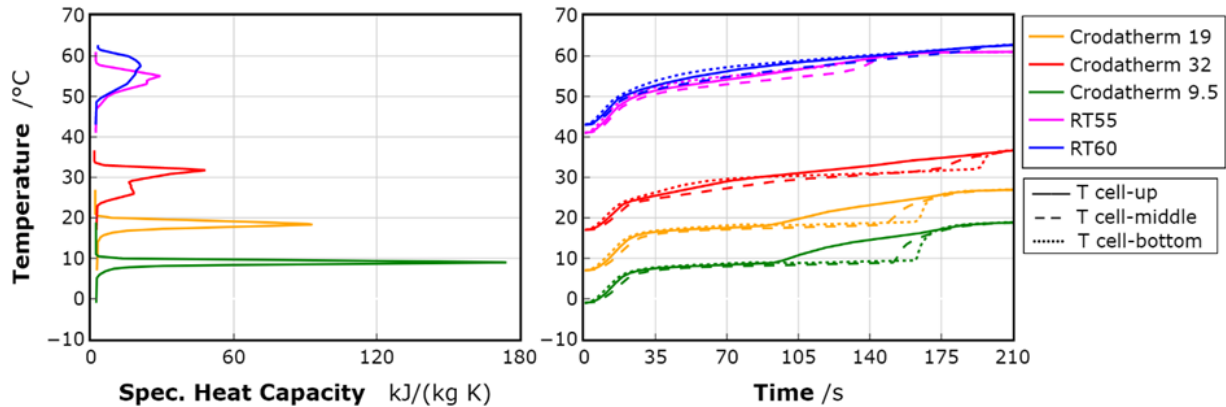


Figure 21. Predicted heat capacities temperatures at upper, middle and bottom cells for five PCMs

For each PCM simulated with the HEX fin geometry, the single phase thermal properties, such as solid and liquid specific heat capacities, liquid density and liquid thermal conductivity, are assumed constant and taken from the sIPCMlib database. Five commercial PCMs are considered for the investigation (Figure 21): Crodatherm 9.5, Crodatherm 19 and Crodatherm 32 are produced by Croda International Plc, while RT55 and RT60 are manufactured by Rubitherm Technologies GmbH. The selection represents different melting behavior, i.e. different phase transition ranges and peak shapes in the apparent heat capacity curves.

Despite the relatively high shape complexity, height, and variations in curvature, all computations showed a good level of convergence. Moreover, it is generally observed that in PCMs showing very sharp heat capacity peaks, the closest cell to the aluminium fin (cell-up) undergoes a faster melting process, followed by cell-middle and cell-bottom. Furthermore, the melting behavior within the domain becomes more homogeneous in PCMs with larger peak areas.

### 8.4.3 Dymola: Modeling of RPW-HEX and fresh water station loop

The modeling of the PCM heat exchanger storage in connection with the fresh water station loop is further modelled in Dymola. The system is represented in Figure 22 and corresponds to a first simplified representation of the “ALL-IN-ONE Solution” design. The PCM heat exchanger is simulated with a unidimensional model, assuming a constant mass flow charging/discharging the storage through one horizontal tube. The heat transfer contribution affecting each PCM layer is simulated only through the y-axis, where the phase fraction of the material varies as a function of temperature from completely solid ( $\xi = 0$ ) to completely melted ( $\xi = 1$ ). The temperature profile for each of the PCM layers is calculated to assess how long the desired temperature of 60 °C is maintained by the material. The material properties for the PCMs are loaded from slPCMLib, thanks to the use of the TIL library. Specifically, the Rubitherm PCM RT60HC is used for the investigation.

