IEA Technology Collaboration Programme

International Energy Agency
Technology Collaboration Programme on Energy Storage
(ES TCP)

Task 40

Compact Thermal Energy Storage – Materials within Components within Systems

Final Report

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Task Manager ES TCP Task 40:
Andreas Hauer
ZAE Bayern e. V.
Germany

Task 40 is a fully joint Task with Task 67 of the IEA Solar Heating and Cooling TCP

SOLAR HEATING & COOLING PROGRAMME
INTERNATIONAL ENERGY AGENCY

AUTHORS (ALPHABETICAL ORDER)

Monica Delgado (Univ. of Zaragoza, Spain), Louis Desgroseilliers (SPF, Switzerland), Reda Djebbar (NRCan, Canada), Stefania Doppiu (CIC EnergiGUNE, Spain), Gerald Englmair (DTU, Denmark), Andrea Frazzica (CNR, Italy), Benjamin Fumey (HSLU, Switzerland), Stefan Gschwander (Fraunhofer ISE, Germany) Andreas Hauer (ZAE Bayern, Germany), Andreas König Haagen (Univ. of the Basque Country, Spain), Daniel Lager (AIT, Austria), Ana Lázaro (Univ. of Zaragoza, Spain), Helena Navarro (Univ. of Birmingham, UK), Christoph Rathgeber (ZAE Bayern, Germany), and Wim van Helden (AEE INTEC, Austria).

CONTRIBUTORS (ALPHABETICAL ORDER)

Alireza Afshari (Aalborg Univ., Denmark), Nidhi Agarwal (Pluss Polymers, The Netherlands), Dylan Bardy (NRCan, Canada), Camila Barreneche (Univ. of Barcelona, Spain), Rocio Bayon (CIEMAT, Spain), Èlise Bérut (LOCIE Laboratory, France), Emiliano Borri (Univ. of Lleida, Spain), Vincenza Brancato (CNR, Italy), Michael Brütting (CAE, Germany), Luisa F. Cabeza (Univ. of Lleida, Spain), Luigi Calabrese (Univ. of Messina, Italy), Luis Coelho (Polytechnic Institute of Setúbal, Portugal), Carolina Costa (Northumbria Univ., UK), José Costa (Univ. of Coimbra, Portugal), Bob Critoph (Univ. of Warwick, UK), Ruud Cuypers (TNO, The Netherlands), Jean Luc Dauvergne (CIC energiGUNE, Spain), Asmira Delic (SINTEF, Norway), Gonzalo Diarce (Univ. of the Basque Country, Spain), Larissa Dietz (DLR, Germany), Yulong Ding (Univ. of Birmingham, UK), Phil Eames (Loughborough Univ., UK), Jonathon Elvins (Swansea Univ., UK), Jianhua Fan (DTU, Denmark), Inés Fernández (Univ. of Barcelona, Spain), Marco Fernandes (Univ. of Coimbra, Portugal), Olav Galteland (SINTEF, Norway), Sebastian Gamisch (Fraunhofer ISE, Germany), Ane Miren García Romero (Univ. of the Basque Country, Spain), Eduardo Jose Garcia-Suarez (CIC energiGUNE, Spain), Adélio Gaspar (Univ. of Coimbra, Portugal), Fabrizia Giordano (AIT, Austria), Dominic Groulx (Dalhousie University, Canada), Saman N. Gunasekara (KTH, Sweden), Andrea Gutierrez (DLR, Germany), Thomas Haussmann (Fraunhofer ISE, Germany), Franz Hengel (AEE Intec, Austria), Sahand Hosouli (Swansea Univ., UK), Henk Huinink (TUE, The Netherlands), Gayaneh Issayan (Univ. of Appl. Sciences Upper Austria), Kévyn Johannes (INSA Lyon, France), Maike Johnson (DLR, Germany), Jochem Jongerius (TNO, The Netherlands), Frieda Kapsamer (TU Vienna, Austria), Sumanjeet Kaur (LBNL, USA), Florian Kerscher (TU Munich, Germany), Franziska Klünder (Fraunhofer ISE, Germany), Lia Kouchachvili (NRCAN, Canada), Yannick Krabben (HSLU, Switzerland), Frédéric Kuznik (INSA Lyon, France), Grégory Largiller (CEA LITEN, France), Nolwenn Le Pierrès (University Savoie Mont Blanc, France), Wenye Lin (Fraunhofer ISE, Germany), Lingai Luo (Université de Nantes, France), Alessandro Maccarini (Aalborg Univ., Denmark), Thomas Manser (NRCAN, Canada), Emanuela Mastronardo (Univ. of Messina, Italy), Chris McNevin (NRCAN, Canada), Harald Mehling (Germany), Candida Milone (Univ. of Messina, Italy), Urška Mlakar (Univ. of Ljubljana, Slovenia), Leander Morgenstern (TU Munich, Germany), Sven Mumme (DoE, USA), Nuria Navarrete (DLR, Germany), Marc Neira i Viñas (Univ. of Barcelona, Spain), Elena Palomo (CIC EnergiGUNE, Spain), Michel Ondarts (University Savoie Mont Blanc, France), Jonathan Outin (University Savoie Mont Blanc, France), Halime Paksoy (Cukurova Univ., Turkey), Anabel Palacios Trujillo (HSLU, Switzerland), Evdoxia Paroutoglu (Aalborg Univ., Denmark), Elpida Piperopoulos (Univ. of Messina, Italy), Rebecca Saldago Pizarro (Univ. of Barcelona, Spain), Rebecca Ravotti (HSLU, Switzerland), Anthony Rawson (DLR, Germany), Jack Reynolds (Swansea Univ., UK), Alenka Ristić (NIC, Slovenia), Jorge Salgado Beiceiro (SINTEF, Norway), Henri Schmit (ZAE Bayern, Germany), Oscar Seco Calvo (CIEMAT, Spain), Ángel Serrano (CIC EnergiGUNE, Spain), Alexis Sevault (SINTEF, Norway), Mina Shahi (Univ. of Twente, The Netherlands), Galina Simonsen (SINTEF, Norway), Jakob Smith (TU Vienna, Austria), Jerome Soto (CNRS, France), Veronika Stahl (DLR, Germany), Adela Svobodova (Univ. of Barcelona, Spain), Handan Tezel (Univ. of

Ottawa, Canada), David Verez (Univ. of Lleida, Spain), Peter Vetter (DLR, Germany), Fride Vullum-Bruer (SINTEF, Norway), Sara Walsh (Swansea Univ., UK), Peter Weinberger (TU Vienna, Austria), Jörg Worlitschek (HSLU, Switzerland), Bernhard Zettl (Univ. of Appl. Sciences Upper Austria), Sai Saran Yagnamurthy (Univ. of Warwick, UK), Laurent Zalewski (Université d'Artois, France), and Gabriel Zsembinszki (Univ. of Lleida, Spain).

CONTENT

LIST OF ABBREVIATIONS

CTES	Compact Thermal Energy Storage
DSC	Differential Scanning Calorimetry
ES	Energy Storage
FTIR	Fourier-transform Infrared Spectroscopy
GUM	Guide to the expression of Uncertainty in Measurement
HD	Hot Disk
HTF	Heat Transfer Fluid
HW	Hot Wire
LFA	Laser Flash Analysis
LN2	Liquid Nitrogen
PCM	Phase Change Material
RH	Relative Humidity
RRT	Round Robin Test
RT	Room Temperature
SAT	Sodium Acetate Trihydrate
SHC	Solar Heating and Cooling
SoC	State of Charge
TCM	Thermochemical Material
TES	Thermal Energy Storage
TGA	Thermogravimetric Analysis
THB	Transient Hot Bridge
TPS	Transient Plane Source
UV/VIS	Ultraviolet–visible Spectroscopy
XRD	X-Ray Diffraction

MAIN RESULTS IN A NUTSHELL

Thermal energy storage (TES) is subdivided into sensible, latent, and thermochemical heat & cold storage. In Task 40, compact thermal energy storage (CTES) materials and components for latent heat & cold storage (phase change materials, PCM) and for thermochemical heat & cold storage (TCM) were in focus. A variety of different material classes is investigated and applied to be used as PCM and TCM in TES systems. New materials, material mixtures, and composites are worked on by a growing community of scientists.

TES components like heat (and mass) exchangers are used to charge and discharge TES units meeting application requirements. Due to the variety of different TES materials, different component concepts are being developed and tested. To enable a performance assessment of components, testing protocols need to pay attention to the material-component interaction.

Task 40 aimed to push forward CTES technology development to accelerate the market introduction through the international collaboration of experts from materials research, components development and system integration, as well as industry and research organisations.

The overall objectives were

1) to better understand the factors that influence the storage density and the performance degradation of CTES materials,
2) to characterize these materials in a reliable and reproducible manner,
3) to develop methods to effectively determine the state of charge of a CTES system, and
4) to increase the knowledge base on how to design optimized heat exchangers and reactors.

Task 40 was divided into five Subtasks. In Subtask A, *Material Characterization and Database*, standardized measurement procedures for CTES materials were developed and validated, and a materials & knowledge database was revised and maintained. In Subtask B, *CTES Material Improvement*, proper strategies that allow for tuning CTES materials' properties to improve their performance in components and systems were identified and analysed. In Subtask C, *State of Charge Determination*, techniques with which the state of charge of a CTES system can be determined in a reliable and cost-efficient way were collected and discussed. The objective of Subtask D, *Stability of PCM and TCM*, was to support R&D on PCM and TCM stability by understanding and classifying the underlying degradation mechanisms. The topic of Subtask E, *Effective Component Performance with Innovative Materials*, was the (evaluation of) material-component interaction for improved system performance.

Task 40, as it was with its predecessors, is built upon a strong collaboration within the international CTES R&D community. The following outcomes were achieved in the five Subtasks.

- Task 40 experts achieved substantial progress in working on standardized measurement methods leading to improved TES material characterization skills of the participating researchers and labs. To this end, round robin tests on thermal conductivity/diffusivity, specific heat capacity of powdery materials, enthalpy change due to sorption or chemical reaction, density, and viscosity were performed. The requirements of a revised CTES material database were defined, evaluated, and summarized in a software requirement specification (SRS) document.
- The information collected regarding CTES material improvement demonstrates how complex the study of these materials is, but also how proper strategies – like material mixtures and composites – allow to obtain materials with tuned properties for potential use in CTES

applications. Open questions cover the definition of guidelines for materials optimization and the quantification of the impact on the TES system.
- A total of twenty-six methods and proofs of concept to effectively determine the state of charge of PCM or TCM systems were collected and classified. Four prototype systems, where a direct interaction of material bulk response with the control system is in place, are presented and discussed.
- The developed approach to map degradation of CTES materials provides a comprehensive overview of the degradation mechanisms and the corresponding degradation factors which are relevant for a specific material or material class. Eleven different examples of CTES materials degradation mapping were elaborated. CTES material stability tests under application conditions can only be carried out reasonably if there is an understanding of the dependencies between degradation factors, degradation mechanisms, and effects on the CTES material and system.
- Performance indicators for PCM allowing a fair comparison of latent heat thermal energy storage units were proposed. This has not been possible so far. For example, a comparison of the average thermal power is strongly influenced by the initial and boundary conditions during the experiment. Three methods were developed by the Task participants to minimize these influences and enable a comparable analysis. For TCM component evaluation, a standardized absorption curve-based performance mapping and a standardized temperature-based test procedure for the sorption heat storage in space heating application were developed.

To disseminate the Task work, Task experts published a technology position paper[1] providing an overview of the compact thermal energy storage technologies market, outlining its importance, potential, and development. The paper addresses policy, decision makers, and influencers and aims to present high-level information as a basis for uptake and further development. It concludes by highlighting actions needed to further exploit thermal energy storages with minimal space requirements and accelerate more efficient energy systems, including sector coupling, with a higher share of renewables.

The work within this Task and its predecessors is establishing the foundation to focus on specific application areas for thermal energy storage. The investigation of the various aspects of material-component interaction is considered as a crucial part of the development and realization of CTES applications.

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[1] SHC Technology Position Paper "Compact Thermal Energy Storage", June 2023, available through SHC Task 67 website.

KEY MESSAGES

General

- Collaboration between material and application experts leads to an improved understanding of material and component design strategies and supports the development of CTES systems.
- Standards to measure material properties and to evaluate components are a prerequisite for constructive discussions among experts and for advancing CTES technologies.

CTES material characterization

- Developed experimental characterization methods (thermal conductivity/diffusivity, specific heat capacity of powdery materials, enthalpy change due to sorption or chemical reaction, density, and viscosity) are the basis for TES material evaluation and comparison.
- Applying a defined uncertainty evaluation according to standards (e.g. ISO/IEC Guide 98-3:2008) is important to develop measurement standards through round robin tests.

CTES material improvement

- A number of innovative and improved CTES materials, e.g. based on material mixtures and composites, were developed and continuously are being developed by the R&D community.
- The definition of guidelines for materials improvement and related KPIs for material performance assessment are a key aspect to guide material development strategies towards system requirements.

State of charge determination

- In flexible heating and cooling systems, *thermal batteries* are needed: TES systems with instantaneous State of Charge (SoC) determination.
- State of charge is a component property (not material) - analogy: electrical battery.
- Reliable SoC determination, based on material bulk response measurements, enables the integration of CTES systems into (digitalized) energy systems.

CTES material stability

- Understanding CTES stability on material level is essential to assess the (long-term) performance of CTES materials in components and storage systems.
- The developed degradation mapping offers an easy-to-use visualization of CTES material stability, thereby supporting the process of CTES material selection under application conditions.

CTES material-component interaction

- The reachable charging/discharging power is strongly influenced by the component (heat exchanger, reactor) design, where the interaction of the CTES material with the component is crucial.
- Uniform test schemes for component evaluation are being established to compare CTES system performance.

EXECUTIVE SUMMARY

1 Short Description of Task 40

1.1 Objectives and Scope

Task 40 dealt with an application-oriented development of innovative and compact thermal energy storage (CTES) materials: Phase Change Materials (PCM) and Thermochemical Materials (TCM). PCM and TCM are studied, improved, characterized, and tested in components. The main components for CTES technologies are heat exchangers and reactors.

The objectives were to have a better understanding of the factors influencing the energy storage density and the performance degradation of CTES materials, to be able to characterize these materials in a reliable and reproducible manner, to have methods to effectively determine the state of charge of a CTES unit, and to have better knowledge on how to design optimized heat exchangers and reactors.

1.2 Organisational Structure

IEA ES TCP Task 40 is a fully joint activity with IEA SHC TCP Task 67.

The work of the Task was split into five Subtasks.

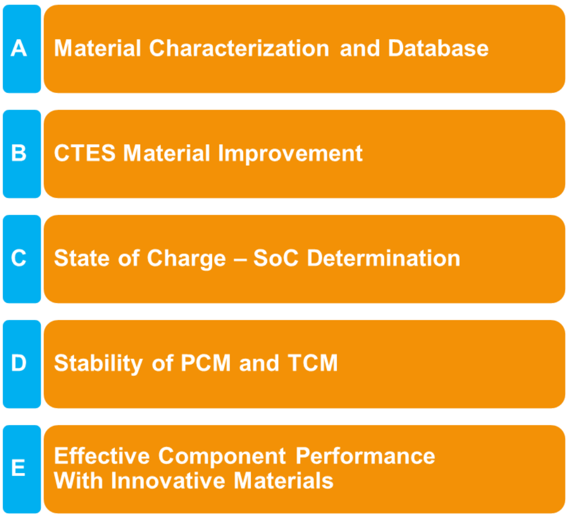


Figure 1-1: Subtask structure.

The Subtask leaders were:

- Subtask A: Daniel Lager, AIT, Austria
- Subtask B: Stefania Doppiu, CIC energiGUNE, Spain
- Subtask C: Gerald Englmair, DTU, Denmark, and Reda Djebbar, NRCan, Canada
- Subtask D: Christoph Rathgeber, ZAE Bayern, Germany
- Subtask E: Ana Lazaro, Univ. Zaragoza, Spain, Andreas König-Haagen, Univ. of the Basque Country, Spain, and Benjamin Fumey from HSLU, Switzerland

1.3 Duration of Task

The beginning of Task 40 was 1 July 2021 and the end 30 June 2024. The work plan was approved by the ES TCP Executive Committee at the 91st ExCo meeting on 7–8 June 2021. It was confirmed by the participants at the kick-off meeting on 27–29 October 2021.

1.4 Experts Meetings

Table 1-1 gives an overview of the expert meetings in this Task.

Table 1-1: Details about the date and location of each expert meeting.

City	Country	Date	# Participants
Vitoria-Gasteiz	Spain	27–29 October 2021	53 (24 on site, 29 online)
Graz	Austria	4–5 April 2022	38 on site
Kassel	Germany	29–30 September 2022	41 on site
Halifax	Canada	24–26 April 2023	37 (30 on site, 7 online)
Lyon	France	2–4 October 2023	35 (29 on site, 6 online)
Lucerne	Switzerland	22–24 April 2024	32 (24 on site, 8 online)

1.5 Participation

Table 1-2 gives an overview about which institution from which country is participating in this Task.

Table 1-2: List of participating institutions and experts per country.

Country	Institution	Representative (name)
Austria	AEE	Wim van Helden, Franz Hengel
Austria	AIT	Daniel Lager, Fabrizia Giordano
Austria	FHOÖ	Gayaneh Issayan, Bernhard Zettl
Austria	TU Wien	Peter Weinberger, Jakob Smith, Frieda Kapsamer
Canada	Dalhousie University	Dominic Groulx
Canada	NRCan	Reda Djebbar, Lia Kouchachvili, Dylan Bardy
Canada	University of Ottawa	Handan Tezel
Canada	Neothermal ES Inc	Louis Desgrosseilliers
Denmark	Aalborg University	Alireza Afshari, Alessandro Maccarini
Denmark	DTU	Gerald Englmair, Jianhua Fan
France	INSA Lyon	Frédéric Kuznik, Kévyn Johannes
France	CNRS	Jerome Soto
France	CEA LITEN	Grégory Largiller
France	LOCIE Laboratory	Èlise Bérut
France	Université d'ARTOIS	Laurent Zalewski
France	Université de Nantes	Lingai Luo
France	University Savoie Mont Blanc	Nolwenn Le Pierrès
Germany	CAE	Michael Brütting
Germany	ZAE Bayern	Andreas Hauer, Christoph Rathgeber
Germany	DLR	Anthony Rawson, Andrea Gutierrez, Maike Johnson, Veronika Stahl, Peter Vetter, Larissa Dietz
Germany	Fraunhofer ISE	Stefan Gschwander, Franziska Klünder, Wenye Lin, Sebastian Gamisch

Germany	TU Munich	Leander Morgenstern, Florian Kerscher
Germany	-	Harald Mehling
Italy	CNR	Vincenza Brancato, Andrea Frazzica
Italy	University of Messina	Luigi Calabrese, Elpida Piperopoulos, Emanuela Mastronardo, Candida Milone
Netherlands	PLUSS Polymers	Nidhi Agarwal
Netherlands	TNO	Ruud Cuypers
Netherlands	TU Eindhoven	Henk Huinink
Netherlands	University Twente	Mina Shahi
Norway	SINTEF	Jorge Salgado Beiceiro, Olav Galteland, Alexis Sevault
Portugal	Polytechnic Institute of Setúbal	Luis Coelho
Portugal	University of Coimbra	José Costa, Adélio Gaspar, Marco Fernandes
Slovenia	National Institute of Chemistry	Alenka Ristić
Slovenia	University of Ljubljana	Urška Mlakar
Spain	University of Barcelona	Ines Fernandez, Camila Barreneche
Spain	CIC energiGUNE	Jean-Luc Dauvergne, Elena Palomo del Barrio, Eduardo Jose Garcia-Suarez, Stefania Doppiu, Ángel Serrano
Spain	CIEMAT	Rocio Bayon, Oscar Seco Calvo
Spain	Universidad del País Vasco UPV/EHU	Ane Miren García Romero, Andreas König-Haagen, Gonzalo Diarce
Spain	University of Zaragoza	Ana Lazaro
Spain	University of Lleida	Luisa F. Cabeza, Gabriel Zsembinszki, Emiliano Borri, David Verez
Sweden	KTH	Saman Gunasekara
Switzerland	HSLU	Benjamin Fumey, Rebecca Ravotti, Yannik Krabben, Jörg Worlitschek
Turkey	Cukurova University	Halime Paksoy
United Kingdom	Loughborough University	Phil Eames
United Kingdom	University Birmingham	Yulong Ding
United Kingdom	University of Warwick	Bob Critoph, Sai Saran Yagnamurthy
United Kingdom	Swansea	Jonathon Elvins, Sara Walsh, Jack Reynolds, Sahand Hosouli
United States	US DoE	Sven Mumme, Sumanjeet Kaur

2 Summary of Subtasks

2.1 Subtask A: Material Characterization and Database

The main objective of Subtask A was to develop and/or validate several standardized measurement procedures for TES materials based on PCM and TCM and to further maintain the existing TES material database.

2.1.1 Standardized measurement procedures and round robin tests

In the preceding TES materials Tasks, new TES materials were identified or developed in research projects of the participating partners. Furthermore, measurement procedures were developed to identify the main physical or chemical parameters. Some of these procedures were already validated and some of them were still at the beginning. In Task 40, round robin tests (RRT) on (i) thermal conductivity and diffusivity, (ii) specific heat capacity, (iii) sorption enthalpy, as well as (iv) density and viscosity of different PCM and TCM were conducted. Depending on the material type and measurement method, different measurement procedures were developed, tested, and evaluated to receive comparable results among the round robin participants. Overall, more than forty organizations from sixteen countries participated in the round robin tests.

The summarized lessons learned from the round robin tests are:

- The equipment variability supposes a challenge to establish a standardized measurement protocol and needs more effort in the beginning of a round robin test.
- Analysis of measurement uncertainty needs to become part of the lab routine. Experimental and systematic uncertainty must be accounted to compare the final results. In some cases, the uncertainty reported was below the equipment error, due to
    - not enough repetitions,
    - not accounted for equipment error,
    - or not enough samples tested.
- The occurrence of water in the sample (especially for TCM, e.g. hydrated or sorption samples) can lead to different sample states in the beginning of the measurement and should be examined in more detail before the measurement.
- It is challenging to have enough participants with comparable instruments participating; meaningful results are only possible with an adequate number of participants.
- Sample preparation and instrument calibration are crucial and to be exercised.