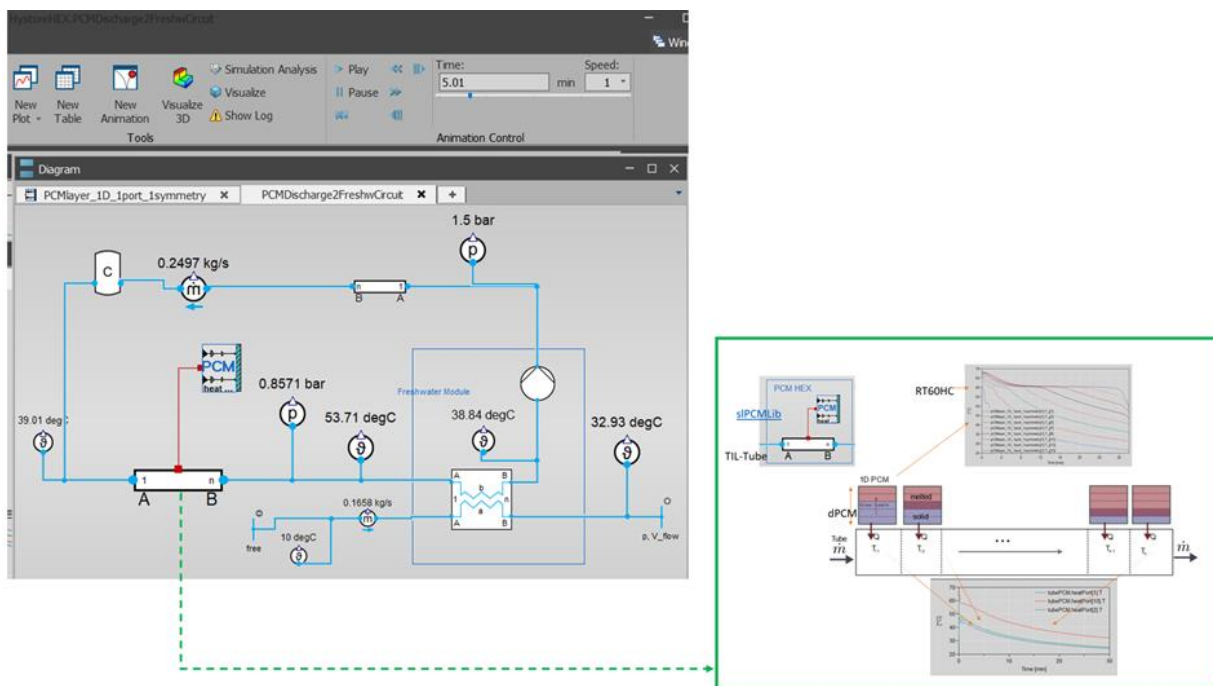


Figure 22. Dymola PCM-HEX and fresh water station loop

As visible in Figure 22, once the water passes through the PCM-HEX a final temperature of around 54 °C is expected to be reached. Being the heat exchanger made of aluminum, this water could not be directly pumped to the final user due to corrosion problems. Therefore, a second loop including a fresh water station is needed to pump the warm water to the tap.

The source code used for Dymola/Modelica is available at slPCMLib, as visible in Figure 23.



## 9. Life Cycle Assessment (LCA)

Life Cycle Assessment (LCA) is a method for evaluating the environmental effect of a product or process from the beginning to the end. It assesses every stage, from raw material extraction to disposal or recycling, with the goal of qualifying and quantifying inputs like energy and outcomes like emissions. By assessing the whole life cycle, it aids in the identification of environmental hotspots and guides impact reduction options.

A product's life cycle usually includes:

1. **material extraction:** this is the process of obtaining natural materials such as minerals, metals and fuels.
2. **manufacture:** known as the production, is the process of transforming the gained raw materials into end products, which frequently involves the use of energy and a possible production of waste and emissions.
3. **package and transport:** this includes moving the materials from industrial facilities to customers, thus resulting in energy consumption and emission release.
4. **use:** consumers or companies use the product with a possible consumption of energy
5. **end of life:** the process of disposing or recycling a product, including waste management and possible environmental impacts

Life cycle assessment (LCA), which is a specific analysis involving quantitative assessments, stems from the broader concept of life cycle thinking (LCT). LCT and LCA give an extensive overview of environmental consequences, including carbon footprint (CF), wastewater management and energy consumption. Their application in e.g. manufacturing industries influences a sustainable decision making of the whole product. [2]

In this chapter, qualitative LCAs, i.e., in LCT, applied to the PCMs considered in HYSTORE project are presented. Qualitative Life Cycle Assessment is a methodology used to evaluate the environmental, social and economic aspects of a product, process or service throughout its life cycle. In this chapter only the environmental impacts of the PCM are described. The LCT here is mainly composed of the key life cycle steps in Figure 24:

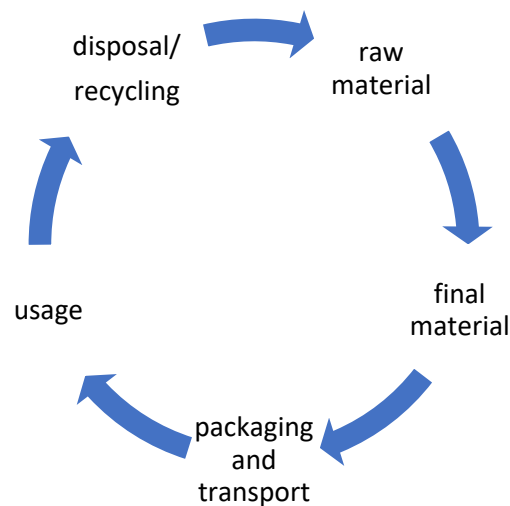


Figure 24. Typical life cycle steps of a product (Conceptualized based on [2])

The following sections represents the LCA of the selected PCMs (RT8HC, RT60HC and SP31) which are chosen for ALL-IN-ONE solution at AIT, PCM HEATING at KTH and LOW TEMP. HEATING at the demosite in Montserrat.