As an example, Figure 2-1 shows the comparison of measured densities of a paraffin melting between 53 and 58 °C. While the liquid densities were in sufficient agreement, the solid densities showed significant deviations. Therefore, the sample preparation and measurement procedure in the solid state was discussed in more depth by the participating experts.

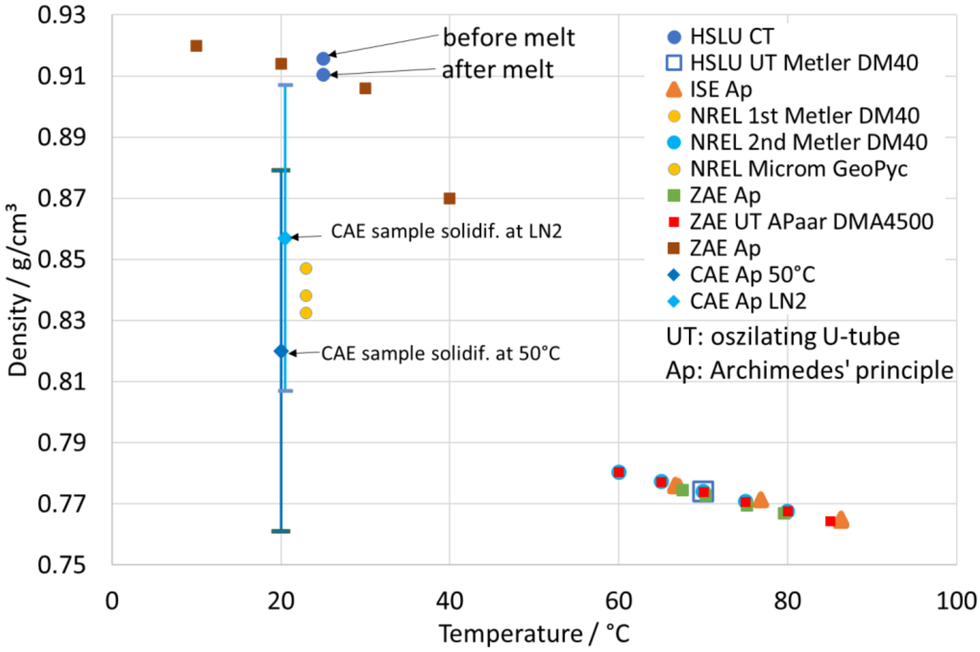


Figure 2-1: Comparison of results of the density RRT.

Summarizing the common topics for future activities:

- An increased number of participants for the round robins to get statistic significant results.
- A defined uncertainty evaluation for all round robin tests according to standards (e.g. ISO/IEC Guide 98-3:2008)
- Exploring new PCM and TCM:
    - Adapt sample preparation procedures for hydrated or sorption materials.
    - Measure PCM with non-Newtonian behaviour in the liquid phase.
- Apply and adapt the methods for high temperature TES materials.

During this Task, round robin test results and improvements for all above mentioned quantities were achieved. The detailed results and measurement procedures can be found in the section 3.1 of the final report.

2.1.2 CTES Materials database and knowledge platform

In the second activity of Subtask A, the requirements of a new *Thermal Energy Storage Material Database* were defined and evaluated. A database has already been developed in the previous Tasks (https://thermalmaterials.org/). This database is to be filled with new data and structurally adapted in the future. One of these structural changes is the link to existing databases such as the *slPCMlib* (https://slpcmlib.ait.ac.at/) database. Several changes of the existing database were proposed to the experts of Subtask A and assessed based on a survey. A *Software Requirement Specification* (SRS) document was created from this survey. The SRS summary is given in section 3.2 of the extended final report and the complete SRS can be found in Appendix 8.1.

Due to budgetary constraints, it was not possible to proceed with the development of an offer from any of the software development firms contacted. Therefore, it was not possible to complete the implementation of the new version of the database.

An outcome for a future task is to implement a reduced number of requirements, while contacting a larger number of software development firms. For this purpose, the developed SRS document constitutes a solid basis to start from, as it follows the conventional IT requirements format needed for database platform development. Starting from the SRS document, the requirement specifications could be further refined to produce an optimized selection that fits within the available budget for the development of the database.

2.2 Subtask B: CTES Material Improvement

The objective of Subtask B was to identify strategies for tuning the properties of CTES materials to improve their performance in components and storage units. This included to discover new potential materials for CTES with the targets of low cost, no toxicity, non-flammable, deployment of natural/bio-based materials; to develop single component materials with changed chemistry through modified structure and multi-component materials with increased storage capacity and enhanced heat and mass transport properties; to evaluate the influence of the synthesis and processing methods on the techno-economic and environmental performances of the materials.

The following CTES materials were considered in Subtask B.

- PCM: solid-liquid and solid-solid transitions, composites and shape-stabilized materials.
- TCM: sorption processes (ad- and absorption) and chemical reactions (mainly gas-solid).

An overview of the CTES materials, the R&D objectives with respect to materials improvement, and possible pathways is given in Figure 2-2.

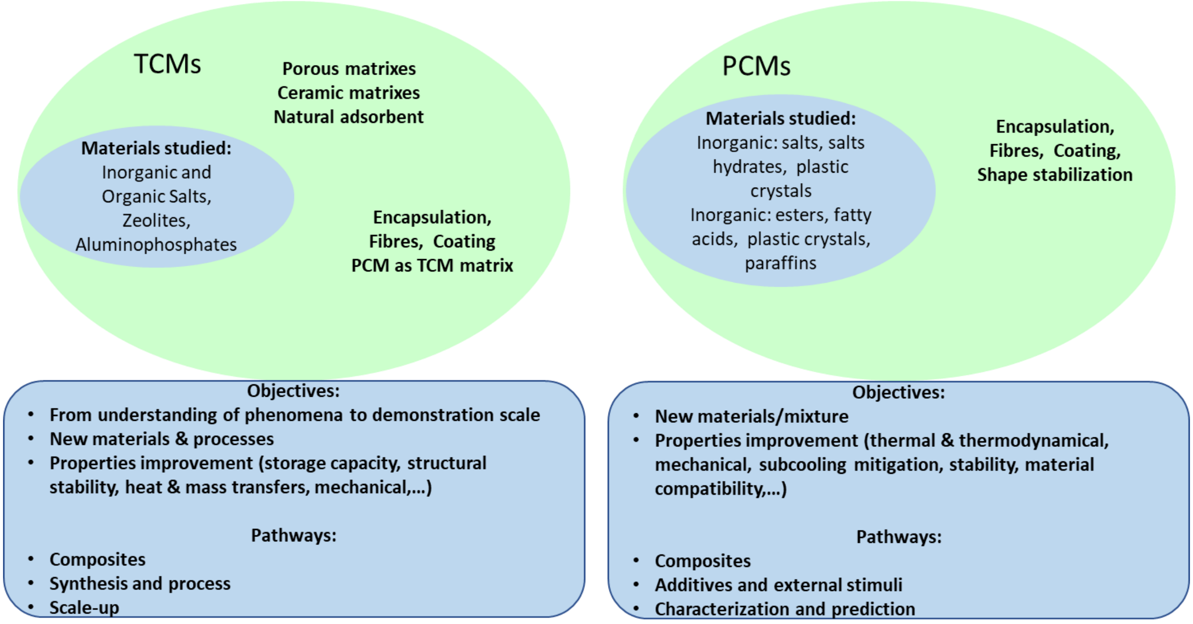


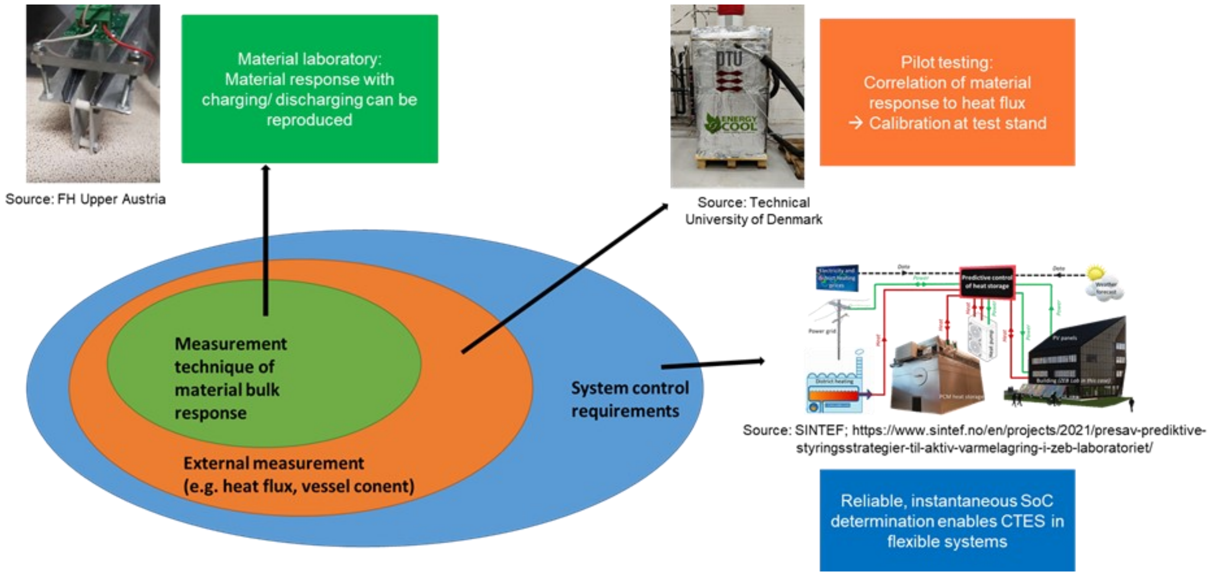
Figure 2-2: Overview of the materials studied in Subtask B.

Section 4 of the extended final report covers the materials studied, as well as the R&D objectives and pathways contributed by the participating experts and institutions.

2.3 Subtask C: State of Charge Determination

The objective of Subtask C was to collect, classify, and disseminate promising techniques with which the state of charge (SoC) of a CTES unit can be determined. Specific activities of Subtask C were to make an inventory of material properties and measurements techniques that can be related to the SoC, to develop methods to link the measured properties to a numerical model of the CTES and use the combination to determine the SoC, as well as to test these in stand-alone storages and possibly in storages integrated in a system.

Subtask C experts defined a *thermal battery* as a TES system with instantaneous SoC determination. Therefore, SoC is a component level property, and its determination utilizes measurement techniques of material bulk response. The following Figure 2-3 defines three distinct levels to the development of SoC determination techniques for PCM and TCM CTES.



Source: FH Upper Austria

Source: Technical University of Denmark

Source: SINTEF; https://www.sintef.no/en/projects/2021/presav-prediktive-styringsstrategier-til-aktiv-varmelagring-i-zeb-laboratoriet/

Figure 2-3. Schematic representation of the 3-level approach for the development of PCM and TCM SoC determination techniques linked to material properties.

The innermost level, *material level*, describes the development of measurement sensors and techniques able to provide data relating to an intrinsic material property of either the PCM/TCM or the external conditions imparting heat/mass to the PCM/TCM that are useful to determine SoC (typically TRL 1–3). The second level, *component level*, describes the development of the *material level* measurement techniques either internal or external to the PCM/TCM able to provide data that is calibrated to either bulk or local SoC determination (typically TRL 4–6). The third level, *system control*, describes the integration of the calibrated SoC determination techniques at the *component level* into a CTES system with electronic control (local or remote) at or near the final CTES configuration for end-use deployment (typically TRL 7–9).

To work towards the objective, Subtask C experts conducted three steps. First, an inventory of promising material properties and related measurement techniques. Regarding PCM, twenty technique submissions were collected. Eleven of them described techniques utilizing temperature measurements of the PCM medium and control volume boundary heat exchange. Regarding TCM, six main TCM SoC measurement techniques were submitted. Most, if not all these methods work at *material level* and used either in a laboratory experimental environment or at pilot scale. The two most promising methods to achieve higher TRL include (i) enthalpy balance SoC determination technique during system operation, and (ii) TCM mass or adsorbate mass balance SoC determination technique. As the second step, a collection of experimental and numerical proofs of concept were presented and explained in more detail. Third, descriptions of application requirements of four prototype systems, where a direct interaction of material bulk response with the control system is in place, were prepared.

2.4 Subtask D: Stability of PCM and TCM

In Subtask D, a better understanding of the stability of PCM and TCM during their lifetime and the development of recommendations for an application-oriented investigation of this stability were addressed. The goal was to support R&D on PCM and TCM with a predictable and improved stability.

Previous works and the state of literature lack differentiating degradation mechanisms, showing which test methods are suitable for determining the respective degradation, and making (material class-specific) recommendations for accelerating measurements.

In Task 40, a CTES material degradation table was proposed to map degradation mechanisms for CTES material classes, and to propose recommendations for stability testing based on simple experiments to faster investigate stability by accelerating degradation. The developed approach to map degradation of CTES materials provides a comprehensive overview of the degradation mechanisms and the corresponding degradation factors which are relevant for a specific material or material class. Such a mapping diagram informs (scheme shown in Figure 2-4) about the effect of different types of degradation on the CTES material and system.

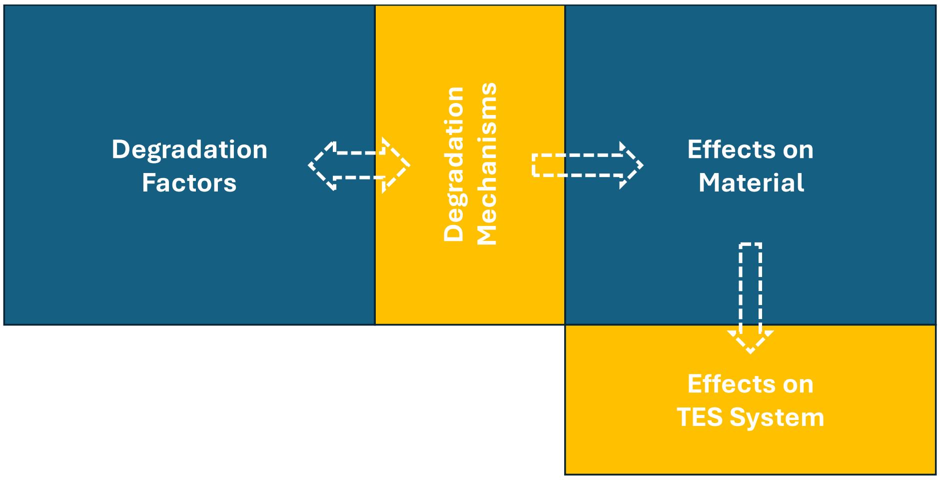


Figure 2-4. Scheme of the degradation mapping diagram to illustrate PCM and TCM stability.

Task experts provided their degradation expertise about the following CTES materials (classes): Organic plastic crystals, lauric and adipic acid, fatty esters, saturated triglycerides, calcium chloride hexahydrate, sodium acetate trihydrate, disodium hydrogen phosphate dodecahydrate, zeolites, potassium carbonate, and sulfates. Evaluating these eleven examples for CTES materials degradation mapping, it became evident that a certain effect on the material (e.g. a transition temperature displacement) can be caused by different degradation mechanisms. In the same way, effects on the storage system performance can usually be attributed to a combination of different effects on material level. In practice, stability tests under application conditions can only be carried out reasonably if there is an understanding of the dependencies between degradation factors, degradation mechanisms, and effects on the CTES material and system. Such an understanding can be summarized and communicated using the developed degradation mapping diagram.

2.5 Subtask E: Effective Component Performance with Innovative Materials

Subtask E focused on material-component interaction for an improved storage system performance. This was attained by defining performance parameters, understanding the mechanisms that determine the performance-based interaction between storage material and components, and identifying methods for improved component and material design. Work was split up between PCM and TCM experts, and the outcomes are presented separately.

2.5.1 PCM

Performance indicators for PCM components (mainly heat exchangers) were defined and agreed upon. These indicators allow a fair comparison of latent heat thermal energy storage units. This has not been possible so far. For example, a comparison of the average thermal power is strongly influenced by the initial and boundary conditions during the experiment. Three methods were developed by the Task participants to minimize these influences and enable a comparable analysis.

The idea behind the first method is to normalize the heat transfer rate $\dot{Q}$ by the volume and a reference temperature difference, calculate a mean value and present the results plotted over a normalized mean value of the capacity flow of the heat transfer fluid in a so-called $\overline{\dot{C}^{\mathrm{norm}}}/\overline{\dot{Q}^{\mathrm{norm}}}$-plot.

The second method, called *three sections approach*, helps finding a suitable stop criterion for calculating a mean value of the power of latent heat thermal energy storage units. Tangents are laid through the inflection points that occur in a characteristic discharge power curve of a latent heat thermal energy storage unit. The discharging process is divided into several sections and the end is determined based on their intersections with each other and with the zero line, respectively.

Depending on the operating conditions, the actual usable heat content of a thermal energy storage can deviate significantly from the theoretical storage capacity calculated from the geometry and material parameters. This can drastically reduce the amount of usable heat, especially at high thermal power rates. The third method is intended to take these dependencies into account. It is based on a small number of standardized charging and discharging measurements with a constant volume flow and constant inlet temperature. The resulting power curves are normalized and converted from the time domain to the energy domain. The curves are plotted in such a way that the actual usable heat content of the storage can be determined for specified values for the set thermal power, the temperature, and the maximum volume flow.

2.5.2 TCM

In the case of TCM components, there is a need for a standardized evaluation of sorption heat storage components and systems with respect to the material performance given by the vapor pressure versus temperature relationship of various concentrations or mass fractions. This standard evaluation will make it possible to quantify development success.

The developed performance mapping technique uses a concentration vs. gross temperature lift diagram, which incorporates the sorbent's equilibrium line and the deviation caused by the non-linear temperature-heat relationship. As shown in Figure 2-5, deviation from the equilibrium indicates performance loss. The performance map of the sorption heat storage is based on a good characterization of the sorption material used.

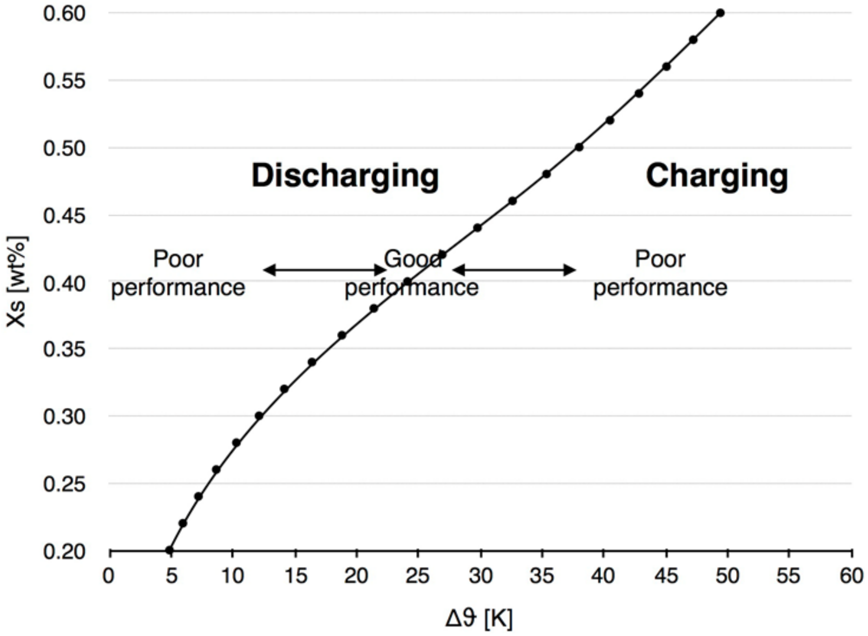


Figure 2-5. Illustration of the mapping procedure, where the x-axis represents the temperature difference between sorbate and sorbent and the y-axis represents the weight percent or mass fraction. Deviation from the theoretical curve indicates loss of system performance.

This mapping helps visualize the operational constraints and the potential performance of the system. There is a non-linear relationship between temperature gain and heat release in all sorption processes. As the sorbent's concentration increases, the temperature gain also increases, but the heat release rate does not linearly follow, leading to potential stagnation in heat transfer, particularly when high-temperature gradients are required. The work emphasizes the importance of operating the system at the minimum necessary temperature rise (gross temperature lift) to optimize heat transfer.

To overcome the problem of incomparable test results from different test methods, a uniform test guideline for building applications was proposed. The proposed guideline defines specific static test temperatures that correspond to realistic operating conditions:

- Desorption: Heat source temperatures are set to a maximum of 95 °C input and 92 °C output, which are conditions achievable by solar thermal systems without exceeding practical limits.
- Condensation: Heat rejection during charging is performed with water-based HTF at 30 °C inlet and 35 °C outlet, in line with standard heat pump conditions (EN 14511).
- Evaporation: Discharge evaporation takes place at 10 °C inlet and 7 °C outlet, simulating typical low temperature ground heat sources in building environments as defined by the EN 14511 heat pump test standard.
- Sorption: Heat absorption also follows the heat pump standard, with HTF temperatures of 30 °C inlet and 35 °C outlet.

This guideline standardizes the evaluation of sorption heat storage systems by ensuring that materials, components, and systems are tested under comparable and realistic conditions. By standardizing test conditions, the guideline facilitates more accurate comparisons of energy density power and temperature gain (gross temperature lift) performance, supporting the advancement of sorption heat storage systems as a viable solution for improving the energy efficiency of buildings.

3 Conclusions

Task 40 advanced the development of compact thermal energy storage by improving material characterization and development, establishing standardized testing methods, and enhancing the understanding of performance degradation. The international collaboration fostered innovation in both materials and components, laying the groundwork for more efficient and reliable CTES systems. These efforts will contribute to accelerating the market integration of CTES technologies and support the broader transition toward sustainable, renewable-based energy systems.