## 9.1. Raw material

The extraction of raw material is a crucial phase in the life cycle of goods and procedures. It has a massive impact on their environmental footprint. It is the first stage of resource extraction from the environment to suit various human needs.

### RT8HC

The life cycle of RT8HC begins with the extraction of different hydrocarbons with a chain length of C14 upto C18. They mainly consist of carbon and hydrogen. These paraffins are part of crude oil and natural gases. The raw material supplier performed a thorough analysis of the individual specifications and grouped the results. They have been generated via Product Carbon Footprint (PFC) calculations using the ISO 14040, 14044 & 14067 standard and TFS guidelines for guidance. The included supplier process steps are extraction of natural resources, processing and the transport to Rubitherm, Berlin. These processes need the input of natural resources and energy. The output are raw materials and energy emissions. Around ~1000 g carbon dioxide (CO<sub>2</sub>) per kg product and ~1000 g CO<sub>2</sub>/kg product are the PFCs of the two used raw materials. The transport to Rubitherm is estimated at ~70 g CO<sub>2</sub>/kg product.

### RT60HC

The life cycle of RT60HC begins with the extraction of different long-chain organic compounds from natural origin e.g. fats or fatty oils. A technical way of production is possible with the hydrogenation of an acid (from natural resources). These processes of extraction or synthesis, hydrogenation and combination need the input of natural resources and energy. The output are a raw material and energy emissions. To get a little bit closer to this important topic a short quantitative analysis was done with the given data of one of our suppliers for raw materials. The material extraction and processing produce ~-300 g CO<sub>2</sub>/kg product, because of the use of renewable resources. The transport emissions amount to ~60 g CO<sub>2</sub>/kg product. The production processes produce ~770 g CO<sub>2</sub>/kg through fuel, steam and electricity. The transport via truck to Rubitherm caused ~70 g CO<sub>2</sub>/kg product.

### SP31

The life cycle of SP31 begins with the production of the sodium salt and the synthesis of a nitrogen additive. These processes need the input of natural resources and energy. The output are raw materials and energy emissions. Due to missing data from the raw material supplier the PFC of these products can not be quantified. Further investigations will be made to get these important data. The assumption is ~130g CO<sub>2</sub>/kg product for the whole transport to the supplier and to Rubitherm.

## 9.2. Final material

In this phase raw materials are transformed into finished goods. Herein several processes working hand in hand to convert the raw material into a usable product.

### RT8HC

The manufacturing of the raw material to the final PCM take place at Rubitherm, Berlin. Afterwards a quality assurance is done. Different measurements like viscosity, density and thermal behaviour are carried out under certain conditions. For producing the final material, the paraffins (which are stored in IBCs) have to be pumped into a mixing reactor. After filling, an electric stirrer starts mixing both components together to a homogenous fluid. This process needs the input of raw material and energy. The output are final material and energy emissions. The PFC for this process amounts to ~5.0 g CO<sub>2</sub>/kg product.

### RT60HC

The manufacturing of the final material take place at Rubitherm, Berlin. For this, the raw material has to be unpacked from its transport container. Afterwards a quality assurance is done. Different measurements like viscosity, density and thermal behaviour are carried out under certain conditions. The raw material then has to be melted in a drum melting system operated by an oil heating



system. Afterwards it is filled in a pre-heated reactor and is stirred for several hours. Different additives like e.g. thickener are added. These manufacturing processes need the input of the raw material and energy for heating, stirring and pumping. The output is the final material and energy emissions like CO<sub>2</sub>. The PFC for these processes amounts to ~153 g CO<sub>2</sub>/kg product.

### **SP31**

The manufacturing of the final material takes place at Rubitherm, Berlin. For this the raw materials have to be unpacked from their transport containers (mostly bags). Afterwards a quality assurance is done. Different measurements like viscosity, density and thermal behaviour are carried out under certain conditions. The raw materials are then filled in a pre-heated mixing reactor and dissolved in hot water. An electrical stirrer is mixing everything together until it is homogenous. These manufacturing processes need the input of raw material and energy for heating and stirring. The output is the final material and energy emissions. The PFC for these processes amounts to ~17.0 g CO<sub>2</sub>/kg product.

## **9.3. Packaging and transport**

This sub-chapter deals with the distribution and delivery of final products to the end-user. The key-role of this step is the protection and transportation of products from the manufacturing facilities to distribution centers.

### **RT8HC, RT60HC, SP31**

The final material will be pumped into drums or in canisters. These containers are stored on a pallet, wrapped with strapping band and foil. Small canisters are packed in cardboard boxes for transportation. The transport is carried out by a truck, over sea or via airplane to the place of destination. A general estimation for the transport to the final destination is due to the multiple variations not possible, but has to be looked at for individual cases. The process step "packaging and transport" needs the input of final material, packaging material and energy. The output are packed and transported material and energy emissions. The PFC for the packaging process amounts to ~0.1g CO<sub>2</sub>/kg product.