The Task achieved good success in enhancing material characterization skills through the development of measurement guidelines and in building a comprehensive knowledge base for state of charge determination techniques. The strong international collaboration within the CTES community was also supported. However, dissemination of lessons learned, broader utilization and expansion of the materials database, and development of guidelines for component design and evaluation fell below expectations. Going forward, two new Tasks will focus separately on TES materials and components to build on the progress made.

3 Subtask A: Material Characterisation and Database

The main objective of Subtask A is to develop and validate several standardized measurement procedures for TES materials based on PCM and TCM and to further maintain existing material databases.

3.1 Standardized measurement procedures and round robin tests

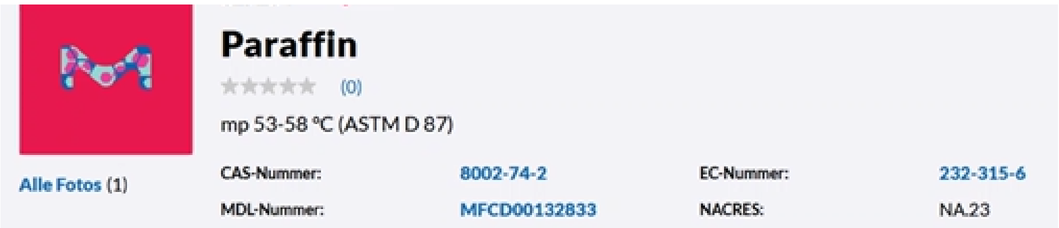
Procedures to measure thermal conductivity and thermal diffusivity of liquids, solids and packed beds (section 3.1.1), specific heat capacity of powdery materials (section 3.1.2), enthalpy change due to sorption or any chemical reaction (section 3.1.3), and thermal expansion, density and viscosity (section 3.1.4) were worked on and further developed.

3.1.1 Thermal conductivity and thermal diffusivity of liquids, solids and packed beds

3.1.1.1 Activities

Measured material

The measured material was a Paraffin supplied by Merck (specifications given in Figure 3-1). All participants purchased the same material to avoid discrepancies as a paraffin is normally supplied as a mixture of different hydrocarbon chains. Participants, who were not able to purchase it, were supplied by others.



Paraffin

(0)

mp 53-58 °C (ASTM D 87)

Alle Fotos (1)

CAS-Nummer: 8002-74-2

EC-Nummer: 232-315-6

MDL-Nummer: MFCD00132833

NACRES: NA.23

Figure 3-1: Paraffin supplier and product reference.

Measurement methods

A total of eight different pieces of equipment were used, based on transient methods and steady-state methods. Three main measuring techniques were used: laser flash analysis (LFA), hot wire (HW), and transient plane source (TPS). Besides, non-commercial equipment was also used in this RRT. The measurement capabilities in this Subtask provided by the participants were the following:

- Measurement of thermal conductivity, thermal diffusivity depending on the equipment
- Sample form/size
    - LFA: solid 12.7 mm ϕ
    - HW: 50 ml
    - Hot Disk (HD): 18 mm ϕ; 6–30 mm ϕ; 4–29 mm ϕ; 2–29 mm ϕ
    - Transient Hot Bridge (THB): 25x25x5 mm; 10x20x3 mm; 20x22x3; 100 mL
- Temperature
    - LFA: RT to 500 °C (-120–2,800 °C)

    - Transient Hot Wire (THW): RT–150 °C (-40–180 °C)
    - TPS: RT to 180 °C (-70–300 °C)
    - THB: -15–200 °C (-150–700 °C)
- Atmosphere
    - Air/ protective gas (nitrogen)
    - Less available: argon and vacuum

Procedures

a) Sample preparation

For the sample preparation, two sets of samples were heated up till fully melted and cooled down following two different cooling rates.

- Heating up to 70 °C (till liquid state) and then cool down at ambient temperature.
- Heating up to 70 °C and then place it in an oven at 50 °C for solidification.

The samples were inspected looking for the formation of bubbles during the cooling process, and density was checked and compared with the provider's specifications.

b) Measurement procedure

A minimum of three samples were tested with three to five values per temperature and sample. Different procedures were established depending on the equipment. As an example, the LFA procedure is summarized below:

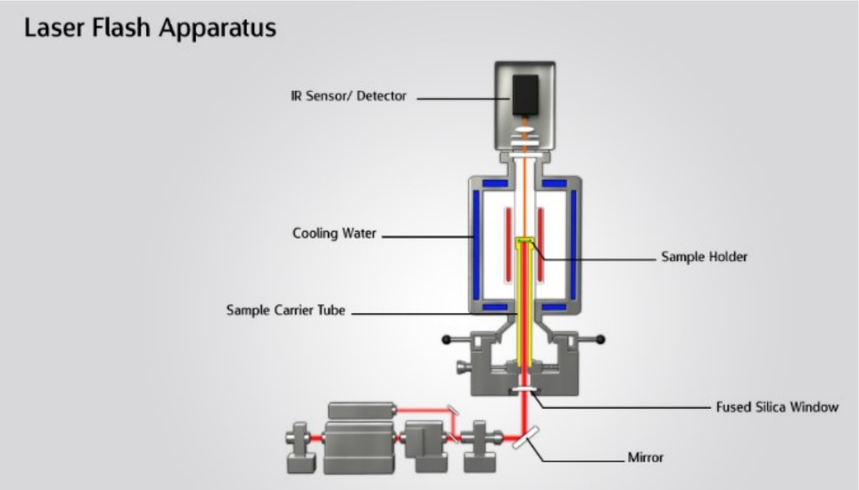


Figure 3-2: Laser Flash Apparatus.

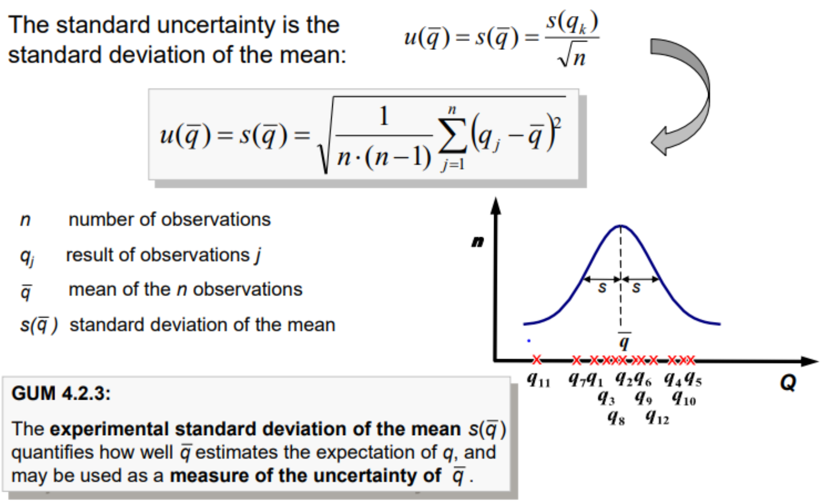
- Focus the laser to a maximal 6 mm (non-focusable LFA: use an aperture with max. 6 mm) to avoid signal superposition with the PTFA ring.
- Use thickness values from the additional information for the thermal diffusivity measurements.
- Perform measurements with at least five shots at 25, 40, and 50 °C with the pulse length and voltage recommended by the software or recommended for polymers by the manufacturer.

After the measurement, provide the information about the pulse voltage, pulse length, pulse area (integral of pulse voltage), and the used evaluation model.

Figure 3-3: LFA samples prepared for the round robin test.

c) Uncertainty analysis

Participants should send the data: mean value and uncertainty following the GUM [1]. The data following that method gives a level of confidence of 95%. The main steps followed are summarized in Figure 3-4 and Figure 3-5.



The standard uncertainty is the standard deviation of the mean:

$$u(\bar{q}) = s(\bar{q}) = \frac{s(q_k)}{\sqrt{n}}$$

$$u(\bar{q}) = s(\bar{q}) = \sqrt{\frac{1}{n\cdot(n-1)}\sum_{j=1}^{n}(q_j-\bar{q})^2}$$

n number of observations

q_j result of observations j

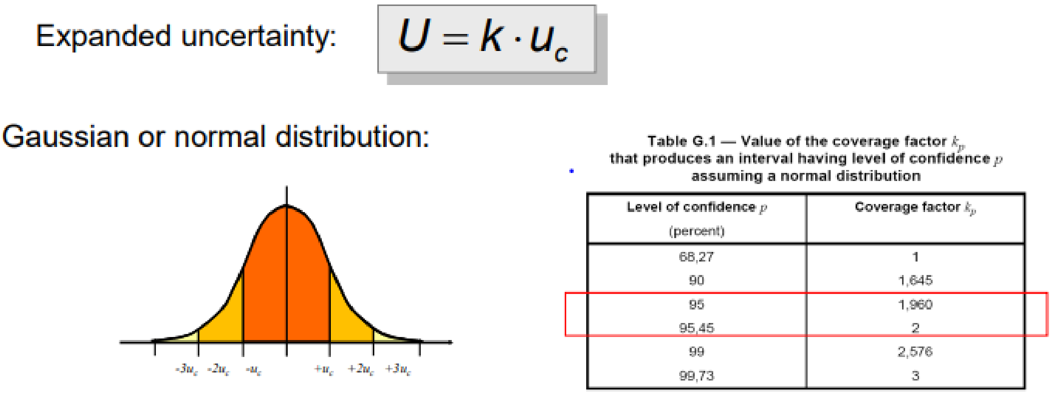
$\bar{q}$ mean of the n observations

$s(\bar{q})$ standard deviation of the mean

GUM 4.2.3:

The **experimental standard deviation of the mean** $s(\bar{q})$ quantifies how well $\bar{q}$ estimates the expectation of q, and may be used as a **measure of the uncertainty of** $\bar{q}$.

Figure 3-4: Standard uncertainty determination of a set of values.



Expanded uncertainty: $U = k \cdot u_c$

Gaussian or normal distribution:

Table G.1 — Value of the coverage factor k_p that produces an interval having level of confidence p assuming a normal distribution

Level of confidence p (percent)	Coverage factor k_p
68,27	1
90	1,645
95	1,960
95,45	2
99	2,576
99,73	3

Figure 3-5: Expanded uncertainty.

Participants

Fifteen institutions participated in this round robin test. The participants in this activity are listed in Table 3-1.

Table 3-1: Participants by institution, country, and contact person.

Country	Organization	Contact person
Germany	DLR	Nuria Navarrete
Germany	Center for Applied Energy Research	Michael Bruetting
United Kingdom	Northumbria University	Carolina Costa
Canada	CanmetENERGY / CanmetÉNERGIE	Reda Djebbar, Lia Kouchachvili
Spain	University of the Basque Country	Gonzalo Diaz
Spain	CIC energiGUNE	Jean Luc Dauvergne
Spain	Universitat de Barcelona	Camila Barreneche
Norway	SINTEF Energy	Asmira Delic
United Kingdom	University of Birmingham	Helena Navarro
Germany	Fraunhofer Institut für Solare Energiesysteme ISE	Thomas Haussmann
Austria	AIT Austrian Institute of Technology GmbH	Daniel Lager
Switzerland	HSLU	Rebecca Ravotti
Spain	Universidad de Zaragoza	Monica Delgado
Italy	CNR	Andrea Frazzica
France	Université d'Artois	Laurent Zalewski

3.1.1.2 Results

LFA results

- Participants: 5
- Procedure
    - Sample size (mm): 12.7–14.8 and 1–2
    - Variable power (50–125%)
    - Number samples: 3–11
    - Repetitions: 3–5

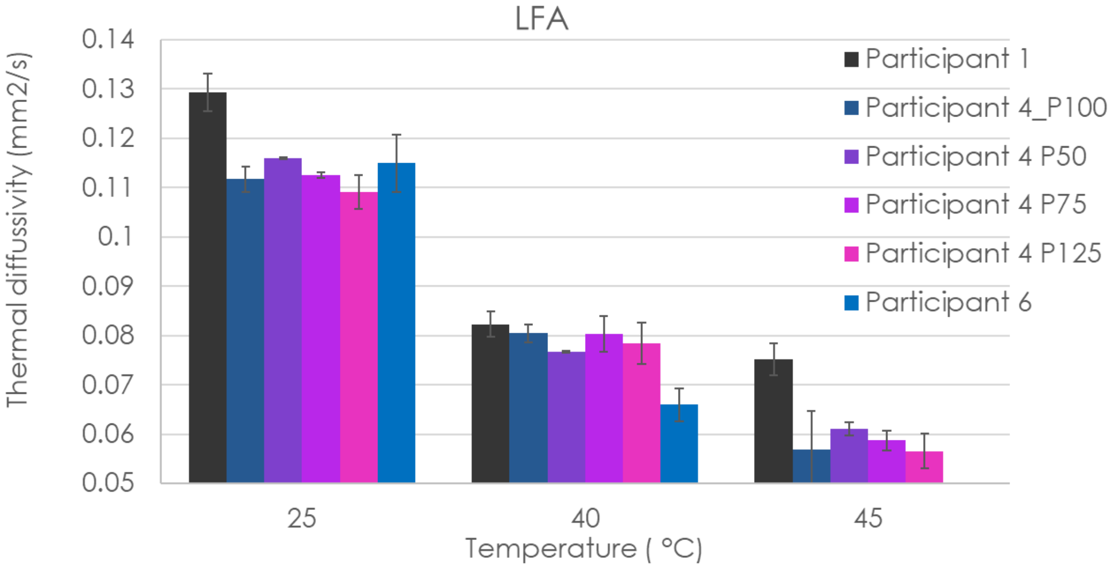


Figure 3-6: LFA results.

The following issues were reported:

- Issues at 50 °C due to the transparency and softening of the samples.
- Sample holder with no transparent windows in a three-layer system.
- Test the samples up to 45 °C, when not possible at 50 °C.

TPS results

- Participants: 5
- Procedure
    - Variable parameters
        - Current (mA): 60
        - Time (s): 30
    - Sample size (mm):
        - P7 50 x 11.5 h[2]
        - P10 70 x 40 x 5–15 h
    - Number samples: 3–4
    - Repetitions: 5

---

[2] h = sample height

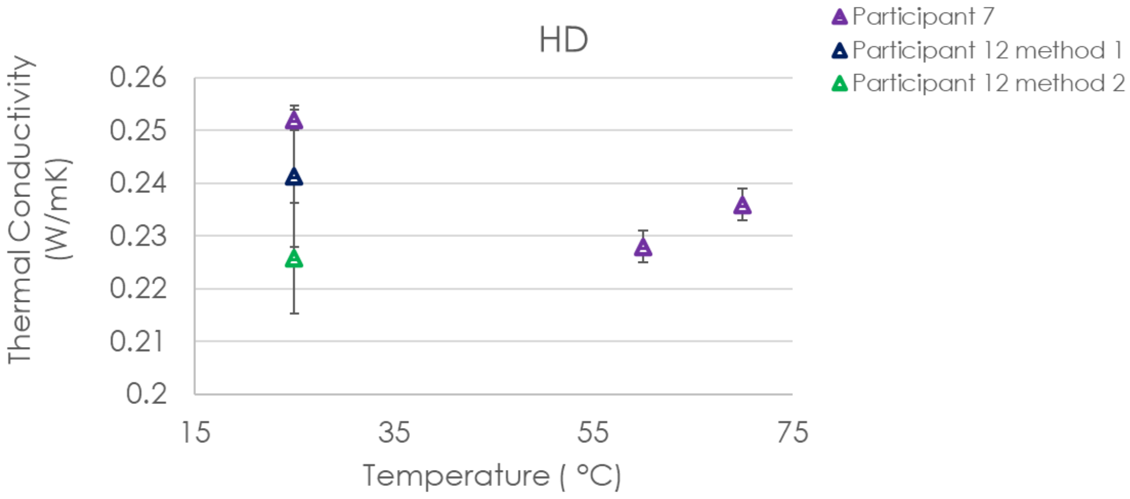


Figure 3-7: Transient plane source results: Hot disk.

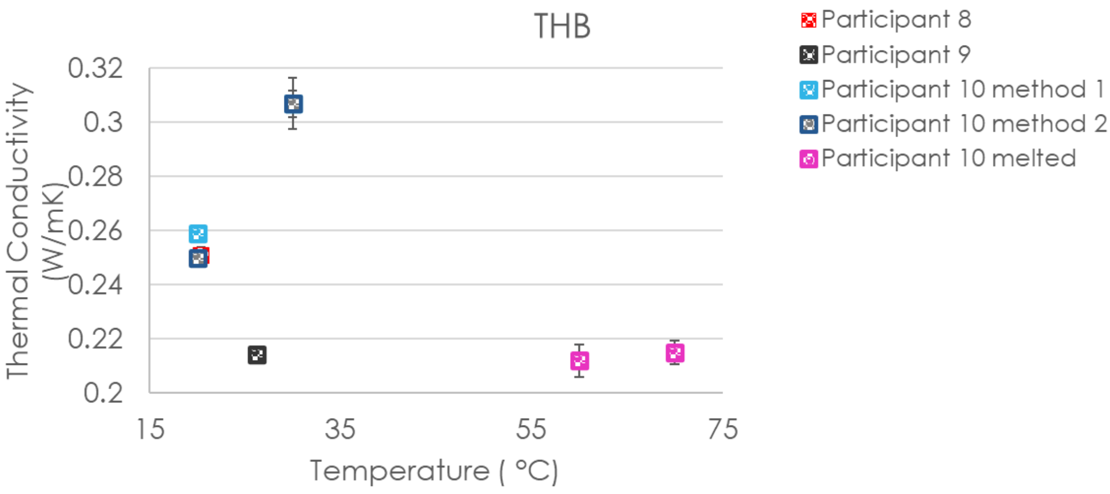


Figure 3-8: Transient plane source results: Thermal hot bridge.

TPS equipment can measure thermal conductivity and thermal diffusivity.

HW results

- Participants: 2
- Procedure
  - Sample size (mm): 34 and 70 h
  - Samples in contact with the sensor.
  - Number samples: 1–6
  - Repetitions: 6

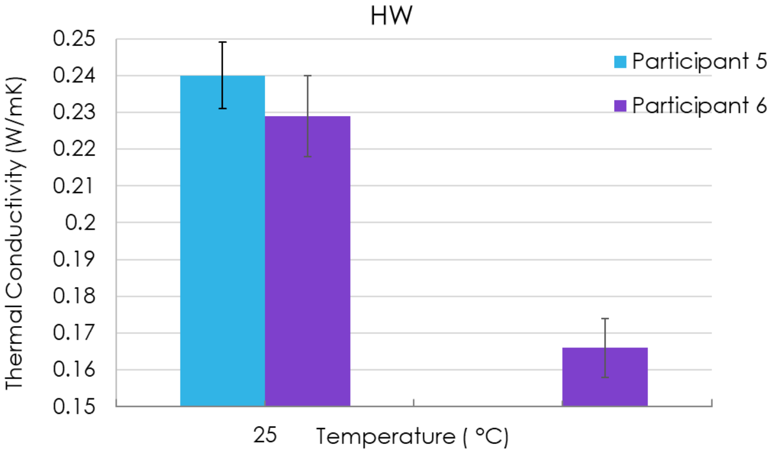


Figure 3-9: Hotwire results.

The following issues were reported:

- Difficult to ensure good contact between sensor and sample.

Other equipment results

- Participants: 3
- Procedure
  - Sample size (mm):
    - GHP 70 x 110 x 6 h
    - GHF 50 x 50 x 6
    - HF 210x140x18, 250x250x20
  - Number samples: 1–3
  - Repetitions: 3

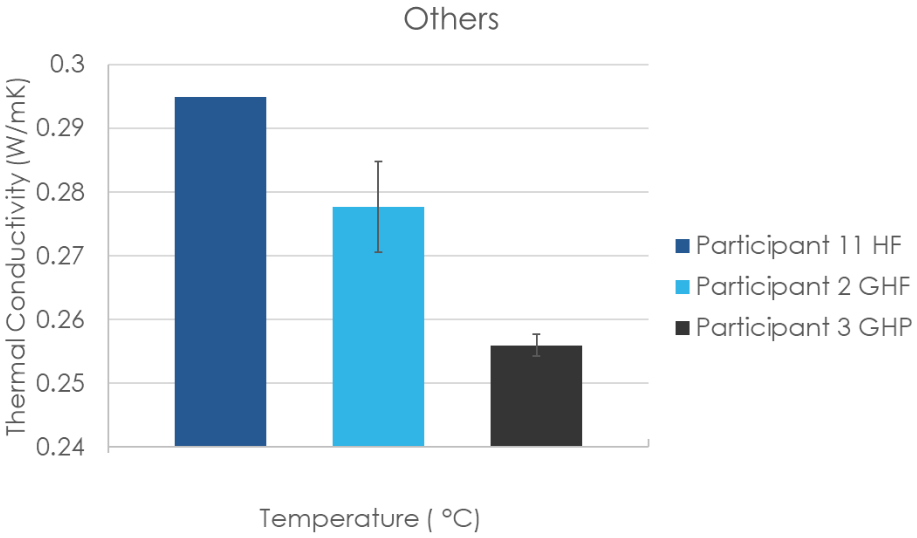


Figure 3-10: Steady-state methods result.

The following issues were reported:

- Difficult to prepare large sample sizes.
    - Large number of samples; long cool-down process; bubble formation.
    - Non-commercial equipment has to be validated.

3.1.1.3 Discussion and Outlook

This RRT presented the following challenges regarding sample preparation, procedure and results analysis that increased uncertainty:

- Equipment: Different equipment based on different methods (transient methods and steady-state methods).
- Sample: Different sample size requires different sample preparation methods, and leads to different cooling rates.
- Procedures: Different equipment requires different procedures (e.g. LFA, HW, and THB).
- Results reporting: Uncertainty assessment was included as another step in the procedure. Both contributions – systematic and experimental uncertainty – were aimed to be included.

Lessons learned:

- Thermal conductivity/thermal diffusivity equipment availability supposes a challenge to establish a standardized measurement protocol. The procedures were split according to the available equipment into LFA, TPS, HW, and other steady-state equipment.
- Both experimental and systematic uncertainty have to be accounted for to compare the results. In some cases, the uncertainty reported was below the equipment error, due to i) not enough repetitions, ii) not accounted for equipment error, or iii) not enough samples tested.