As an intermediate summary the product carbon footprint for RT8HC from raw material to packaging process amounts to ~2.075 g CO<sub>2</sub>/kg product from "cradle to gate" at Rubitherm.

As an intermediate summary the product carbon footprint for RT60HC from raw material to packaging process amounts to ~753 g CO<sub>2</sub>/kg product from "cradle to gate" at Rubitherm.

As an intermediate summary the product carbon footprint for SP31 from raw material to packaging process amounts to ~147 g CO<sub>2</sub>/kg product (without energy emissions of synthesis) from "cradle to gate" at Rubitherm



## 9.4. Use of the Product

The usage of the final product describes the period during which a final product is applied by the end-user. Important steps are the operation, maintaining and (possible) energy consumption.

### RT60HC

This section specifically concerns the chosen PCM RT60HC for HYSTORE PCM Heating solution at KTH and for the “ALL-in-ONE Solution” at AIT.

In the PCM Heating solution, RT60HC will be used for space heating applications. It also can serve as a potential PCM for any other heating or cooling applications, provided the heating/cooling need is covered by its phase change temperature range (overall at: 56-62 °C, as presented in Deliverable 2.2 report, section 7.2.2.3). These could be e.g., but not limited to, other space heating applications, as pre-heating steps for domestic hot water supplies, and possibly some industrial cooling and pre-cooling processes. This might be also of interest for thermal management of e.g. electronics, given the temperature is suitable.

Concerning the application conditions in this specific PCM Heating Solution, the PCM will be melted in an oven. This will be done batch-wise, PCM contained in metal Jerry cans each of ~20 L volume, to fulfill the final total LHTES volume which is in the order of 500-800 L. The molten PCM will be then poured into the LHTES unit or capsules (based on the optimal heat exchanger geometry that will be chosen later in HYSTORE project). Afterwards, the LHTES unit will be kept closed and operated in thermal cycles as dictated by the PCM Heating application, thus with minimal interactions with the outside air. The operating temperature range would be maximum 15-85 °C in these use cycles. The LHTES and thus RT60HC PCM are anticipated to undergo very many complete (i.e., one full melting and freezing per day) cycles and possibly over a lifetime of 15-20 years (thus ~5000-7500 cycles in total). The 50+ cycles tested and reported in Deliverable 2.2 show consistent performance upon cycling. Backed by these results and the fact that it undergoes minimal exposure to external ambient conditions, it can be expected to show negligible to minimal degradation within this lifetime.

The “ALL-in-ONE Solution” developed at AIT includes a Refrigerant-PCM-Water heat exchanger (RPW-HEX) connected to the fresh water station circle, which delivers domestic hot water to the user thanks to a closed loop (see scheme in Figure 25).

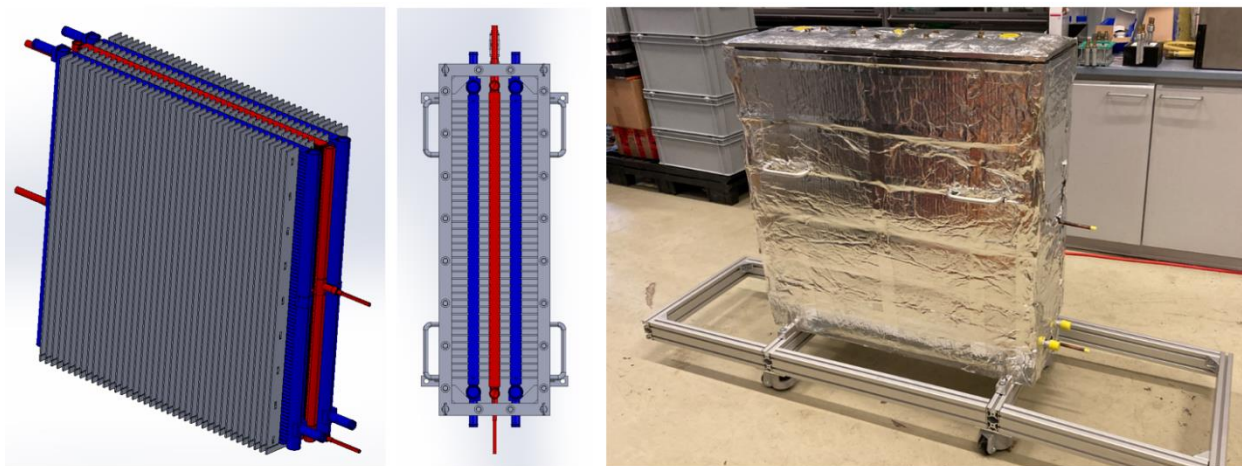


Figure 25. CAD drawing and laboratory set-up at AIT of RPW-HEX storage

The PCM is filled from the top of the storage maintaining an additional upper volume between the PCM and the lid, to allow its volume expansion during the melting process without physical deformation of the storage container. After filling, minimal interactions with the outside environment are expected for the PCM. A total of 10 temperature sensors and one pressure sensor are located directly in contact with the PCM in order to monitor its state of charge and its changes over time and number of cycles, e.g. this way it is possible to detect the degradation of the material.