Future actions agreed upon:

- Increase the number of repetitions and tests of different samples at the same conditions.
- Account for the equipment error by testing a standard (different from the one used for calibrating the equipment) under the same test conditions for the RRT.
- Statistical analysis of the data to compare the use of different equipment and techniques.
- Explore other PCM.
- Test TCM.

3.1.2 Specific heat capacity of powdery materials

3.1.2.1 Activities

Measured materials:

- Anhydrous strontium bromide ($SrBr_2$);
- Strontium bromide hexahydrate ($SrBr_2 \cdot 6H_2O$),
- Synthetic zeolite Z-13X.

The materials were purchased from Sigma Aldrich (now Millipore Sigma).

Proposed Measuring Procedures:

Steps:

- Instrument calibration (temperature, sensitivity).
- Baseline runs.
- Reference material run.
- Sample preparation.
- Sample run and specific heat (c_p) evaluation.

Instrument calibration

Temperature calibration is recommended with the following reference materials.

Table 3-2: Temperature calibration reference materials for the RRT of the specific heat capacity.

$SrBr_2$	**$SrBr_2 \cdot 6H_2O$**	**Z-13X**
High melting temperature reference materials: Tin, Bismuth, Zinc, Lead, etc.	Low melting temperature reference materials: Gallium, Biphenyl, Indium, etc.	High melting temperature reference materials: Tin, Bismuth, Zinc, Lead, etc.

- Calibration of the DSC signal's sensitivity is recommended.
- Due to high thermal conductivity, aluminum (Al) crucibles with Al lids are recommended.
- Temperature and sensitivity calibration should be performed with the same heating (h.r.) and cooling rates (c.r.).
- h.r. of 1 K/min and c.r. of 1 K/min (with LN2) or 3 K/min (with compressed air) are recommended.
- c_p evaluation is recommended in the following temperature range:

Table 3-3: Temperature range of evaluation for the RRT of the specific heat capacity.

$SrBr_2$	**$SrBr_2 \cdot 6H_2O$**	**Z-13X**
125–180 °C	25–40 °C	RT–250 °C

Baseline runs

- Place the empty Al crucible with the lid on both sides of the sample holder of the instrument, tear the crucible masses.
- Run the baseline. The temperature and sensitivity calibration options should be checked.

Table 3-4: Baseline runs to be applied for the RRT of the specific heat capacity.

$SrBr_2$	$SrBr_2\cdot 6H_2O$	Z-13X
a. Heat to 180 °C.	a. Cool the instrument down to -5 °C.	a. Heat to 300 °C.
b. Isothermal 1 min	b. Isothermal 15 min to stabilize the temperature	b. Isothermal 1 min
c. Cool down to 25 °C.	c. Heat to 40 °C.	c. Cool down to 50 °C.
d. Isothermal 1 min.	d. Isothermal 1 min.	d. Isothermal 1 min.
e. Repeat steps a–d to get a stable c_p reading between 125 and 200 °C.	e. Repeat steps a–d to get a stable c_p reading between 25 and 40 °C.	e. Repeat steps a–d to get a stable c_p reading between 100 and 250 °C.

Cool down to room temperature.

Reference material run

- Remove the crucible lid from the sample side of the sample holder.
- Place inside a Sapphire reference and run the test (steps a–f).
- As a reference material, use synthetic sapphire with 99.9% or higher purity.

Sample preparation

Table 3-5: Instructions for sample preparation for the RRT of the specific heat capacity.

$SrBr_2$	$SrBr_2\cdot 6H_2O$	Z-13X
Dry "as received" anhydrous $SrBr_2$ to remove any moisture that was absorbed by the specimen while loading into the crucible: Heat the sample in the open crucible to 180 °C and hold isothermally under the pressure of 10 mbar until the mass of the simple stabilizes; open the furnace, remove the sample, and seal it instantaneously OR prepare the sample inside the glovebox if available.	Use "as received" commercial material.	Z-13X received from Sigma Aldrich in pellets (d=1.6 mm), will be grinded in a mortar into powder and packed in the Al crucible. Another option is to prepare the pellets from this powder with a diameter close to the diameter of the crucible. Determine the sample's dry mass by heating it in the open crucible (or covered with the punched lid) to 350 ˚C and keep at this temperature until the mass stabilizes (~ 1 h). Open the furnace and apply the lid instantaneously if the sample was dried in an open crucible.

Sample run c_p evaluation

- Replace the reference material with the sample (use the same crucible/lid).
- Repeat the run at least with three different specimens and compare c_p.
- Repeat the steps a–f.
- Report results (template in Figure 3-11).

Organization:	
DSC instrument: • Manufacturer • Model	
Reference materials for calibration	
Sapphire dimensions • Diameter • Height • Mass	
Sample preparation conditions • Temperature • Pressure • Time	
Crucible/lid • Material • Diameter • Height • Mass	
Gas • Flow rate	
Cooling method • Cooling rate	
Heating Rate	

c_p evaluation							
Material	m (mg) before measurement	m (mg) after measurement	c_p (J/gK) at temperature (°C)				U_{cp} (J/g)
			T_1	T_2	T_3	Other temperatures	
1							
2							
3							

Figure 3-11: Reporting template for the specific heat RRT.

Participants

Eight labs participated in the anhydrous $SrBr_2$ c_p measuring procedure.

Table 3-6: Participants of $SrBr_2$ c_p RRT.

Country	Organization	Contact person
Austria	AIT Austrian Institute of Technology GmbH	Daniel Lager
Switzerland	HSLU	Rebecca Ravotti
Austria	TU Wien	Peter Weinberger Jackob Smith
USA	The US.DOE – LBNL	Sumanjeet Kaur
Canada	CanmetENERGY	Reda Djebbar Lia Kouchachvili
Spain	University of Barcelona	Rebecca Saldago Pizarro Inés Fernández Marc Neira i Viñas Adela Svobodova
Germany	Fraunhofer-ISE	Thomas Haussmann Stefan Gschwander
Germany	Center for Applied Energy Research e. V.	Michael Brütting

Three labs participated in the $SrBr_2{\cdot}6H_2O$ c_p measurement procedure.

Table 3-7: Participants of $SrBr_2{\cdot}6H_2O$ c_p RRT.

Country	Organization	Contact person
Canada	CanmetENERGY	Reda Djebbar; Lia Kouchachvili
Spain	University of Barcelona	Rebecca Saldago Pizarro; Inés Fernández; Marc Neira i Viñas; Adela Svobodova
Germany	Fraunhofer-Institute for Solar Energy Systems ISE	Thomas Haussmann; Stefan Gschwander

Three labs participated in the zeolite 13X c_p measurement procedure.

Table 3-8: Participants of zeolite 13X c_p RRT.

Country	Organization	Contact person
Canada	CanmetENERGY	Reda Djebbar; Lia Kouchachvili
Austria	AIT Austrian Institute of Technology, GmbH	Daniel Lager
Germany	Fraunhofer-Institute for Solar Energy Systems ISE	Thomas Haussmann; Stefan Gschwander

3.1.2.2 Results

Out of eight participated labs, three were equipped with the Netzsch STA, three with the TA DSC, one with the Mettler Toledo DSC, and one is unknown. All labs used Al crucible, and N_2 gas flow except one lab using Helium. The heating rate varied (1, 10, and 20 K/min); the cooling rate also varied (2, 3, 10, and 20 K/min). The flow rate of gases was also different (10, 20, 40, 50, and 100 mL/min).

$SrBr_2$

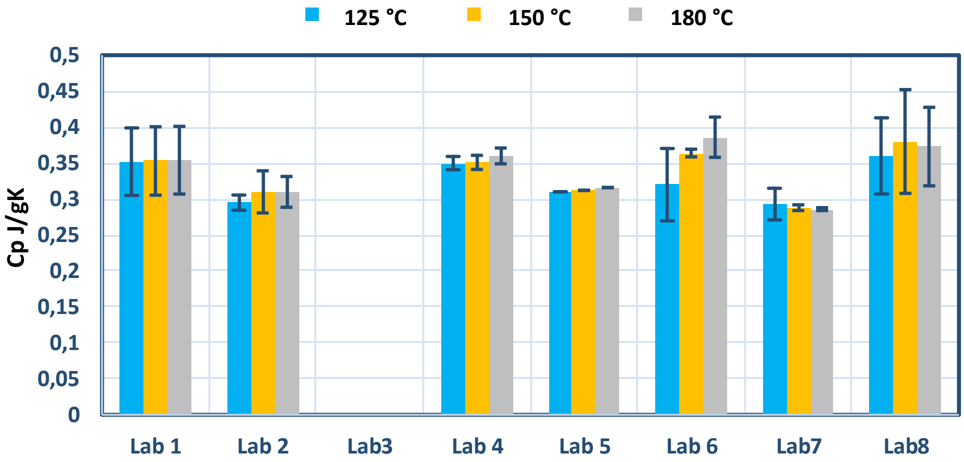


Figure 3-12: Results of the RRT of the specific heat capacity of $SrBr_2$.

Results from lab 3 are excluded as they are a way off from the rest of the labs' results. From these results, the assigned values (mean value for all labs at a defined temperature) for the specific heat for $SrBr_2$ are:

$c_p(125\ °C) = 0.326\ J\ g^{-1}\ K^{-1}$

$c_p(150\ °C) = 0.337\ J\ g^{-1}\ K^{-1}$

$c_p(180\ °C) = 0.341\ J\ g^{-1}\ K^{-1}$

According to ISO 13528 "Statistical methods for use in proficiency testing by interlaboratory comparison" [2], a z-score can be evaluated to assess the comparability of results. $z \leq |2,0|$ means that the performance is satisfactory, a value $|2,0| < z < |3,0|$ means that the performance is questionable, and $z \geq |3,0|$ means the performance is unsatisfactory.

In the case of the specific heat capacity of $SrBr_2$, since all labs show a z-score $z \leq |2,0|$, a good performance of every participant and comparable results in that round robin test were obtained. That means reliability is given for nearly all measurements/participants here.

$SrBr_2·6H_2O$

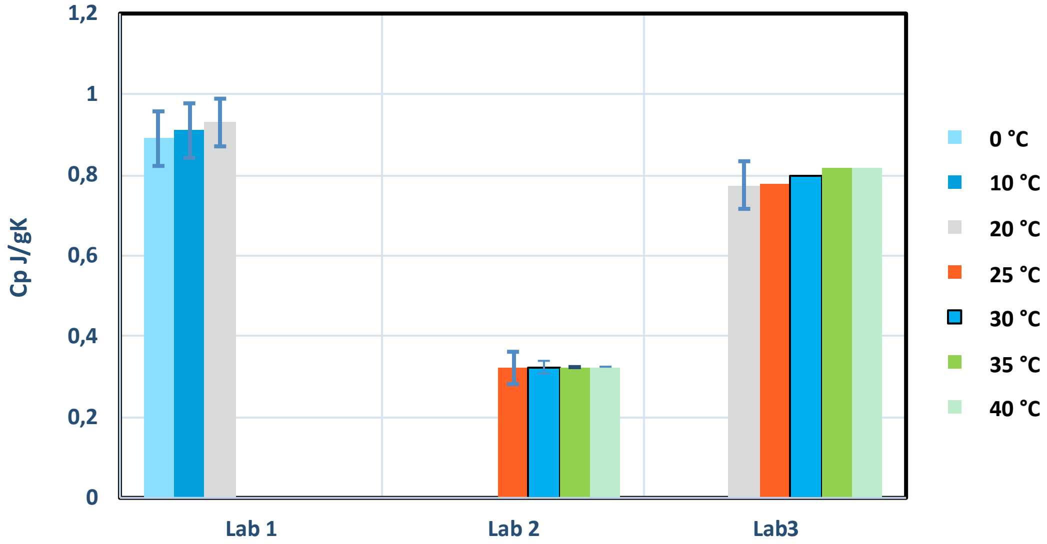


Figure 3-13: Results of the RRT of the specific heat capacity of $SrBr_2·6H_2O$.

Results of $SrBr_2·6H_2O$ are still not comparable due to problems with the hydrate sample preparation. These results cannot be used to evaluate a z-score for the lab performance.

Zeolite 13X

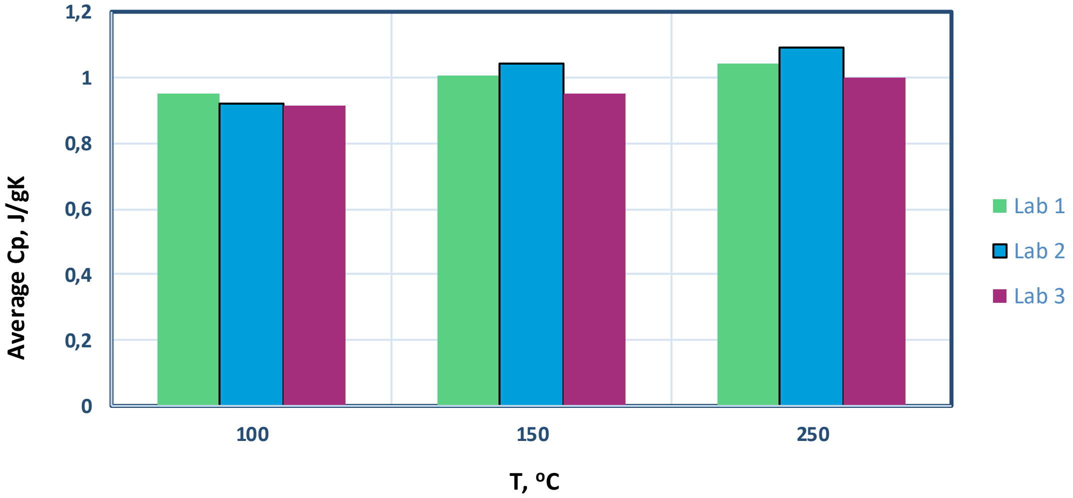


Figure 3-14: Results of the RRT of the specific heat capacity of zeolite 13X.

From these results, the assigned values (mean value for all labs at a defined temperature) for the specific heat for zeolite 13X are:

$c_p(100\ °C) = 0.929\ J\ g^{-1}\ K^{-1}$

$c_p(150\ °C) = 0.998\ J\ g^{-1}\ K^{-1}$

$c_p(250\ °C) = 1.002\ J\ g^{-1}\ K^{-1}$

With these results the z-score can be evaluated. In this case, since all labs show a z-score $z \leq |2{,}0|$, a good performance of every lab in that round robin test was achieved.

3.1.2.3 Discussion and Outlook

In the first round, eight participants joined the $SrBr_2$ round robin test. This is already a representative number of results for statistical analysis. The results showed a good comparability and a good z-score (satisfactory performance) for all participants.

The $SrBr_2$ hydrate measurements showed strong deviations. These may be connected to different hydration states in the measurement. Due to that, the sample preparation and measurement procedure routines must be corrected.

For the zeolite 13X round robin test, only three participants shared their data, which can be connected to the late beginning of the round robin test during the Task. Nevertheless, the defined procedure and the results showed a good comparability and a low z-score for all participants.

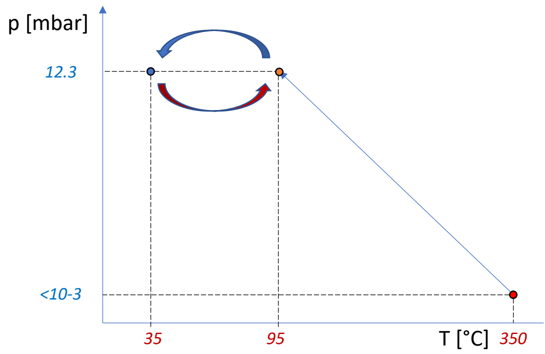
For future activities, especially the occurrence of water in the sample (hydrated or sorption samples) should be examined in more detail. Also, the application of the measurement routines for higher temperature were not covered in this or previous Tasks.

3.1.3 Enthalpy change due to sorption or any chemical reaction

The aim of this activity was to perform a round robin test focused on the evaluation of a standardized procedure for the measurement of the sorption enthalpy. Starting from previous experiences, it was agreed to define a simplified procedure, which is easier to implement, in order to get replicable results.

3.1.3.1 Activities

The selected material for the RRT was a standard zeolite 13X, available on the market and commercialized by Sigma Aldrich (https://www.sigmaaldrich.com/AT/de/product/sigald/334340), using water vapour as working fluid for the sorption process. The selected simplified procedure was based on a single adsorption/desorption cycle under isobaric conditions. The full set of operating conditions of each step is represented in the following schematic as well as in the table, specifying more in details the operating conditions to apply (Figure 3-15).



Phase	Temperature [°C]	Pressure [mbar]	Duration	Heating/cooling rate	Crucible material
Desorption	350 °C	< 10-3	> 6 h (dry mass)		Aluminum (preferred)
Equilibrium	95 °C	12.3	Until stabilization		Aluminum (preferred)
Adsorption	95->35 °C	12.3	Until stabilization	5 K/min (same as the calibration)	Aluminum (preferred)
Desorption	35->95 °C	12.3	Until stabilization	5 K/min (same as the calibration)	Aluminum (preferred)

Figure 3-15: Defined standardized testing conditions for the sorption enthalpy RRT.

Many partners were initially involved in the activities, but the tests were performed only by four partners, due to delays and/or lack of funding: CNR, University of Messina, Austrian Institute of Technology, and NRCan.

CNR was not able to provide data for the analysis. The achieved results were not accurate enough due to a major issue with the instrumentation. Accordingly, only AIT, UNIME, and NRCan data were analyzed. Among the three partners, only AIT was able to accurately follow the planned procedure (temperature range 90–35 °C, vapor pressure of 12.3 mbar). As reported in Figure 3-16, three consecutive tests were carried out to evaluate the replicability of the measurement.

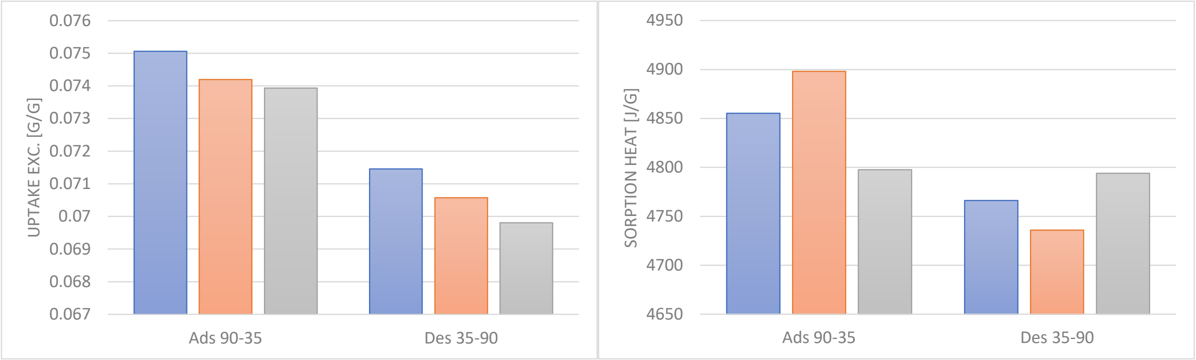


Figure 3-16: Replicability analysis of uptake variation (left-hand side) and sorption heat (right-hand side) for three consecutive tests performed by AIT.

The results were satisfactory, with a maximum deviation among the tests of around 1%, with a deviation between ad-/desorption heat of 2% and ad-/desorption uptake exchange of 5%.

The tests performed by UNIME and NRCan deviated from the nominal ones. For UNIME, the following conditions were applied: Temperature range 95–35 °C, vapor pressure 17 mbar. For NRCan, the temperature range was 95–25 °C at a vapor pressure of about 25 mbar. This was caused by specific features of the available equipment at the respective labs. Nevertheless, a comparison was made, reported in Figure 3-17. A quite good agreement between AIT and UNIME measurements was achieved, with deviations in the range 12% for the water uptake variation and 18% for the sorption enthalpy. Due to the large difference in operating conditions, the results from NRCan were significantly deviating from the others.

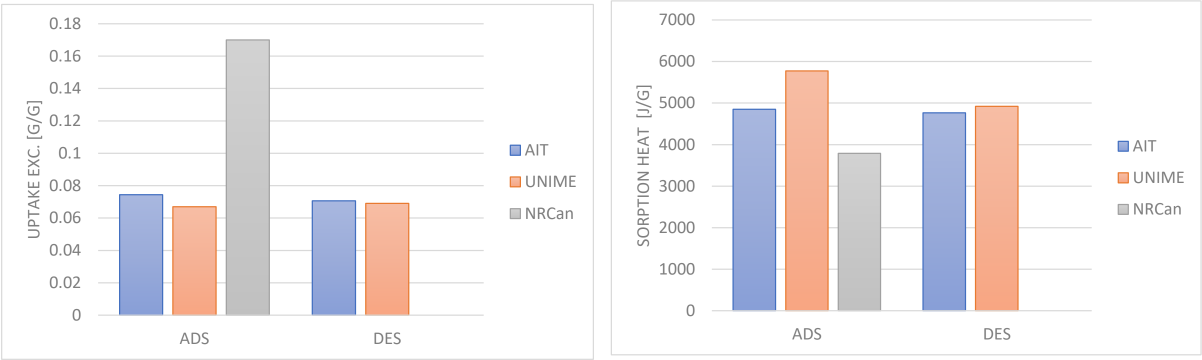


Figure 3-17: Comparison analysis of uptake variation (left-hand side) and sorption heat (right-hand side) for the average data obtained by AIT, UNIME, and NRCan.

3.1.3.2 Discussion and Outlook

As experienced in the past, coming to a common methodology to measure sorption enthalpy is not an easy task. It depends a lot on the performance of the different equipment available in the laboratories and the ability of these instruments to carefully follow the planned conditions. Moreover, the lack of specific funding for some of the involved partners to perform the planned activities is limiting the efforts that can be put into the measurement and analysis campaign.

Nevertheless, the initial results, at least for the partners able to complete them, show some acceptable agreement, even using different apparatuses. This is a first step which demonstrates the possibility of reaching useful results.