Specifically, the LHTES is heated up by the heat pump modul within a temperature range of 20 – 70 °C (charging period), ensuring the complete melting of the PCM (RT60HC). Once the storage gets to the homogeneous temperature of 70 °C, the fresh water station pump is activated with a flow rate of 2 – 25 l/min and the discharge of the PCM takes place. In the final use the charge and discharge operation can be characterized by tests defined in norm ÖNORM EN 16147.

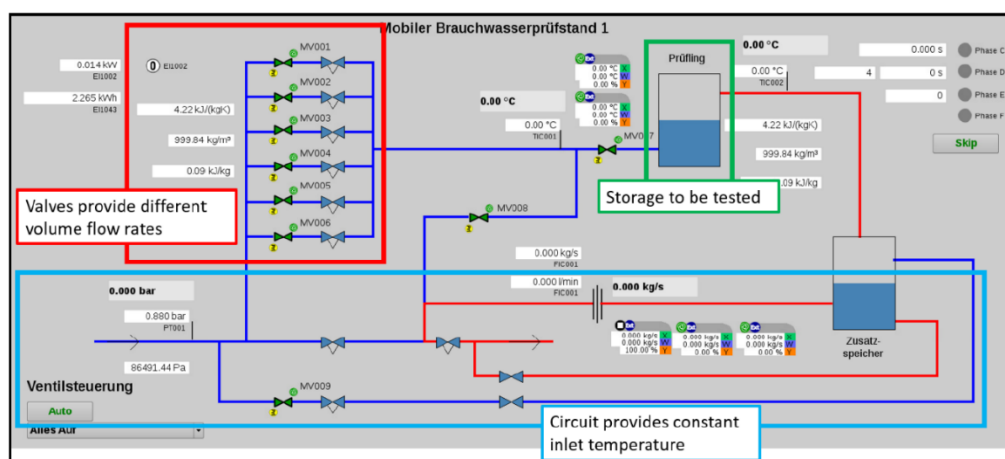


Figure 26. Hydraulic connections to perform charging and discharging tests

Similarly to the space heating solution at KTH, the RPW-HEX storage is expected to undergo up to two melting and solidification cycles per day over a lifetime of 15-20 years, reaching a total of ~7000-10000 cycles.

## 9.5. Reuse and recycling

This phase of LCA is crucial to the whole assessment as the used materials are splitted up from disposal and being reintegrated into the production process. To reduce the PFC, the used materials are collected, sorted, processed and reprocessed for minimizing waste production.

To have a minimal life-cycle impact, at the end-of-life (EoL) of the PCM in LHTES, recovery, reuse and recycling are the most preferred and prioritized options. In the PCM Heating solution, in case of the PCM in a tank LHTES where the HEX is submerged, the recovery is straightforward and will be with high recovery rates. If the PCM would however be encapsulated and then submerged in HTF, the recovery would be more tedious (to take the PCM out of the capsules) and may have somewhat lower recovery rates. Avoiding too intricate and complex geometries may contribute here for better EoL PCM recovery rates. Once the PCM at EoL is recovered, it could be reused for other TES or thermal management applications, or if not: as feedstock in chemical and other industries, if it has not considerably degraded. RT60HC is a relatively bulky molecule, which however has the potential to be broken down and used as raw material to chemicals industry e.g. in solvents production. As RT60HC is anticipated to have sound cycling stability, higher recovery, reuse and recycling potential is expected.

As a thermal management PCM (e.g. in electronics cooling), the amount of PCMs used per electronic unit will vary greatly depending on the type of electronic devices (e.g. small portable batteries of super-capacitors and stationary batteries, and mobile phones to data centers). This will thus also decide how easy or difficult it is to extract and recover the PCM at the EoL of its intended thermal management application. In smaller devices, extracting small amounts of PCMs may not be as cost-effective or technically feasible as that with large devices. This will impact the recovery options as well as the quality of the PCM at EoL that is recovered, thus affecting its reusability (again for TES applications, or as a feedstock (a secondary raw material) to chemical industries) and recycling. The CF of these processes will also play a major role, which could be increasingly embedded in the processing and recovery costs (with increasingly stringent climate regulations etc.), thus affecting the cost-effectiveness of these different recovery, reuse and recycle routes.

## 9.6. Disposal

This part represents the end-of-life of the product, if recycling and reuse is not possible. If products have reached their end-of-life different methods like landfilling or incineration are common.