Possible future activities could be focused on enlarging the number of laboratories involved in the testing campaign, using different apparatuses under the proposed simplified protocol. Once the approach is validated, it can be extended to a wider set of conditions and different materials to reach a common approach to be considered by the scientific community.

3.1.4 Thermal expansion, density and viscosity

3.1.4.1 Activities

Density

Measured material:

In the RRT for density, measurements in the liquid and solid phase were carried out and compared on a paraffin wax CAS 8002-74-2 (melting temperature 53–58 °C).

Procedure and methodology:

Different methods were used to characterize the actual density of the solid and liquid phase:

- Computer tomography
- Oscillating U-tube
- Archimedes principle
- Pycnometer

No procedure was specified for this RRT, participants were asked to use their usual method.

Participants:

- HSLU- Lucerne University of Applied Sciences and Arts
- Fraunhofer ISE - Fraunhofer-Institut für Solare Energiesysteme
- NREL - National Renewable Energy Laboratory (NREL)
- ZAE Bayern
- CAE – Center for Applied Energy Research

Viscosity

Measured materials:

- Standard oil S3 from Paragon Scientific to check the performance of the viscometers/ rheometers. Measurement at 80 °C.
- A paraffin with a melting temperature range between 53–58 °C (CAS 8002-74-2).

Procedure and methodology:

- Shear sweep:
    - Geometry used in case of rheometers: plate
    - Gap: 500–1,000 µm
    - Temperature: 70 °C (paraffin in the melted phase)
    - Time for thermal stabilization: 5 minutes
    - Shear rate range: 0.001–1,000 s^{-1}
    - Mode: logarithm

  - Points per decade: 10
  - Sample period: 10 s

- Temperature ramp:
  - Conditioning step at 85 °C during 20 minutes. No shearing.
  - Cooling at 0.5 K/min and 100 s^{-1} from 85 down to 60 °C.

Participants:

Table 3-9 compiles the institutions involved in the viscosity RRT together with instrument used.

Table 3-9: Participants of the viscosity RRT.

Institution	Instrument	Methodology
Fraunhofer ISE	MCR 502, Anton Paar	Controlled stress rheometer
HSLU	MCR 302, Anton Paar	Controlled stress rheometer
Northumbria University	Brookfield DV-E digital viscometer	Viscometer
NREL	Haake Mars 60	Controlled stress rheometer
University of Zaragoza	AR-G2, TA Instruments	Controlled stress rheometer

3.1.4.2 Results

Density:

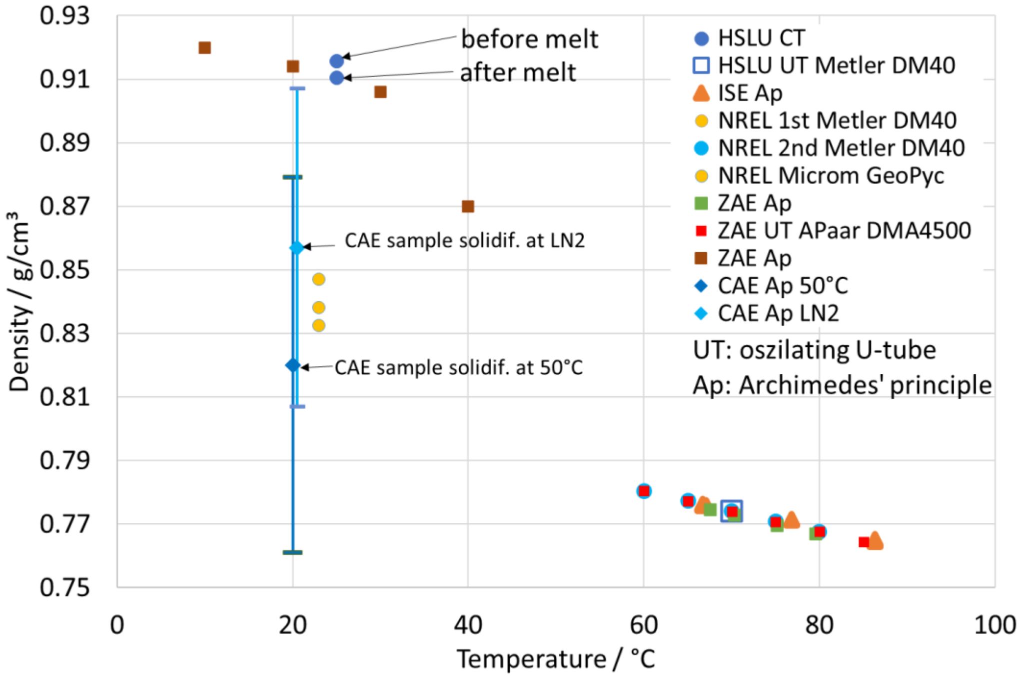


Figure 3-18: Results of the density RRT.

As Figure 3-18 shows, the results in the liquid phase are comparable, while there are strong variations for the solid samples. Due to that, no further investigations for the PCM liquid measurements were done and the focus shifted to the solid-state measurements.

A new procedure based on the Archimedes principle was documented and sent to all participants based on the results from ZAE:

Measurement setup

Figure 3-19: Balance with installed density kit (upper left). Holders for floating and sinking samples (upper right). Setup for measurements at different temperatures (lower left and right).

The balance is put on a shelf with a hole and the holder is hung on the bottom hook of the scale. If there is a floating sample, as is the case here with paraffin, you need a weight on top of the sample holder to push the sample down. To measure paraffin, desalinated water is used as fluid. The double-walled vessel is tempered by a circulator to adjust the temperature. During the setting of the temperature, the bath is stirred by a magnetic stirrer and the sample is floating in the liquid. During measurement, the stirrer is switched off. The height of the vessel can be adjusted with the X-table.

Sample preparation

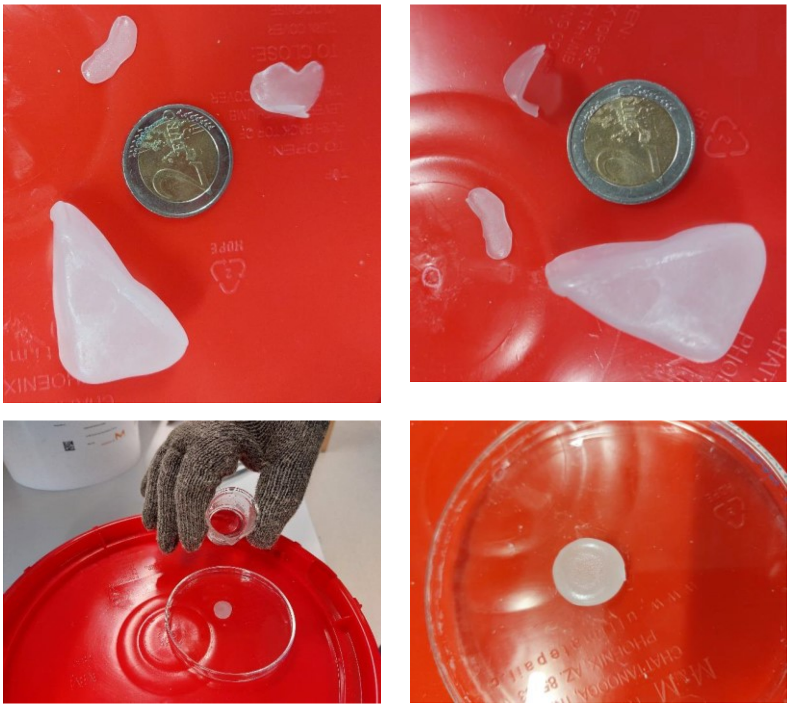


Figure 3-20: Used samples (upper left and right); casting a sample (lower left and right).

Samples used: The large one is a chunk as delivered with smoothened surface; two small samples prepared as described below. After measuring them at 40 °C they are deformed. For the large sample (~10 cm^3), ZAE used a piece from the delivered paraffin and smoothed the surface with a hot air blower. This is necessary so that no air bubbles adhere to the sample during the measurement. Perhaps this is a little annealing or tempering of the sample.

For smaller samples (~1-3 cm^3) ZAE poured melted paraffin onto the bottom of a Petri dish to get round, plate-shaped samples. As a result, the sample crystallizes mainly from below and the thin soft skin on the surface can move downwards, so that no voids are created in the sample. After complete crystallization, the sample can be easily detached from the Petri dish. ZAE smoothed the surface here as well with the hot air blower.

After measuring the different samples at room temperature, which lead to pretty much the same result, ZAE used only small samples for the other temperatures, because temperature adjustment is much better with the small samples and the measuring procedure is much easier. During the measurements, ZAE was unable to detect any significant differences in the density of the samples, despite their distinctly different appearance (the large sample had white inclusions). The measurement at 40 °C is in the range of the first phase change. Here, the sample becomes noticeably softer, so that deformation cannot be prevented. This makes the reaching of a temperature equilibrium much more difficult and thus the error in the measurement increases considerably.

Viscosity:

If the viscosity values obtained by each institution in the shear sweep experiment (Table 3-10) are considered, the average viscosity value is 4,712 mPa·s with a standard deviation of 0,177 mPa·s.

Table 3-10: Average viscosity for the paraffin at 70 °C calculated according to the procedure defined in Annex 29.

Institution	Viscosity (mPa·s)
Fraunhofer ISE	4,57
HSLU	4,87
Northumbria University	4,91
NREL	4,51
University of Zaragoza	4,70

Figure 3-21 presents the results of the temperature ramp experiment, which also includes the steady state viscosity values obtained from the previous experiment. Higher values are observed for the measurements from Northumbria University, consistent with the shear sweep experiment. Additionally, higher deviations are noted at higher temperature for NREL.

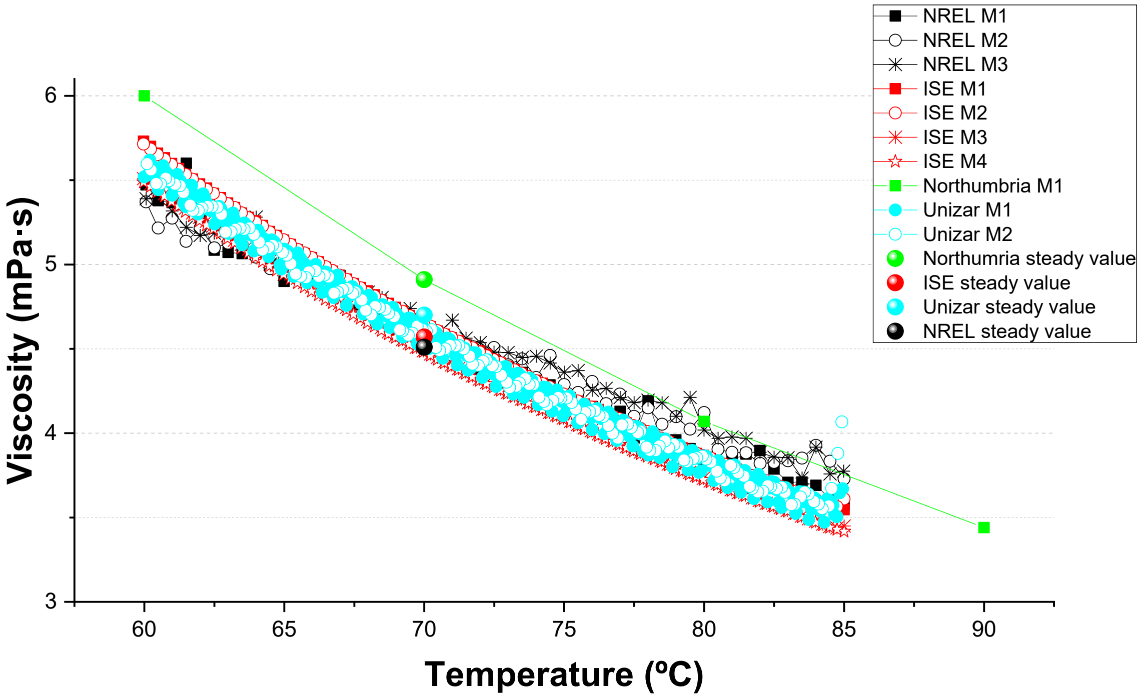


Figure 3-21: Viscosity based on temperature for the paraffin. Shear rate=100 s^{-1}.

3.1.4.3 Discussion and Outlook

Density:

The density measurements of the liquid showed comparable results. Therefore, no adaption of existing procedures was done. The density measurements in the solid phase have shown that there are still strong variations and that further investigations should be conducted. The proposed procedure for the Archimedes principle was developed and sent to the participants. New results based on this procedure have not yet been published by the other participants. This could be one of the first activities in a successor Task.

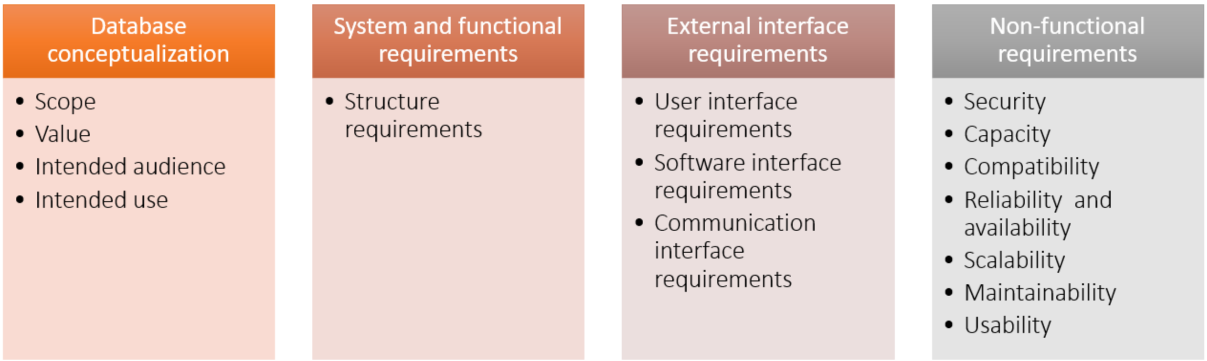
Viscosity:

It can be stated that the measurement procedure is adequate for measuring paraffins in the molten phase. So far, octadecane, RT70, and the paraffin detailed in this report have been successfully measured. At this stage, viscosity measurements of other PCM families following the proposed measurement protocol should be considered. Furthermore, it would be interesting to characterize other storage materials that may exhibit non-Newtonian behavior (e.g. PCM slurries) to determine how the measurement protocol should be adapted.

3.2 CTES Materials database and knowledge platform

3.2.1 Activities

As part of the development of the data knowledge platform for PCM and TCM, the features of the new version of the CTES materials database "thermalmaterials.org" have been defined. The definition of the new requirements for the CTES materials database consisted of four main phases, as shown in Figure 3-22.



Database conceptualization	System and functional requirements	External interface requirements	Non-functional requirements
• Scope • Value • Intended audience • Intended use	• Structure requirements	• User interface requirements • Software interface requirements • Communication interface requirements	• Security • Capacity • Compatibility • Reliability and availability • Scalability • Maintainability • Usability

Figure 3-22: Definition of new requirements for CTES database.

During the database conceptualization phase, the general scope of the new version of the CTES materials database has been identified, in relation to its intended use and audience. Although the general purpose of the database remains consistent with its previous version, the added value expected from this new iteration is mainly related to its accessibility, i.e., making data and information environments convenient and easily usable. This could be achieved, for example, by improving the process by which users can submit measurement data to the database or access any relevant information. Furthermore, the structure of the database has been revised in relation to the different types of CTES materials and the most relevant parameters for their thermophysical characterization. Finally, attention has been given to the role and positioning of the database within the wider framework of a materials data platform, to which other already existing databases with similar objectives could contribute in synergy with each other's.

The set of changes and recommendations for the new version of the database can be classified as follows:

1. **System and functional requirements:** This entails the structure requirements, including the change, integration or remotion of content from the database.
2. **External interface requirements:** This entails the new accessibility features of the database (user interface requirements), the connections between the database and other software components and platforms (software interface requirements), and the communication functions between the database and the user (communication interface requirements).

3. **Non-functional requirements:** This entails the database's operation capabilities and limitations.

Under the lead of AIT and Fraunhofer ISE, several activities were carried out to compile a list of relevant changes for each of the requirements, to which the task participants have actively contributed.

A summary of the activities is presented in Table 3-11:

Table 3-11: Summary of activities carried out to define new requirements for CTES database.

Activities	Lead	Total number of participants
Brainstorming session during online meeting	AIT and Fraunhofer ISE	Approximately 20 participants
Brainstorming session during T67T40 Expert Meeting	AIT	Approximately 40 participants
Compilation of survey "Proposed Changes to PCM/TCM Database"	AIT	11 participants
Elaboration and implementation of inputs from brainstorming sessions and survey	AIT and Fraunhofer ISE	3 participants
Writing of the software requirements specification document (SRS)	AIT and Fraunhofer ISE	3 participants
Search for software interface development firms that could implement the database requirements	AIT and Fraunhofer ISE	3 participants
Online meeting with software interface development firms to define an offer	AIT and Fraunhofer ISE	3 participants

First, the general requirements for the database were defined through online and in-person brainstorming sessions during the Task Expert meeting held in Lyon in October 2023. The discussions resulted in a list of requirements for the CTES materials database. At the end of the last in-person brainstorming session, the participants were asked to indicate their preference (yes/no) and the priority they attributed to each requirement (from 0 to 5) by compiling a survey. Once the key requirements were selected and ranked in order of importance, they have been further elaborated by AIT and Fraunhofer ISE and formalized into the Software Requirements Specification document (SRS), available in the Appendix (section 8.1). In parallel, AIT and Fraunhofer ISE have been in contact with software interface development firms that could implement the database requirements. Therefore, bilateral meetings have been conducted with the scope to further screen and select the most relevant requirements in light of their cost and, eventually, to draw an offer.

3.2.2 Results

The main requirements identified for the new version of the CTES database are summarized as follows:

System and functional requirements:

- Introduction of new data types and format for PCM & TCM, for example: material class (filter), company product (switch), description of degradation process (text), chemical formula (string), molecular weight (number), CAS Nr. (string), chemical structure (string) etc.

- Introduction of detailed information about measurements which do not follow the DSC measurement standard developed in the framework of IEA ES Annexes 24 and 29, and IEA SHC Task 42.
- Introduction of information on users actively contributing to the database, including references to relevant projects and research activities of interest for the database.
- Introduction of information to other databases and platforms, which could work in synergy with the CTES materials database, and according to the FAIR data principles.
- Introduction of publication list containing papers, reports, public documents etc. which used or contributed to the CTES materials database.

User interface requirements:

- The CTES materials database must be organized according to a matrix format, divided into: “super-topic” (Home), “topics” (Compare and Explore, Measurements Standards, Wiki, Workshops, Publications, Database Network) and “databases” (PCM Database, TCM Database).
- The CTES materials database interface must include a new section "Compare and Explore" to simultaneously plot different measurements already loaded in the database.
- The CTES materials database must be organized with a hierarchical tabulated structure, moving from general to progressively specific levels information: from overview table to list of datasets, to table of measurements, to plots.
- The CTES materials database interface must include filters and switches to select the measurements.
- The CTES materials database must contain specific requirements and procedures for uploading measurements for TCM.
- The CTES materials database must be able to automatically generate plots in a predefined format and visualize them on demand in the graphical interface.

Software interface requirements:

- Introduction of hyperlinks to other databases and platforms, which could work in synergy to the CTES materials database, according to the FAIR data principles.

Communication interface requirements:

- The CTES materials database must automatically generate e-mail newsletters to be sent periodically according to the user wishes.

For a more detailed explanation of each requirement, please refer to the requirements specification document (SRS) in Appendix 8.1.

3.2.3 Discussion and Outlook

The main outcome of the activities is the finalization of the Software Requirements Specification document (SRS) for the new version of the CTES materials database. The document details all the requirements identified as highly relevant by most of the task members who participated in the database survey.

Due to budgetary constraints, it was not possible to proceed with the development of an offer from any of the software development firms contacted. Therefore, it was not possible to complete the implementation of the new version of the database.

A possible outcome for a future Task is therefore to implement a reduced number of requirements, while contacting a larger number of software development firms. For this purpose, the developed SRS document already constitutes a solid basis to start from, as it follows the conventional IT requirements format needed for database platform development. Starting from the SRS document, the requirement specifications could be further refined to come up with an optimized selection that fits within the available budget for the development of the database.

Finally, collaboration with other existing databases and platforms which share similar scope, use, and audience with the CTES materials database, is encouraged for future tasks. This approach would make the database more robust and in synergy with the current wider framework of platforms following the FAIR data principles.

3.3 References

[1] W. Schmid (EURAMET), S. Mieke (PTB), M. Hoxha (DPM), GUM (Guide to the expression of Uncertainty in Measurement) © EURAMET e. V. 2015

[2] [ISO] INTERNATIONAL ORGANIZATION FOR STANDARDIZATION. ISO 13528: 2015. Statistical methods for use in proficiency testing by interlaboratory comparison. ISO, 2015.

4 Subtask B: CTES Material Improvement

4.1 Introduction and Objectives

4.1.1 Why CTES Materials Improvement?

The identification of suitable materials and processes to be used in thermal energy storage applications is an up-to-date research topic. The development of new materials or the optimization of the existing ones, to match the TES application requirements, is fundamental to help the large use of TES technologies in the present and the future [1-4]. Concerning materials optimization, the main objective is the development of high performant TES materials that can strongly impact the efficiency of the TES system thus contributing to cheaper the technology. Moreover, the simplification of the storage concept and the TES system design is also crucial. To reach these objectives, multiple improving/modification paths can be followed. On one side, the synthesis of materials with energy densities as high as possible (compact storage) and suitable thermophysical properties. On the other side, the use of encapsulation and shape stabilization approaches to avoid heat exchangers or dealing with liquid phases in case of solid-liquid PCM. This could also help solving possible compatibility issues of the TES material with the heat transfer fluid and containment materials.

The optimization paths depend, and can be substantially different, on the type of material considered (PCM, TCM) and the objective targeted. This may include, on one hand, the preparation of materials with the highest enthalpies (reaction, transition) and tailored temperatures, and, on the other hand, an adjustment of the thermophysical properties [5] (e.g., thermal conductivity, specific heat, …) and achieving a reversibility of the processes at the selected conditions (e.g., mitigation of supercooling, avoiding degradation thus increasing durability). As an example, Figure 4-1 reports examples of increasing the enthalpy of transition/reaction and tuning the working temperature of PCM and TCM. The picture collects the main strategies explored in Subtask B and is included in a scientific article[3].

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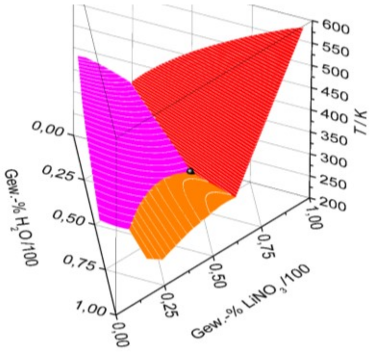
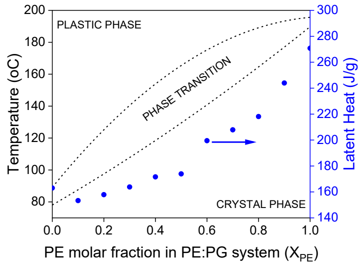
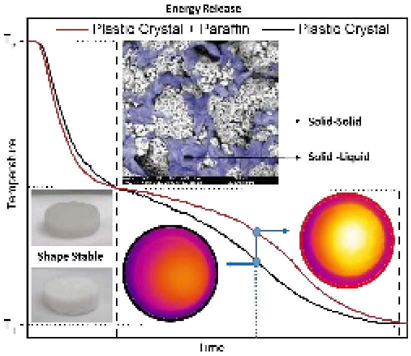
[3] Ristić, A., Mal, S., Zabukovec Logar, N., Bérut, E., Bois, L., Outin, J., … & Doppiu, S. (2024). Improving Materials for Compact Thermal Energy Storage: Two Case Studies on Tailor-Made Polyalcohol Mixtures (PCMs) and Composites of Chlorides Confined in Gamma-Alumina or Silica-PEG (TCMs). *ACS Applied Energy Materials*, *7*(20), 9242-9254. https://pubs.acs.org/doi/abs/10.1021/acsaem.4c01702

	Materials	Process	Improving strategies	Expected results
PCM	Fatty acids, Esters, Paraffins, Salt hydrates, Natural oils (15–20 °C)	Solid-liquid		- Latent heat enhancement - Tuning melting temperatures - Supercooling mitigation
	Novel ternary mixtures of salt hydrates, salts, and water (-70–120 °C)	Solid-liquid	Theoretical prediction and experimental determination of solid-liquid phase diagrams: 	- Tuning melting temperatures
	Plastic Crystals (40–200 °C), Ionic Plastic Crystals (20–120 °C)	Solid-solid	Blends of plastic crystals: 	- New solid-solid molecules with high latent heat and tuned transition temperatures
	Combining solid-liquid and solid-solid PCM	Composites		- Latent heat enhancement - Shape stabilization - Solving compatibility issues
	Hybrid PCM-TCM concept: S-L and S-S PCM as a TCM (salt hydrates) matrix			- Properties improvement (thermal & thermodynamical, mechanical, supercooling mitigation, stability, material compatibility)

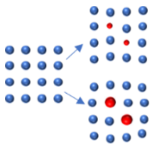
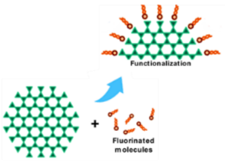
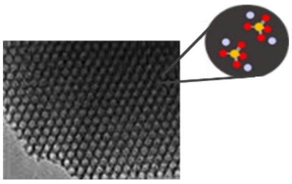
	Materials	Process	Improving strategies	Expected results
TCM	Oxides, hydroxides, Inorganic and Organic Salts, Hierarchical Zeolites, Hierarchical Alumino-phosphates,	Sorption and/or chemical reactions (pure materials	 Doping  Functionalization	• Increasing reaction enthalpy, tuning temperature, improving stability • From understanding of phenomena to demonstration scale.
	TCM in porous matrixes (Salt hydrates) Polymers based encapsulation salt hydrates Natural-based adsorbent TCM as host matrices (salt hydrates e.g., $MgCl_2$, $CaCl_2$, etc.)	Combining sorption and chemical reactions (Composite Materials)	 Mixing active materials	Design smart TCM composites with: • High reaction enthalpies • Tailoring hydrophilicity • Enhanced heat and mass transfer • Enhanced thermal conductivity • New “natural” highly stable composites with high chemical storage capacity

Figure 4-1: Tailoring enthalpies and working temperatures of PCM and TCM.

4.1.2 Objectives

The main objective of Subtask B was to define proper strategies that allow to tune CTES materials properties to improve their performance at component and storage system level. This is a paramount aspect for TES materials when the existing (commercial) ones does not show the properties (chemical and physical) that satisfy the application requirements. Following this target the specific objectives of this Subtask were identified as following:

- Developing of new materials for CTES (low cost, no toxicity, non-flammable, natural/raw materials).
- Synthesis of novel single-component materials with changed chemistry through modified structure.
- Developing multi-component materials (composites) with increased storage capacity and enhanced heat and mass transport properties.
- Evaluating the influence of the synthesis and processing methods on the final techno-economic and environmental performances of the materials.

These aspects (all or in part) are covered by the Subtask B participants in their research activities. This includes the use of different types of materials working in different ranges of temperatures and, depending on the specific case, undergoing phase transitions (PCM based materials) and chemical reactions (TCM based materials). The approaches used to develop the targeted materials and the type of modifications needed are different depending on the process considered (PCM or TCM). When defining the goal of this Subtask, two different key aspects and activities, divided in different subsections, were highlighted.

- B.1 Exploring potential materials for CTES

Objective B1: Tailor made materials with tuned thermodynamic properties (high energy storage capacity, working temperature aligned with the application).

- B.2 Improving the performances and increasing versatility: Advanced composites for CTES and best conditioning

Objective B2: Improved materials in terms of energy storage capacity and heat and mass transfer ability. Look for best conditioning in view of their integration into application.

The materials targeted in Subtask B are PCM focusing both on solid-liquid and solid-solid transitions as well as composites or shape-stabilized derived materials, and TCM focusing both on sorption processes (ad- and absorption) and chemical reactions (mainly gas-solid systems). In Figure 4-2, the general overview of the materials studied and the improving paths explored are reported. Figure 4-2 shows the types of materials explored and their optimization paths to tune key properties to match the targeted application requirements. In general, this is one focal point of the discussion trying to link material development with application-oriented requirements. Some more details relevant to the materials studied will be given in section 4.2.

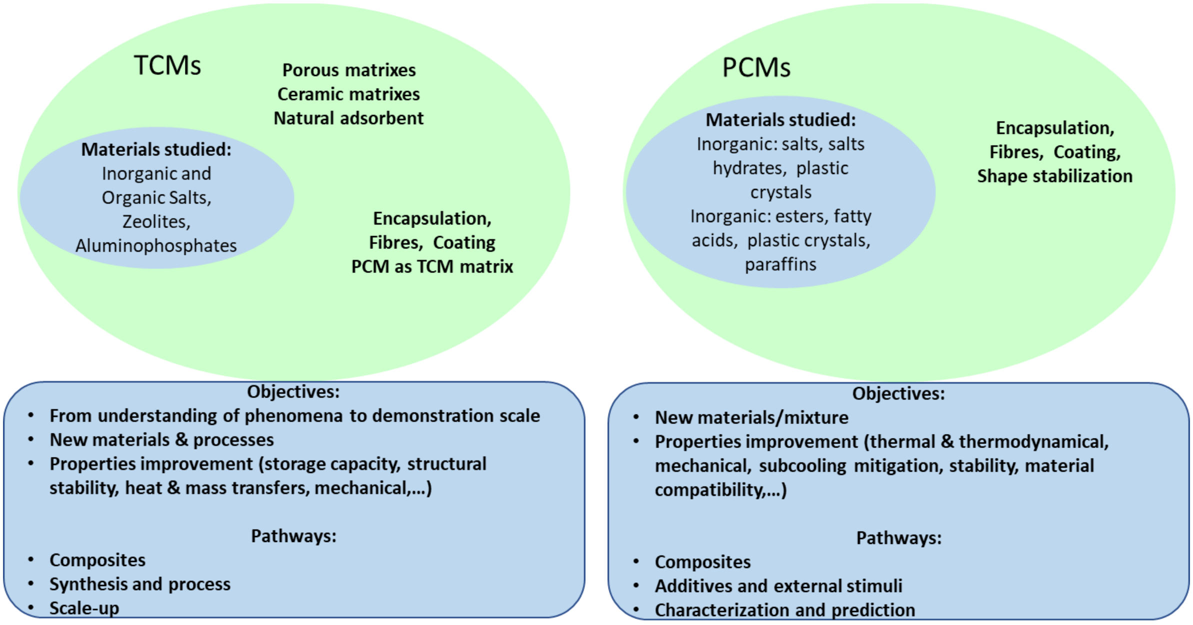


Figure 4-2: Overview of the materials studied in Subtask B.

As an example, the materials modification (optimization) strategies are summarized in Figure 4-3. The research work includes **Tailoring energy density/working temperature** by crystal structure modification, functionalization, using nanostructured materials, and new composite materials designed by mixing active materials; **Enhance heat and mass transport** properties by i) adding highly conductive materials, ii) infiltration in highly conductive matrixes, and iii) materials with high thermal conductivity (foam/fibres); **Best integration into the application** by i) shape-stabilization, ii) granulation with active and inactive binders, iii) coatings, and iv) monoliths.

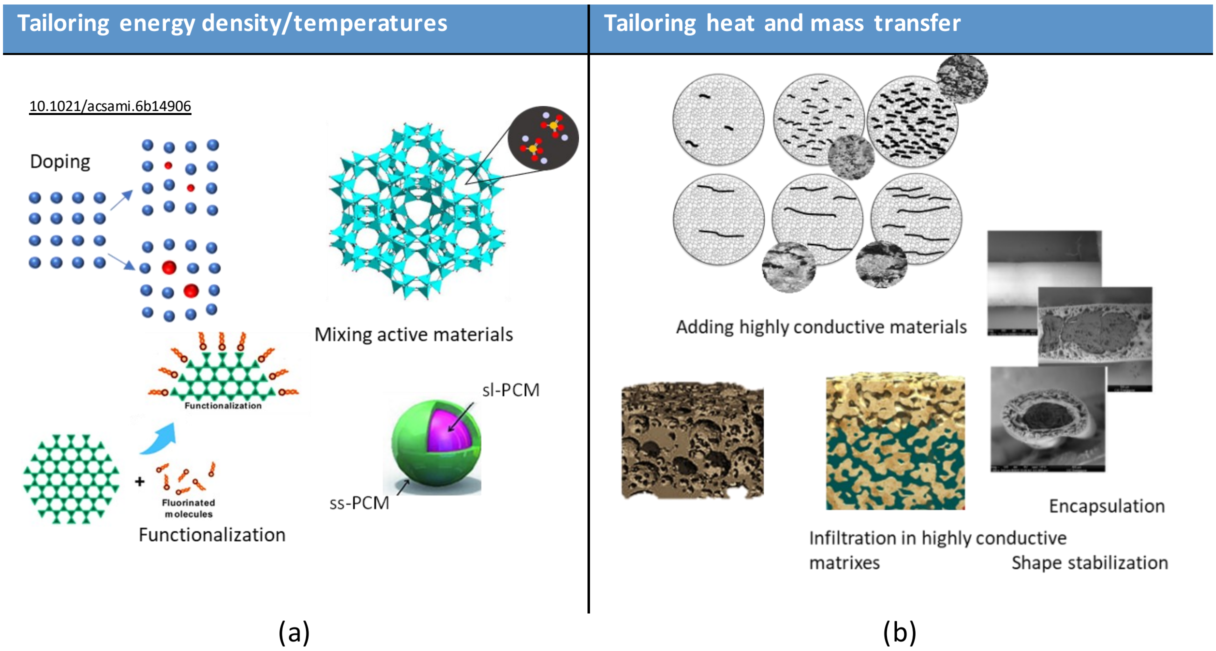


Figure 4-3. Materials modification strategies studied in Subtask B.

In Subtask B, the expertise of around twenty institutions and experts in the field of thermal energy storage was shared to start the discussion about the definition of guidelines and strategies for materials improvement.

Following this strategy, the work of Subtask B included the building of a map of all the materials studied by the experts involved including i) the types of materials, ii) the improving strategies, iii) the main goals of the research, and iv) the application addressed. This work allowed to identify synergies between the different research entities to prepare joint documents containing key information for material development summarising the most relevant findings of the experts participating to Subtask B. At the same time, the key concept on how to quantify how the materials improvement can impact the TES system was deeply discussed. This is still an open discussion between the experts trying to define proper ways to address it.

The organizations that participated to Subtask B are listed in the following Figure 4-4.

Figure 4-4. Organizations participating to Subtask B.

4.2 Overview of experience and map of CTES improvement

The map of materials studied in Subtask b is given in Table 4-1.

Table 4-1: Expertise on CTES materials improving/optimization.

Institution / Project name	PCM/TCM	Short description of the materials	R&D objectives	Pathways
CETHIL Heat Transfer and Energy Processes in Buildings and their Environment)	TCM	**Ceramic/hydroscopic salt** composite with multi porosity	• Elaboration of ceramic pastes for 3D printing • Improving mechanical properties • Multi porosity matrices • Understanding of heat and mass transfer	Composite materials
		Zeolite coating via a polymer	• Coating permeability to steam • Mechanical strength enhancement • Adherence of coating after thermal and sorption cycles	Composite materials Reactive coating
		Encapsulation of salt hydrates by polymer	• Enhanced mechanical resilience of the grains • Understanding of heat and mass transfer • Chemical heat enhancement	Coating formulation Composite materials
University of Applied Sciences Upper Austria	TCM	**Salt in porous matrix-** Composites for low-temperature TES (40–150°C)	• Improving mechanical stability • Sorption capacity enhancement	Salt-mixtures (diff. synthesis methods) and composite (fiber) development
ZAE Bayern PCM based on salt-water systems	PCM	**Mixtures of salt hydrates, salts, and water** as “new” PCM (-70–120 °C); systems with up to three different salts and water	• Solid-liquid phase diagrams: Theoretical predication and experimental determination • Identification of eutectic mixtures • Tests of nucleating agents to promote crystallization	Solid-liquid phase diagrams: Theoretical prediction and experimental determination

Institution / Project name	PCM/TCM	Short description of the materials	R&D objectives	Pathways
CIC energiGUNE PCM-based **solid-state** thermal batteries	PCM	**Inorganic Plastic Crystals** for TES at high temperature (450–650 °C)	- Improving mechanical properties - Thermal conductivity enhancement - Multi-responsive features	Composite materials
		Organic Plastic Crystals for TES at medium temperature (40–200 °C)	- Supercooling mitigation - Enabling direct contact with water/steam - Thermal conductivity enhancement - Latent heat enhancement - Multi-responsive features	External stimuli Protective coatings Composite materials
		Ionic Plastic Crystals for TES at low-to-medium temperature (20–120 °C)	New molecules undergoing solid-state phase transitions with high latent heat	Rational design and synthesis
TU Wien/NIC Ljubljana/AEE INTEC Design of Smart HeatStock TCM composites	TCM	Composite TCM based on **g-Al_2O_3 covered by in-situ $AlPO_4$** and additionally **coated with hygroscopic salts**	Boosting the thermochemical heat storage capacity	Composite materials
HSLU Optimization and development of PCM	PCM	**Organic (esters) and inorganic (salt hydrates)** PCM with low to medium temperature (-15–80°C)	- Study of the polymorphic transformations and ways to control them - Study on the optimization of materials in terms of improved stability (i.e. kinetics, segregation, accelerated long term testing)	Usage of additives In-depth characterisation development of new methodologies

Institution / Project name	PCM/TCM	Short description of the materials	R&D objectives	Pathways
NIC Slovenia Research programme “Nanoporous materials”	TCM for low temperature TES	**Hierarchical aluminophosphates** (60–90 °C)	- Water adsorption capacity / storage improvement - Tailoring hydrophilicity	Green synthesis Recycling Low cost reactants Shaping
		Composites with salt hydrates / aluminophosphates (80–120 °C)	- Water adsorption capacity / storage enhancement - Mass and heat transfer enhancement - Thermal conductivity enhancement	Preparation paths, Green synthesis, Low cost reactants
		ZIFs (80–100 °C)	- Ethanol adsorption capacity enhancement - Tailoring structure	Green synthesis
		Porous matrices (60–100 °C)	- Tailoring structural properties - Water and heat transfer enhancement	Design and monitoring of synthesis parameters
TNO / compact loss-free heat batteries based on salt hydrates	TCM	**Salt hydrates and salt hydrate composites** (Salt hydrate + additive to improve cyclability); Optimization of size/shape of solid materials for optimal performance	- Increase of Energy storage density from material to system level - Optimized module and system lay-out for increased performance and potential series production - Demonstration of systems in relevant use-cases - Spin-out of technologies for future market uptake	Materials and composites testing, small-scale (flexible) module testing, system integration and optimization, demonstration.

Institution **/ Project name**	**PCM/TCM**	**Short description of the materials**	**R&D objectives**	**Pathways**
University of Ottawa (uOttawa) Design of composite TCM Materials	TCM	Composite materials made out **of salt hydrates + host material + encapsulating material**	Increasing the energy storage density for commercialization	Composite materials
UniMe Development of hybrid and novel TCM	TCM	**Inorganic salt hydrates** in macroporous foams	- Inhibiting deliquescence-related issues - Preventing agglomeration phenomena - Correlation between energy storage capability and macro-micro-structure of the composite	Confinement in a macroporous foam semipermeable to water vapor
		Organic salts	- Identification of novel organic salts - Characterization & Testing	Rational design and synthesis
Eindhoven University of Technology (Applied Physics)	TCM	**Salt hydrates** for low temperature TES (30–100°C). For the built environment.	- Understanding reaction kinetics - Improving power output by doping - Making stable mm-sized composite particles for reactors (reinforced, encapsulated) - Behavior of particle beds	Multiscale experimental approach

Institution / Project name	PCM/TCM	Short description of the materials	R&D objectives	Pathways
BCES (University of Birmingham) PCM-based composite	PCM	**PCM composites**, by using **by-products such as red mud or fly-ash** among others. From medium to high temperature.	Improving cyclability and material compatibility.	Formulation optimization. Scale-up.
	TCM	**TCM composite** at medium temperature by using **ceramic matrix and by-products.**	Special focus on formulation optimization and novel manufacturing routes.	Manufacturing routes. Formulation optimization. Scale-up.
	PCM/TCM	Combination of **S-L and S-S PCM** as a TCM matrix at medium temperature (salt hydrates).	Improving cyclability and material compatibility.	Composite materials. Manufacturing routes. Formulation optimization. Scale-up.
University of Warwick / Sorption heat pump systems (Mission Innovation)	TCM	Resorption of ammonia between salts: $CaCl_2$, $MnCl_2$, $BaCl_2$, NH_4Cl, NaBr	PoC heat pump and thermal transformers with power density > 1kW/litre	ENG (Sigratherm) matrix to promote thermal conductivity.
University of Warwick / HP-FITS	TCM	NaOH – H_2O absorption heat storage	Link to a domestic heat pump for demand side management	Novel absorber and evaporator designs, possible use of additives/mixtures

Institution / Project name	PCM/TCM	Short description of the materials	R&D objectives	Pathways
NRCan Low-cost high-performance thermal energy storage materials	TCM	• Natural-based adsorbent TCM as host matrices for medium temperature (up to 250 °C): ○ High-purity crystal zeolites ○ Forest waste residues ○ Vermiculite Host matrices to be loaded with salt hydrates (e.g., $MgCl_2$, $CaCl_2$, etc.)	• Identification of promising natural-based host matrices for composite materials development • Investigating shaping techniques (granulation/agglomeration) • Investigating hydrothermal and structural stability of the developed materials • Thermal conductivity enhancement • Structural and surface measurements characterization (BET surface area, pore size & distribution, SEM) Elemental analysis (XRD, XRF, and EDX)	Composite materials
Aalborg University / Energy reduction for cooling using PCM in 2-pipe chilled beam systems	PCM	PCM with a phase change temperature range: 15–20℃ • Organic paraffins RT18, RT15 • Organic fatty acids Pure Temp 18, Pure Temp 15, • Salt hydrate SP15 • Coconut oil • Tamanu oil	• Identification of examined PCM long term stability in pure form • Identification and characterization of eutectic mixtures • Identification and characterization of PCM encapsulated in electrospun fiber matrices • Study of optimization of thermal properties for future use of PCM in LHTES application	• Thermograms of PCM in pure form, eutectic mixtures and encapsulated in electrospun fiber matrices. • Theoretical prediction of PCM applicability in LHTES application

In Table 4-1, the materials studied (PCM or TCM), the R&D objectives, and the pathways to reach the objectives are reported for all participating institutions. This confirms the deep interest around materials optimization for TES applications. As already reported in Figure 4-1, the materials studied are both organic based and inorganic based and the preferred modification path is given by the development of different types of composites depending on the optimization targeted (increase energy density, improve thermophysical properties, or best integration into the TES system).

Considering the modification paths reported in Figure 4-3, the major focus to improve the energy density and tailor the working temperature is towards the development of composite materials by mixing active materials (Figure 4-3 (a)). This means that all the materials in the composites have to undergo a phase transition or a chemical reaction in the same range of temperature, contributing to the overall energy density. As two examples, the infiltration of salt hydrates in to porous structure (e.g. zeolites, aluminophosphates) or the mixing of solid-solid and solid-liquid based PCM (Figure 4-3 (a)). This optimization path presents many challenges including the "perfect reactivity" and reversibility of the material involved and, at the same time, the materials have to be compatible and do not interact too strongly leading to possible deviations negatively influencing their stability/durability. Another goal achieved by the development of "ad hoc" composites is obtaining materials with improved thermophysical properties to enhance the heat and mass transport (Figure 4-3 (b)). For example, this includes a small addition of highly conductive materials, the infiltration into porous matrixes or the encapsulation of the material into highly conductive fibres. In general, the objective is to minimize the amount of inert materials to impact the energy density of the composite as less as possible. Also in this case, many aspects have to be considered to ensure the short- and long-term stability without a significant degradation of the materials performance.