As an organic compound, RT60HC has a relatively high energy capacity, when considering incineration to recover energy. At its end of life of use in LHTES (or another TES or thermal management) solution, if it is found to be too degraded or contaminated due to some

unavoidable reasons, it could be thus sent for ultimate disposal for incineration for energy recovery. Examples for this route are waste incineration plants for combined heat and power production (CHP). CO<sub>2</sub> emissions from these incinerations bring about a considerable CF however. Incineration of these EoL PCMs in CHP or similar plants that are coupled with carbon capture and storage (CCS) or even better, with carbon capture, utilization and storage (CCUS) [3] would enable minimizing the CF in this life cycle step.

RT60HC does not contain minerals or metallic compounds and hence would produce minimal amount of bottom ashes and which are also typically not hazardous. Therefore, the ashes generated from the PCM are expected to have minimal environmental impact after incineration and would require minimal landfilling. RT60HC itself would not risk landfilling as it is, for its high energy capacity. An exception here would be that the PCM is contaminated with a very hazardous compound. This however is also very unlikely in the intended thermal applications.

## 9.7. Summary LCA

In this section a qualitative LCA was performed for three final chosen PCMs RT8HC, RT60HC and SP31. The steps from natural resources, raw material, final material, packaging & transport, usage, reuse & recycling, and disposal are described. Though it is a qualitative assessment some data for carbon footprints could be included through the calculations of energy consumption while processing from raw material to packaging & transport. The calculated carbon footprints for these steps "raw material" to "packaging and transport" are summarized in the Table 9.

The main environmental hotspot identified was the raw material extraction. It can be seen that the biobased RT60HC has a lower environmental impact than the RT8HC. De Garcia et al. presented in their study that "the use of hydrated salts presents manufacturing impact about 75% lower than paraffins" [4]. The SP31(\*) data are for now incomplete and for this a comparison is yet not possible but a lower impact than paraffins can be estimated.

Table 9. carbon footprints for RT8HC, RT60HC and SP31

<b>Carbon footprints [g CO<sub>2</sub>/kg product]</b>	<b>RT8HC</b>	<b>RT60HC</b>	<b>SP31*</b>
<b>Raw material</b>	2070	600	(130)
<b>Final material</b>	5	153	17
<b>Packaging &amp; transport</b>	0.1	0.1	0.1
<b>total</b>	2075.1	753.1	147.1

## 10. Conclusion

Within the work of this deliverable 2.1, the following are achieved, fulfilling the plans and commitments of it quite successfully to a great extent, such as:

- The specified criteria were met in the final selection of biobased PCMs, which exhibit high storage capacity, an appropriate temperature range, non-corrosive characteristics towards the HEX (polymer and aluminium) and storage material, exceptional cycle stability, and absence of phase separation.
- The final data from bench-scale testing of **RT57HC** and **RT60HC** at KTH, as detailed in Deliverable 2.2, are summarized in 7.4, with minor adjustments from previous reports regarding heat loss. However, due to uncertainties in specific heat capacities and the approximate mass of stainless steel LHTES container and HEX parts, there are overestimations in PCM heat storage capacities, especially in the heating cycles. Despite this, PCM-TES capacity data for cycling performances remain consistent and comparable across all tested cycles (27 for RT57HC and 53 for RT60HC), demonstrating satisfactory **cycling stability** for both PCMs.
- The PCM **RT60HC**, a biobased organic material, meets all requirements with its high heat storage capacity, non-corrosive nature, and sharp enthalpy peaks. It's chosen as the final phase change material for solution I: **ALL-IN-ONE** and solution III: **PCM HEATING**
- The PCM **RT8HC**, with a high heat storage capacity of 190 kJ/kg and no corrosive effects on metals, is liquid at room temperature, making it easy to handle. It meets all requirements and performed well in tests with an aluminium heat exchanger for solution I **ALL-IN-ONE** (cool side).
- The PCM **SP31**, an inorganic material with a high heat storage capacity exceeding 200 kJ/kg, is solid at room temperature and exhibits corrosive effects on metals. Recommended with a polymer storage and heat exchanger, it fulfils all requirements for low-temperature heating PCM. Tested successfully in Rubitherm's small storage for solution II **LOW-TEMP HEATING**, SP31 will demonstrate its power at the demosite in Montserrat.
- **sIPCMlib** is a PCM library offering **code for calculating thermophysical properties** in Python, Matlab, Modelica/Dymola, and Ansys Fluent. It aids in heat transfer modeling and analysis of PCM-enhanced materials. The users can select PCMs based on various criteria, with relevant information displayed. An overview table summarizes main properties, including phase transition details and metadata. Information on measurement procedures and data processing is also provided.

## 11. References

- [1] T. Barz, A. Bres and J. Emhofer, sPCMLib: A Modelica Library for the Prediction of Effective Thermal Material Properties of Solid/Liquid Phase Change Materials (PCM), 2022, pp. 63-74.
- [2] J. Ren, Life Cycle Sustainability Assessment for Decision-Making, 2020.
- [3] IEA (International Energy Agency), "IEA 50 - Carbon Capture, Utilisation and Storage," 22 02 2024. [Online]. Available: <https://www.iea.org/energy-system/carbon-capture-utilisation-and-storage>.
- [4] D. Garcia, "Life Cycle Assessment of the inclusion of phase change materials (PCM) in experimental buildings," *Energy and building*, vol. 42, no. 9, pp. 1517-1523, 2010.