Another important aspect is the production of composites for the efficient integration of the TES material into the system. The strategy in this case could be taking advantage of the composites developed to improve materials properties that can be directly used into the system. This includes for examples the shape stabilization or the encapsulation techniques. This is a key aspect for the development of the TES technologies since a TES material in direct contact with the heat transfer fluid would contribute to the simplification of the systems (no heat exchanger needed) thus lowering the cost.

Keeping in mind this TES material improving philosophy, the discussion during the period of the Task touched different crucial points.

The key discussion points were:

- What is the impact of materials improving on the TES system?
- How to define materials improving guidelines depending on the application addressed?

So far, these questions have not an answer – but the discussion with the experts led to the definition of possible ways to approach them.

On one side, the first step was a crossing Subtasks (B, D, and E) brain storming discussion to define KPIs at component level linked to material properties. To this end the proposal by Christoph Rathgeber (ZAE Bayern) was discussed and then presented to all the experts in expert meeting in Kassel

(September 22). Table 4-2 reports the classification of CTES properties on material level and KPIs on component level.

Table 4-2: Classification of CTES properties on material level and KPIs on component level.

CTES characteristic	**Property on material level (*PROP*)**	**KPIs on component level (*KPI*)**	**Direction of optimization**
Amount of energy stored per mass or volume	• Melting enthalpy of PCM (per mass or volume) • Max. reaction enthalpy of TCM (per mass or volume) • Cp	• Storage capacity (per mass or volume)	Towards *PROP* (*KPI* always less than *PROP*)
Energy uptake and release rate	• Thermal conductivity • Thermal conductivity normalized by ? • Mass transfer • Kinetics?	• Power (normalized) during charging/discharging	To be increased towards application requirements
Stability	• Change of material properties with – number of charging/discharging cycles – (testing) time	• Change of storage capacity or power with – number of charging/discharging cycles – (operation) time	Towards "no change"
Costs	• Costs per mass or volume of CTES material • Costs per specific enthalpy change	• Costs per 1 kWh of capacity • Costs per 1 kW of power	To be decreased towards application requirements

The discussion raised many concerns demonstrating how complex it is to approach this problem that and many other aspects should be taken into account. For example:

- The impact of encapsulation/shape stabilization on storage capacity is important.
- Materials development can strongly impact the system cost (eliminate heat exchanger): Shape stabilization/encapsulation compatibility with the HTF.
- Add the concept of efficiency at component and material level.

Finally, the key concept to quantify how the materials improvement can impact the TES system is still an open discussion between the experts. As a first attempt, it was decided to follow two different approaches for TCM and PCM. In case of TCM, the preparation of a joint document led by Frederic Kuznik (INSA Lyon) on "TCM materials into system" was discussed. In case of PCM, as suggested by Elena Palomo del Barrio (CIC energiGUNE), the approach to follow is building Ragone plots [6] (example in Figure 4-5) for selected materials and properties. The corresponding article [6] states that "geometry, material properties and operating conditions all contribute to the energy and power trade-off of a phase change thermal storage device. This thermal storage Ragone framework enables a clear comparison method between different thermal storage materials and designs". This approach could be helpful guiding the materials scientist towards the development of the "right materials" with optimum properties adapted to the application requirements.

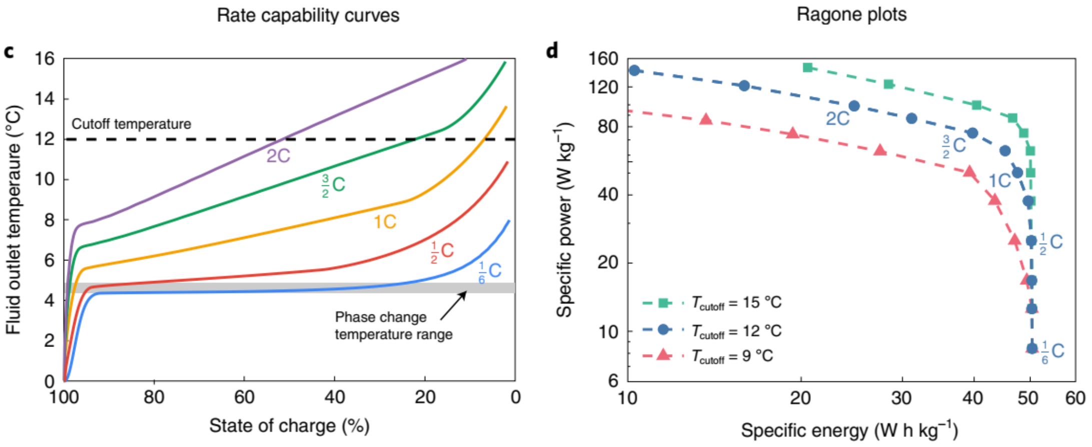


Figure 4-5: Example of rate capability and Ragone plots for thermal energy storage.

In particular, it was decided to prepare a map of materials including, for example, all the work done concerning the use of carbon based materials to improve PCM properties. The key parameters collected will be used in a numerical model (for a certain system configuration) to build Ragone plots (specific power versus specific energy). This could be a first step to define the state of the art related to those specific materials. This approach could be extended to other classes of materials and properties in a second stage. The final goal is both to have a clear picture of the degree of development reached up to now but also the definition of guidelines for materials improvements when considering certain applications.

Unfortunately, for both cases (TCM and PCM), due to lack of time and resources, this planned work was not carried out even if it remains of great interest.

4.3 Conclusions

The development of optimized TES materials will continue to be a key topic until the commercialization of a large number of TES systems covering the needs of a wide range of applications. The information collected in Subtask B demonstrates how complex the study of these materials is, but also how proper strategies of improvement allow to obtain materials with tuned properties for potential uses in applications. There are still many open questions especially concerning the definition of guidelines for materials optimization and the impact on the TES system.

4.4 Key messages

The key messages of Subtask B are the following:

- The development of performant TES materials is an up-to-date research topic for the implementation of efficient and low cost TES systems
- The definition of guidelines for materials improvement are a key aspect to guide the materials development strategies towards the system requirements
- There is a growing effort to enhance TCM with strategies that differ significantly from those traditionally employed for PCM.

- Despite several years of work on improving PCM and TCM, new strategies for designing and developing PCM and TCM with tailored properties continue to emerge.
- It's essential to define targeted KPIs helping to identify where efforts for improvement need to be intensified or where the impact of this improvement has minimal effect on the overall system performance

4.5 References

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5 Subtask C: State of Charge Determination

5.1 Background & Objective

Subtask C focused on the collection, classification, and dissemination of the most promising methods to effectively determine the state-of-charge (SoC) of PCM and TCM CTES systems. In particular, the identification of suitable methods for determining SoC in either PCM or TCM CTES is a crucial foundation for the digitization of energy storage systems.

Subtask C was executed in three steps: Inventory Survey, Collection of Experimental and Numerical Proof of Concept, and Descriptions of Application Requirements. This section captures the collective outputs from all three steps.

5.2 Subtask Contributors

The following Table 5-1 lists the experts and their institutions who contributed to Subtask C.

Table 5-1: Task experts with state-of-charge experience; investigated PCM and TCM; applied testing devices and experimental conditions (sorted alphabetically by country).

Country	Institution	Field	Experts
Austria	AEE INTEC	TCM	Wim van Helden, Franz Hengel
Austria	University of Applied Sciences Upper Austria	PCM/TCM	Gayaneh Issayan, Bernhard Zettl
Austria	TU Vienna	TCM	Peter Weinberger, Jakob Smith
Canada	Dalhousie University (LAMTE)	PCM	Dominic Groulx
Canada	Neothermal Energy Storage Inc.	PCM	Louis Desgrosseilliers
Canada	NRCan CanmetENERGY-Ottawa	TCM	Reda Djebbar, Chris McNevin, Thomas Manser
Denmark	Technical University of Denmark (DTU)	PCM	Gerald Englmair
Germany	German Aerospace Center (DLR)	PCM/TCM	Andrea Gutierrez, Maike Johnson
Germany	-	PCM	H. Mehling
Germany	University of Bayreuth	PCM	Marco Griesbach, Andreas König Hagen
Germany	Fraunhofer ISE	PCM	Sebastian Gamisch
Germany	ZAE Bayern	PCM	Christoph Rathgeber
Italy	CNR	TCM	Andrea Frazzica
Italy	University of Padova	PCM	Carolina Mira-Hernández
Netherlands	TNO	TCM	Ruud Cuypers; Jochem Jongerius
Norway	SINTEF Energy Research	PCM	Jorge Salgado Beceiro, Olav Galteland
Slovenia	NIC Slovenia	TCM	Alenka Ristic
Spain	Universitat de Lleida (UDL)	PCM	Gabriel Zsembinszki, Emiliano Borri
Spain	University of the Basque Country	PCM	Gonzalo Diarce

Switzerland	Lucerne University of Applied Sciences and Arts	TCM	Benjamin Fumey, Yannick Krabben
UK	Birmingham Centre for Energy Storage (BCES), School of Chemical Engineering, University of Birmingham	TCM	Helena Navarro
UK	Swansea University	TCM	Jonathon Elvins
USA	US DOE; US DOE labs (LBNL and ORNL)	PCM/TCM	Sven Mumme, Sumanjet Kaur, Tim Laclair; Youngsup Song

5.3 Definitions

The following definitions were applied in Subtask C.

- Thermal Battery: A TES with instantaneous SoC determination
- State of charge determination utilizes measurement techniques of material bulk response.
- State of charge is a component level property (analogy: electrical battery).

5.3.1 State of charge

The SoC of energy storage systems (electrochemical, thermal, kinetic, gravitational) can be broadly defined in Eq. (6.1) as the quotient of either the residual (discharge) or accumulated (charge) energy capacity ($E(t)$) to the maximum system energy storage capacity (E_{max}), normally expressed as a percent value:

$$SoC = \frac{E(t)}{E_{max}} \% \tag{6.1}$$

Both $E(t)$ and E_{max} are determined with respect to reference states that define the anticipated lower and upper bounds of operating conditions that produce energy transfer.

With respect to CTES, these energy capacities are expressed primarily using system relative enthalpy, ΔH, as the active PCM/TCM are either exclusively in the solid/liquid phases in closed systems with only modest variations in internal pressure or constitute open systems energy balances around the principal heat exchangers due to the conveyance of either liquid or vapor thermal storage species across its boundaries (e.g., PCM slurry or TCM).

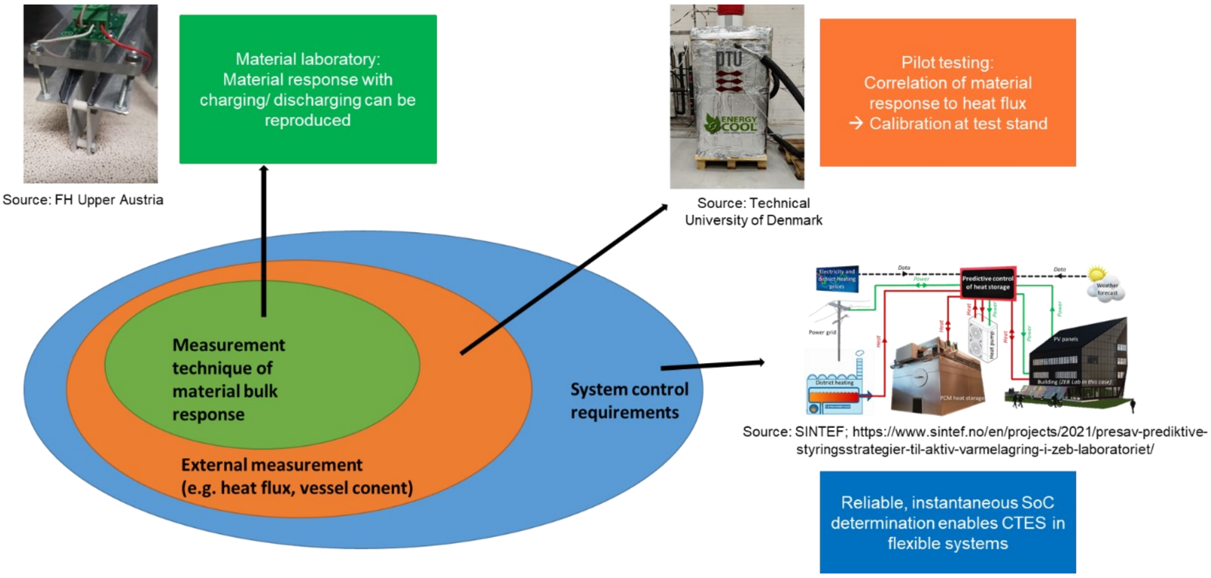
At a system level, the energy storage capacities of CTES are extensive properties that include both the active PCM/TCM species and smaller contributions of sensible energy storage capacities from the materials of construction that belong passively to the heat exchange network between the CTES and the external energy sink/source. However, to generalize methods of SoC determination suitable for either PCM or TCM CTES, Subtask C focused exclusively on the techniques used to quantify the ΔH contributions to the CTES from the active PCM or TCM species only. Quantifications of the passive sensible storage capacities, while not difficult to model, require specific knowledge of a CTES' construction and the relationship of these materials to the CTES' heat exchange network, which therefore cannot be generalized.

The extensive nature of determining the PCM/TCM energy capacities also necessitates the ability to either directly measure the active material's bulk (i.e., average) energy capacity or to approximate it from an array of spatially discrete (i.e., local) measurements along the principal directions of both thermal and concentration gradients in the CTES.

Two difficulties arise in both PCM and TCM CTES to quantify the residual/accumulated energy capacities: 1) path dependence (e.g., heat exchange history, supercooling/nucleation history), and 2) bulk averaging of local independent variables. In contrast, a CTES' maximum system energy storage capacity can be more easily quantified as an idealized representation of the CTES (i.e., uniform temperature, pressure, concentrations) at its lower and upper limit operating conditions.

5.3.2 Research classification

Members of Subtask C have collectively defined three distinct levels to the development of SoC determination techniques for PCM and TCM CTES (Figure 5-1).



Source: FH Upper Austria

Source: Technical University of Denmark

Source: SINTEF; https://www.sintef.no/en/projects/2021/presav-prediktive-styringsstrategier-til-aktiv-varmelagring-i-zeb-laboratoriet/

Figure 5-1. Schematic representation of the 3-level approach for the development of PCM and TCM SoC determination techniques linked to material properties.

The first, innermost level, given the shorthand description of "Material Level", describes the development of measurement sensors and techniques able to provide data relating to an intrinsic material property of either the PCM/TCM or the external conditions imparting heat/mass to the PCM/TCM that are useful to determine SoC. Developments characterized by this stage belong generally to TRL 1-3, meaning the exploration of the fundamental basis for the technique as well as proof-of-concept using either lab evaluation or numerical simulation.

The second level, given the shorthand "Component Level", describes the development of the "Material Level" measurement techniques either internal or external to the PCM/TCM able to provide data that is calibrated to either bulk or local SoC determination. Development characterized by this stage generally belongs to TRL 4-6, meaning that basic component integration has been demonstrated in either a simulated or controlled environment.

The third and final level, given the shorthand "System Control", describes the integration of the calibrated SoC determination techniques at the "Component Level" into a fully integrated CTES system with electronic control (either local or remote) at or near the desired final CTES configuration for end-use deployment (TRL 7-9). Some activities at this level might involve the development of model predictive control (MPC) or the generation of other forms of "digital twins" representing the dynamic response of the PCM/TCM CTES.

5.4 Inventory of Promising Material Properties and Related Measurement Techniques

5.4.1 Survey of past and current studies among Task experts

Member participants of Subtask C were surveyed to provide suitable examples of SoC determination techniques for PCM/TCM CTES. These could either be SoC techniques personally utilized by the member participants, those of which they were familiar from the research literature, or those for which they could reasonably hypothesize a novel approach.

Table 5-2: Overview of all 21 contributors to the inventory table.

County	Institution	Field
Austria	AEE INTEC	TCM
Austria	University of Applied Sciences Upper Austria	PCM/TCM
Austria	TU Vienna	TCM
Canada	Dalhousie University (LAMTE)	PCM
Canada	Neothermal Energy Storage Inc.	PCM
Canada	NRCan	TCM
Denmark	Technical University of Denmark (DTU)	PCM
Germany	German Aerospace Center (DLR)	PCM/TCM
Germany	H. Mehling	PCM
Germany	University of Bayreuth	PCM
Germany	Fraunhofer ISE	PCM

County	Institution	Field
Germany	ZAE Bayern	PCM
Italy	CNR	TCM
Netherlands	TNO	TCM
Norway	SINTEF Energy Research	PCM
Slovenia	NIC Slovenia	TCM
Spain	Universitat de Lleida (UDL)	PCM
Spain	University of the Basque Country	PCM
Switzerland	Lucerne University of Applied Sciences and Arts	TCM
UK	Birmingham University	TCM
UK	Swansear University	TCM

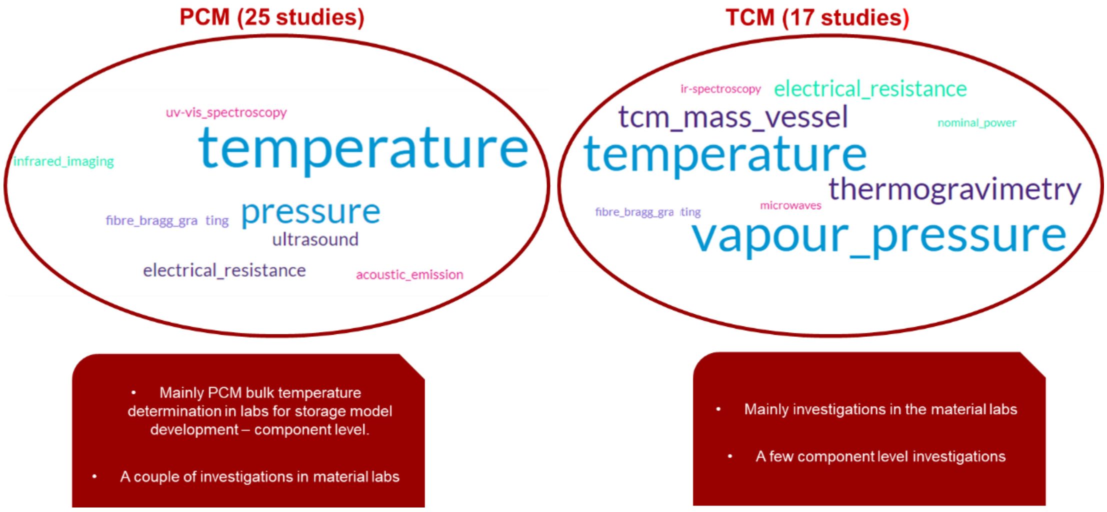


Figure 5-2. Measurement techniques applied by Task experts (weighted).

Figure 5-2 shows a summary of the main measurement techniques applied by Task experts with the most used weighted and highlighted in bigger fonts.

Regarding PCM, 20 technique submissions were collected from 11 participants. Amongst these submissions, 11 described techniques utilizing temperature measurements of the PCM medium and control volume boundary heat exchange, 1 exclusively utilizing temperature measurements of the PCM, 4 utilizing volumetric changes of the PCM, 3 utilizing acoustic properties of the PCM, and 1 utilizing the electrical conductivity of the PCM. In general, the temperature/control volume and temperature-only approaches have been more broadly utilized and achieved higher TRL than most of the other techniques.

Regarding TCM, six main TCM SoC measurement techniques were submitted by eleven participants. Most, if not all these methods were performed at the material level and used either in a laboratory experimental environment or at pilot scale and therefore will need further validation at the higher TRL. A few methods were applied at component level. The two most promising methods that could achieve rapidly higher TRL included (i) enthalpy balance SoC determination technique during system operation. This SoC determination method was tested by five participants; and (ii) TCM mass or adsorbate mass balance SoC determination technique, which was reported by at least four participants. Other interesting SoC determination methods being investigated and reported by participants include (iii) temperature of the TCM bulk material and adsorbate vapor pressure of the TCM bulk material, (iv) adsorbate volume change during operation, (v) electric, and (vi) spectroscopic properties measurement of the TCM unit bulk materials.

5.4.2 Internet survey using ChatGPT (October 2023)

Several, specific search questions were applied. A list of measurement techniques was obtained, but no examples/ detailed references are possible. The list was tailored/revised by Task experts.

List of measurement techniques:

5.4.2.1 PCM Applications

The application of measurement techniques in thermal energy storage (TES) systems using phase change materials (PCM) can vary depending on the specific requirements and the scale of the system. In practice, several of the mentioned measurement techniques can be applied in TES systems, but their usage may depend on factors such as the intended application, budget constraints, and the need for precision. Here's a breakdown of which techniques are commonly used in practice:

1. **Temperature measurement:** Monitoring temperature is a fundamental and widely used technique in TES systems. It is a straightforward and cost-effective method to assess the state of charge. Temperature sensors, such as thermocouples or resistance temperature detectors (RTDs), are commonly employed in TES systems.
2. **Thermal energy flow measurement:** Measuring the thermal energy flow is also a common practice in TES systems. Heat flux sensors, calorimeters, and flow meters are frequently used to monitor energy input and output during charging and discharging processes.
3. **Differential Scanning Calorimetry (DSC):** DSC is a precise laboratory technique and is not typically used in real-time monitoring of TES systems in practical applications. It is more often used for material characterization and research purposes.
4. **Ultrasonic techniques:** Ultrasonic sensors can be applied in TES systems for measuring density or compressibility changes in the PCM, but their usage may be less common compared to temperature or thermal flow sensors.
5. **Acoustic emission:** Acoustic emission techniques are less common in practical TES systems, primarily because they require specialized equipment and are often used for research purposes rather than real-time monitoring.
6. **Electrical resistance measurement:** While changes in electrical resistance can occur during phase transitions in some PCM, this technique is not commonly employed in practical TES systems due to the need for specialized equipment and potential safety concerns.
7. **X-ray imaging:** X-ray imaging techniques are not typically used for routine monitoring of TES systems. They are more commonly used for research and visualization purposes.