## Appendix

### Modelica/Dymola code from slPCMLib for PCM RT60HC

```

within slPCMLib.Media_Rubitherm_RT;
package Rubitherm_RT60HC "Rubitherm GmbH, RT60HC; data taken from: Rubitherm
datasheet."
  extends slPCMLib.Interfaces.partialPCM;

  // -----
  redeclare replaceable record propData "PCM record"

    constant String mediumName = "RT60HC";
    // --- parameters for phase transition functions ---
    constant Boolean modelForMelting = true;
    constant Boolean modelForSolidification = true;
    constant Modelica.Units.SI.Temperature rangeTmelting[2] =
{3.2314999999999998E+02, 3.3614999999999998E+02}
      "temperature range melting {startT, endT}";
    constant Modelica.Units.SI.Temperature rangeTsolidification[2] =
{3.2414999999999998E+02, 3.3514999999999998E+02}
      "temperature range solidification {startT, endT}";

    // --- parameters for heat capacity and enthalpy ---
    constant Modelica.Units.SI.SpecificHeatCapacity[2] cpS_linCoef =
{2.0000000000000000E+03, 0.0000000000000000E+00}
      "solid specific heat capacity, linear coefficients a + b*T";
    constant Modelica.Units.SI.SpecificHeatCapacity[2] cpL_linCoef =
{2.0000000000000000E+03, 0.0000000000000000E+00}
      "liquid specific heat capacity, linear coefficients a + b*T";
    constant Modelica.Units.SI.SpecificEnthalpy phTrEnth =
2.6452741843501542E+05
      "scalar phase transition enthalpy";

    // --- reference values ---
    constant Modelica.Units.SI.Temperature Tref = rangeTmelting[1]
      "reference temperature";
    constant Modelica.Units.SI.SpecificEnthalpy href = 0.0
      "reference enthalpy at Tref";

  end propData;

  // -----
  redeclare function extends phaseFrac_complMelting
    "Returns liquid mass phase fraction for complete melting processes"

```



```

protected
  constant Integer len_x =    data_H.len_x;
  constant Real  data_x[:] =  data_H.data_x;
  constant Real  data_y[:] =  data_H.data_y;
  constant Real  m_k[:] =    data_H.m_k;
  constant Real  iy_start[:] = data_H.iy_start;
  constant Real  iy_scaler =  data_H.iy_scaler;
algorithm
  (xi, dxi) := slPCMLib.BasicUtilities.cubicHermiteSplineEval(T-273.15,
    len_x, data_x, data_y, m_k, iy_start, iy_scaler);
end phaseFrac_complMelting;

// -----
redeclare function extends phaseFrac_complSolidification
  "Returns liquid mass phase fraction for complete solidification processes"
protected
  constant Integer len_x =    data_C.len_x;
  constant Real  data_x[:] =  data_C.data_x;
  constant Real  data_y[:] =  data_C.data_y;
  constant Real  m_k[:] =    data_C.m_k;
  constant Real  iy_start[:] = data_C.iy_start;
  constant Real  iy_scaler =  data_C.iy_scaler;
algorithm
  (xi, dxi) := slPCMLib.BasicUtilities.cubicHermiteSplineEval(T-273.15,
    len_x, data_x, data_y, m_k, iy_start, iy_scaler);
end phaseFrac_complSolidification;

// -----
package data_H "spline interpolation data for heating"
  extends Modelica.Icons.Package;
  constant Integer len_x =    14;
  constant Real[14] data_x =  {5.000000000000000E+01,
5.262500000000000E+01, 5.487500000000000E+01, 5.662500000000000E+01,
5.862500000000000E+01, 5.987500000000000E+01, 6.037500000000000E+01,
6.062500000000000E+01, 6.087500000000000E+01, 6.112500000000000E+01,
6.162500000000000E+01, 6.187500000000000E+01, 6.287500000000000E+01,
6.300000000000000E+01};
  constant Real[14] data_y =  {0.000000000000000E+00, 1.2768133011999999E-
02, 3.0590439165999999E-02, 3.1892708887999999E-02, 8.1894258654999996E-02,
1.8696226150299999E-01, 3.4794026749599999E-01, 4.9334748718600002E-01,
5.2575078416099996E-01, 4.2847607736799997E-01, 8.0679170413999995E-02,
2.7444280046999999E-02, 0.000000000000000E+00, 0.000000000000000E+00};
  constant Real[14] m_k =    {0.000000000000000E+00, -
7.7469021709999997E-03, 1.3460511043999999E-02, 2.0528986514000001E-02,
1.4122573055000000E-02, 1.9670756622700000E-01, 4.3056625883200000E-01,
4.5832549208200002E-01, -1.7171492437800001E-01, -6.9228207596699998E-01, -
5.7698655226600004E-01, -8.0073094742000001E-02, 0.000000000000000E+00,
0.000000000000000E+00};

```

```

constant Real[14] iy_start = {0.000000000000000E+00, 2.113299531800000E-
02, 6.082627954599999E-02, 1.135116233270000E-01, 2.290317626710000E-01,
3.727923532790000E-01, 5.011987536240000E-01, 6.058506928179999E-01,
7.360659620370000E-01, 8.576322518790000E-01, 9.820856642359999E-01,
9.929750821770000E-01, 1.000000000000000E+00, 1.000000000000000E+00};
constant Real    iy_scaler = 9.9652958170012729E-01;
end data_H;

// -----
package data_C "spline interpolation data for cooling"
extends Modelica.Icons.Package;
constant Integer len_x = 14;
constant Real[14] data_x = {5.100000000000000E+01,
5.262500000000000E+01, 5.387500000000000E+01, 5.437500000000000E+01,
5.562500000000000E+01, 5.812500000000000E+01, 5.962500000000000E+01,
6.037500000000000E+01, 6.062500000000000E+01, 6.112500000000000E+01,
6.137500000000000E+01, 6.162500000000000E+01, 6.187500000000000E+01,
6.200000000000000E+01};
constant Real[14] data_y = {0.000000000000000E+00, 1.473675938800000E-
02, 0.000000000000000E+00, 0.000000000000000E+00, 1.573716089800000E-02,
4.331200130099999E-02, 1.046550129940000E-01, 3.380330174260000E-01,
5.451401370949999E-01, 6.144896125609999E-01, 4.447538937439999E-01,
2.230650738789999E-01, 5.118391292700000E-02, 0.000000000000000E+00};
constant Real[14] m_k = {0.000000000000000E+00, 1.639196281600000E-
02, 0.000000000000000E+00, 0.000000000000000E+00, -3.730016791999999E-03,
2.093706080099999E-02, 9.849759814599999E-02, 6.035244742209999E-01,
6.850749219830000E-01, -5.439222927100000E-01, -8.292524079919999E-01, -
8.015412098430000E-01, -5.965166476169999E-01, 0.000000000000000E+00};
constant Real[14] iy_start = {0.000000000000000E+00, 8.299241811000000E-
03, 1.955284323900000E-02, 1.955284323900000E-02, 2.979123595800000E-02,
9.026493627800000E-02, 1.859220158909999E-01, 3.271121337019999E-01,
4.361995634840000E-01, 7.491735402400000E-01, 8.819882215030000E-01,
9.646510394330000E-01, 9.975972015349999E-01, 1.000000000000000E+00};
constant Real    iy_scaler = 9.9195728546595674E-01;
end data_C;

// -----
redeclare function extends density_solid "Returns solid density"
algorithm
rho := 8.500000000000000E+02;
end density_solid;
// -----
redeclare function extends density_liquid "Returns liquid density"
algorithm
rho := 7.500000000000000E+02;
end density_liquid;
// -----

```

```

redeclare function extends conductivity_solid "Returns solid thermal
conductivity"
algorithm
  lambda := 2.0000000000000001E-01;
end conductivity_solid;
// -----
redeclare function extends conductivity_liquid "Returns liquid thermal
conductivity"
algorithm
  lambda := 2.0000000000000001E-01;
end conductivity_liquid;

annotation(Documentation(
  info="<html>
  <p>
  This package contains solid and liquid properties for the PCM:
  <strong>RT60HC</strong> from manufacturer: <strong>Rubitherm
  GmbH</strong>.<br>
  Basic characteristics are the material class: unknown, and encapsulation:
  multiple options available<br> The data is taken from: Rubitherm datasheet -
  last access 2023-05-23.<br><br>
  <br><br>
  The package contains phase transition functions for
  <ul>
  <li>complete melting      : true</li>
  <li>complete solidification: true</li>
  </ul></p><p>
  <p>
  Code export from <strong><u>slPCMLib database</u></strong> on 2023-12-
  08.<br><br>
  See:<br>
  Barz, T., Bres, A., & Emhofer, J. (2022).
  slPCMLib: A Modelica Library for the Prediction of Effective
  Thermal Material Properties of Solid/Liquid Phase Change
  Materials (PCM).
  In Proceedings of Asian Modelica Conference 2022 (pp. 63-74).
  Linköping University Electronic Press.
  <a href>https://doi.org/10.3384/ecp19363</a>.
  </p>
  </blockquote>
  </p></html>",
  revisions="<html>
  <ul>
  <li>file creation date: 2023-12-08 </li>
  </ul>
  </p></html>"));
end Rubitherm_RT60HC;

```

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