8. **UV-Vis Spectroscopy and MRI:** These techniques are generally not used in practical TES systems due to their complexity, cost, and limited applicability in real-time monitoring.

In practice, temperature measurement and thermal energy flow measurement are the most employed techniques for assessing the state of charge in TES systems using PCM. These methods provide valuable information for controlling and optimizing the operation of the system. The choice of technique will depend on the specific requirements of the application and the available resources.

5.4.2.2 TCM Applications

The choice of measurement methods in large-scale thermochemical heat storage (TCS) systems depends on various factors, including the specific technology, application, and goals of the project. Some methods may be more promising than others based on the following considerations:

1. **Temperature measurement:** Temperature measurement is a fundamental and widely applicable technique in TCS systems. It provides essential data for monitoring the progress of reactions and ensuring safe operation. Temperature sensors are commonly used in both lab-scale and large-scale TCS systems.
2. **Calorimetry:** Calorimetry is highly promising, especially for understanding the heat flow associated with chemical reactions. In large-scale TCS systems, calorimetric techniques can provide valuable information about energy storage and release, aiding in system optimization.
3. **Pressure measurement:** Pressure measurement is particularly relevant for gas-phase reactions in large-scale TCS systems. It can help ensure safety and provide insights into the state of the storage material.
4. **X-ray imaging (XRD and X-ray CT):** X-ray techniques offer non-invasive visualization of chemical species and structural changes within the storage material. They can be valuable for quality control, fault detection, and process optimization in large-scale TCS systems.
5. **Chemical composition analysis (spectroscopy):** Spectroscopic methods, such as FTIR or Raman spectroscopy, are powerful for monitoring chemical composition changes. They can be promising in cases where detailed chemical analysis is critical for understanding reactions.
6. **Gravimetry:** Gravimetric measurements can be useful when mass changes are significant in large-scale TCS systems, such as in reactions involving solid-gas interactions or material loading/unloading.
7. **Electrical conductivity:** Electrical conductivity measurements may be promising in certain TCS systems where electrical properties change significantly during reactions, allowing for non-invasive SoC assessment.
8. **Optical imaging:** Optical microscopy and imaging can provide valuable visual insights into material behaviour and structural changes within large-scale TCS systems, aiding in quality control and system monitoring.
9. **Chemical sensors:** Chemical sensors can be tailored to specific chemical species or properties, making them promising for real-time monitoring of critical parameters in large-scale TCS processes.
10. **Heat flow measurement:** Heat flux sensors and calorimeters are promising for large-scale TCS systems to quantify heat flow and optimize energy storage and release.

5.4.3 Theoretical aspects on material level

5.4.3.1 PCM SoC

Regarding the determination of ΔH in PCM CTES, the component of latent heat of phase transition (Δh_{trns}) is normally responsible for most of the useful energy capacity in the CTES, while the contributions from sensible energy can sometimes be neglected if the CTES is operated around T_{trns} in a limited temperature range. Eq. (6.2) describes the relative, specific enthalpy (Δh) of an idealized, either pure or eutectic ($\Delta h_{mix} = 0$), solid/liquid PCM while Eq. (6.3) describes the relative, specific enthalpy of an idealized binary mixture PCM ($\Delta h_{mix} = 0$) operating within the liquidus dome adjacent to the component undergoing phase transition (see Figure 5-20; e.g., salt hydrate with excess water):

$$\Delta h(T, T_{\mathrm{ref}}, \partial) = \partial\left(\Delta h_{\mathrm{trns}} + \int_{T_{\mathrm{ref}}}^{T} C_{\mathrm{p,l}}dT\right) + (1-\partial)\int_{T_{\mathrm{ref}}}^{T} C_{\mathrm{p,s}}dT \qquad (6.2)$$

T, T_{ref}, ∂, $C_{\mathrm{p,s}}$ and $C_{\mathrm{p,l}}$ refer to the PCM temperature, reference temperature used for relative enthalpies (i.e., temperature at which Δh_{trns} is expressed), liquid phase fraction ($0 \leq \partial \leq 1$) and solid and liquid PCM phase specific heat capacities (mixture average properties for eutectics), respectively, and,

$$\Delta h\left(T, T_{ref}, \partial, w_0, w_{A,c}\right) = \left(\partial + \frac{w_0}{w_{A,c}} - 1\right)\left(\Delta h_{trns,A} + \int_{T_{ref}}^{T} C_{p,l,A}dT\right) + (1-\partial)\int_{T_{ref}}^{T} C_{p,s,A}dT + \left(1 - \frac{w_0}{w_{A,c}}\right)\int_{T_{ref}}^{T} C_{p,l,B}dT \qquad (6.3)$$

w_0, $w_{\mathrm{A,c}}$, and subscripts A and B refer to the component A mixture-average mass fraction, mass fraction composition of pure species A ($0 < w_{\mathrm{A,c}} < 1$ for coordination compound A – e.g., salt hydrates, where A represents the anhydrous salt – or $w_{\mathrm{A,c}} = 1$ for single component pure PCM species A), the phase transition species and passive, single-phase species, respectively. Such a system as is represented by Eq. (6.3) has been described in the literature as a "heat of dissolution" PCM system [1].

At $T = T_{\mathrm{trns}}$ in Eq. (6.2), there is only one remaining degree of freedom, ∂, which is independent of T, but dependent only on the PCM's heat transfer history (path dependent).

In Eq. (6.3), w_0 and $w_{\mathrm{A,c}}$ are fixed, known values, ∂ and $T = T_{\mathrm{sat}}$ vary throughout the phase transition process. Utilizing the binary, equilibrium phase diagram for species A and B (see example in Figure 5-20), the Lever rule (Eq. (6.4)) can be used to express ∂ as $f(w(T_{\mathrm{sat}}))$, meaning that T_{sat} is the only remaining independent variable describing Δh of the PCM in Eq. (6.3):

$$\partial = \frac{w_{\mathrm{A,c}} - w_0}{w_{\mathrm{A,c}} - w(T_{\mathrm{sat}})} \qquad (6.4)$$

Therefore, as it is the only transient variable multiplying Δh_{trns} in both Eqs. (6.2) and (6.3), ∂ is effectively the dominant variable in determining SoC in PCM CTES and that temperature measurements in the case of PCM whose energy balances are described by Eq. (6.2) provide only limited ability to discern the PCM's SoC in actual practice.

5.4.3.2 TCM SoC

With respect to TCM, one common class of equilibrium chemical reactions can be generalized as:

$$A \cdot mB_{(\mathrm{s})\mathrm{or}(\mathrm{aq})} + nB_{(\mathrm{v})} \leftrightarrow A(m+n)B_{(\mathrm{s})\mathrm{or}(\mathrm{aq})} \qquad (6.5)$$

Species A and B form coordination compounds (e.g., hydrates or ammoniates). The contributions of latent heat in these cases come from the combination of the heat of reaction (Δh_{rxn}) and the heat of evaporation or sublimation (Δh_{vap} or Δh_{sub}) of species B, thus increasing its magnitude in comparison to the latent heat of transition for PCM. For simplicity, however, the heat of reaction (Δh_{rxn}) will be used to express the sum of both quantities, equal to the enthalpy change between the products and reactants in their indicated states of matter in Eq. (6.5).

Therefore, in the case of TCM, the relative specific enthalpy can therefore be approximated from the reaction yield of species B (θ):

$$\Delta h = \theta \Delta h_{\mathrm{rxn}} \tag{6.6}$$

and

$$\theta = \frac{\Delta[B]}{\Delta[B]_{\max}} \tag{6.7}$$

Where $\Delta[B]$ indicates the change in either concentration or partial pressure of species B and $\Delta[B]_{\max}$ indicates the maximum possible change in either the concentration or partial pressure of species B, given the constraints of the limiting reactant in the TCM CTES, assuming chemical activity coefficients equal to 1 (ideal mixture assumption). While θ can also be determined using the coordinated species in Eq. (6.5), it is often more practical to determine the concentration of species B from measurements of partial pressure (e.g., electrical capacitance).

For TCM CTES, θ is therefore the dominant variable in determining SoC.

5.5 Selected Proof of Concepts

A survey was conducted, aiming to summarize the state of knowledge on measurement techniques of material bulk response (first level - Material) as well as correlation of material bulk response with external measurements (second level - Component).

For PCM, the differentiation of material and component level is sufficient to group the information. For TCM, a more detailed approach for closed and open systems with fixed bed or transported storage material was discussed. In the following sections, a summary of selected examples in order by measurement technique - 1. Material level example**,** 2. Component level example - are reported**.**

5.5.1 Latent Thermal Energy Storage

The following sections identify the fundamental bases for SoC determination techniques practiced in the lab or by PCM TES developers that are reported in the literature, and those indicating promise for exploitation. Their advantages and limitations are also discussed.

The techniques discussed were largely focused on the correlation of a state property to the PCM phase fraction that is contrasted between the solid and liquid phases, as well as techniques derived on the basis of calorimetry to determine the system's accumulated energy.

Detailed discussions of exclusively lab-based SoC determination techniques of limited commercial applicability were not included in this report (e.g., viscosity, dielectric strength).

5.5.1.1 Acoustic Wave Amplitude Attenuation (Material Level)

Amongst the state variables examined in the literature for PCM SoC determination, one research team was found to have evaluated the ability to discern phase fraction based on acoustic wave attenuation through a lab-scale TES enclosure with internal tube coil heat exchanger [2], as seen in Figure 5-3. The proposed technique was motived by simplicity of SoC measurement configuration and use of inexpensive transducers and sensors.

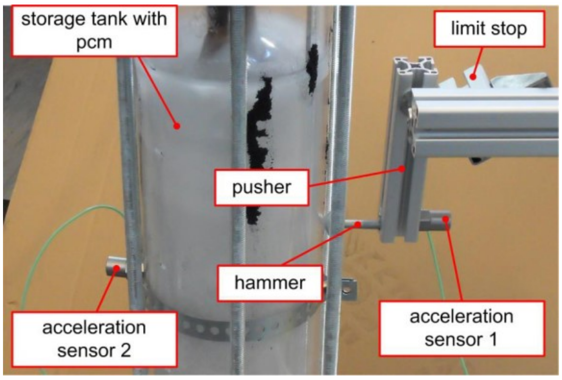


Figure 5-3. Undisclosed organic PCM (assumed paraffin) lab scale TES used to evaluate acoustic wave attenuation for SoC determination [2].

The researchers hypothesized that acoustic wave transmission through a PCM TES would predictably vary in amplitude (i.e., attenuation) at a receiver positioned on the opposite side of the PCM TES from the acoustic source in response to the PCM phase fraction. However, wave attenuation implies wave scattering/absorption, for which there are several fundamental processes and underlying causes/independent variables that risk obfuscating SoC determination, therefore making it an unreliable technique to determine SoC in a PCM TES. For example, wave scattering is a function of the signal wavelength and the population of particle sizes [3] which for PCM TES is path dependent on the heating/cooling history of the PCM, and therefore an unreliable basis to determine a system state variable such as the phase fraction. Wave scattering is an interfacial phenomenon rather than a bulk behaviour, and is therefore fundamentally unsuitable for PCM SoC determination, for which both phase fraction and particle size distribution vary independently throughout PCM TES operation, coinciding predictably only at full PCM charge (complete fusion), therefore unable to provide any reliable intermediate measurement of SoC. Wave scattering (e.g., using visible or infrared light) is employed in other measurements of relative material content (concentration, turbidity), but normally in very fine particle suspensions and colloidal mixtures wherein particle size distributions can be more easily characterized within a nominal size range.

As seen in the results obtained by the researchers in Figure 5-4, there is insufficient correlation between acoustic wave amplitude and PCM TES bulk SoC, producing even an inverse response for wave periods > 2.6 ms (< 380 Hz). There is little evidence in Figure 5-4 of a regime of gradual response in measured signal to phase fraction.

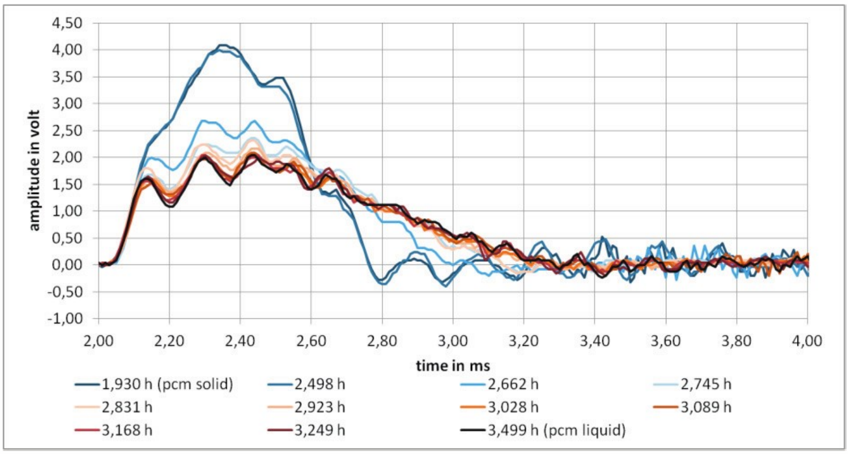


Figure 5-4. Transient response of acoustic wave attenuation, varying by source signal wave period indicated in ms [2].

While the ambition of acoustic wave attenuation for PCM SoC determination were well intentioned, the underlying principles leave too much uncertainty and path dependence to result in a reliable and predictable technique for SoC determination to warrant widespread implementation into PCM TES.

5.5.1.2 Acoustic Wave Time-of-Flight (Material Level)

In contrast to acoustic wave attenuation mentioned above, the hypothesis that acoustic wave transmission time-of-flight can be correlated reliably to PCM TES bulk phase fraction is supported by fundamental physics and material science. While this has been proposed only in the literature as a passing thought, neither a detailed treatise nor demonstration of the proof-of-concept has yet been reported in the literature. A first attempt to do so is presented here in the hope to motivate PCM researchers/developers to undertake a proof-of-concept evaluation and to report it in the literature.

At its most simple, acoustic time-of-flight can be simplified as a 1D, direct line-of-sight kinematic model as illustrated in Figure 5-5, in which there are fixed and variable material domains (vessel walls, HX, PCM liquid and PCM solid), each with their own characteristic times-of-flight and lengths, denoted t and L. In reality, however, the situation is more complex and it will be a question primarily of signal disambiguation in order to obtain the signal corresponding to the proposed simple model. The anticipated competing signals are those caused by both distinct and hybrid parallel paths with varying physical path lengths and phase fractions of PCM to those of the target direct line-of-sight as well as signal noise from internal wave reflection and signal amplitude attenuation due to both absorption/scattering. As measurements can be obtained in either of two modes (through or reflective), they each represent possible strategies of decreasing signal noise and disambiguating the desired signal path to those alternative paths mentioned here. The selection of signal frequency represents a further strategy to promote increased signal response from the desired line-of-sight path of acoustic transmission by subduing the effects of absorption/scattering as was shown in Figure 5-4. Furthermore, as time-of-flight is expected to be measured most reliably using intermittent emission pulses so that the delay between the source and the receiver can be more accurately determined, parametric variation in the durations of the on and off pulses represent an additional tool to improve the signal-to-noise relationship of this method.

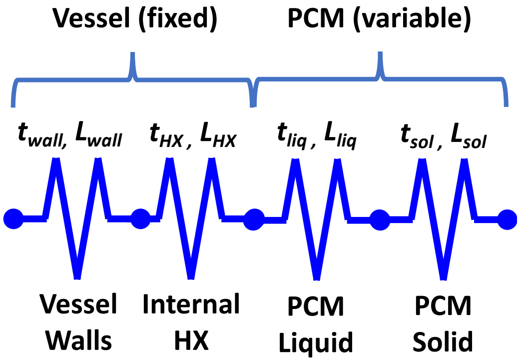


Figure 5-5. Simplified 1D kinematic model of PCM TES time-of-flight for SoC determination.

Eqs. (6.8) to (6.11) outline the simplified kinematic equations from which the volumetric phase fraction, ∂_{vol}, would be ascertained, in which v denotes the intrinsic speed of sound within each domain. Note that the spatial distribution of the PCM phases has no influence on the overall time of flight, meaning that it is inherently a bulk material response and is therefore represented only by the total relative quantities of each phase, represented by L_{liq} and L_{sol}.

$$t_{\text{total}} = t_{\text{vessel}} + t_{\text{PCM}} \tag{6.8}$$

$$t_{\mathrm{PCM}} = t_{\mathrm{sol}} + t_{\mathrm{liq}};\ t_{\mathrm{i}} = L_{\mathrm{i}}/v_{\mathrm{i}} \tag{6.9}$$

$$\partial_{\mathrm{vol}} = \frac{L_{\mathrm{liq}}}{L_{\mathrm{PCM}}};\ L_{\mathrm{PCM}} = L_{\mathrm{liq}} + L_{\mathrm{sol}} \tag{6.10}$$

$$\partial_{\mathrm{vol}} = \frac{v_{\mathrm{liq}} v_{\mathrm{sol}}}{L_{\mathrm{PCM}}(v_{\mathrm{sol}} - v_{\mathrm{liq}})} t_{\mathrm{total}} - \frac{v_{liq}(v_{\mathrm{sol}} t_{\mathrm{vessel}} + L_{\mathrm{PCM}})}{L_{\mathrm{PCM}}(v_{\mathrm{sol}} - v_{\mathrm{liq}})} = m t_{\mathrm{total}} - b \tag{6.11}$$

Examining Eq. (6.11), it can be seen that this technique has the potential advantage of a linear response of ∂_{vol}, and hence SoC, with respect to the measured t_{total} as all other quantities represent fixed physical parameters and intrinsic material properties. In fact, through suitable calibration – assuming that sufficient signal strength, low noise, and signal disambiguation are achievable and provided that $|v_{\mathrm{sol}} - v_{\mathrm{liq}}| >> 0$ – it would be possible simply to infer the linear equation parameters of fit m and b in Eq. (6.11) rather than needing to obtain these through rigorous measurements of both material properties and physical design of the PCM TES.

Figure 5-6 represents evidence that has been found in the literature to support the assumption that a sufficiently large contrast between characteristics speeds of sound in each the liquid and solid PCM phases is possible in some PCM, in particular organic PCM. Using the compressed liquid in Figure 5-6 as a simple analogue for the density difference that would be observed between liquid and solid phase PCM, a 6% difference in PCM density (typical of many PCM) can correspond to a 24% difference in their characteristic speeds of sound.

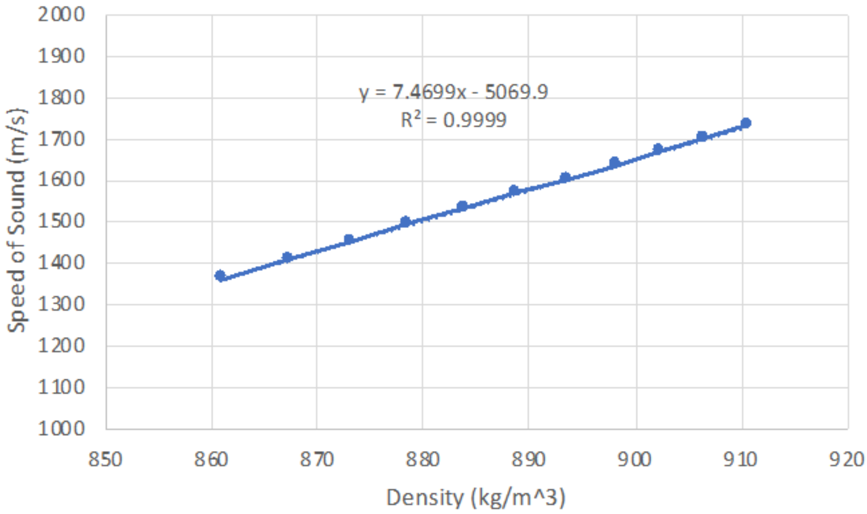


Figure 5-6. Speed of sound for compressed liquid ethyl myristate (fatty acid ester) at 293.15 K. Data from [4].

5.5.1.3 Optical (Material Level)

Conventional digital photography has been used in PCM lab evaluations to obtain detailed spatial distribution of the solid and liquid phases and tracking the shape and evolution of the two-phase interface (aka, phase front). Doing so requires a digital camera positioned from the PCM vessel within its focal range and that the PCM vessel have at least one solid wall composed of transparent material with easily removable thermal insulation. As is illustrated in Figure 5-7, this is normally performed to track the phase transition process along a vertically oriented surface that is normal to the direction of heat transfer, and therefore is best suited for both simple vessel and HX geometries. Using this technique for determination of SoC relies on assuming heat transfer symmetry along the depth axis so that a planar 2D sample can be used uniformly to represent the phase distribution within a 3D TES vessel. This technique, while very simple and spatially accurate for lab evaluations is fundamentally impractical for field operation of PCM TES and for SoC determination to be used to trigger a desired control system response. It also lacks data relating to the sensible energy content in each phase of the PCM.

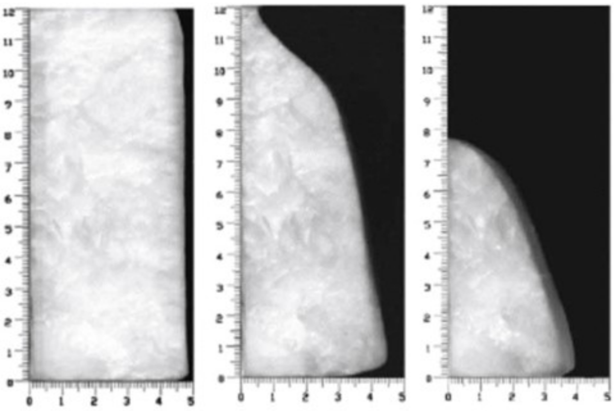

a) 10 min b) 90 min c) 170 min

Figure 5-7. Tracking dynamic changes in the phase distribution of lauric acid (dodecanoic acid) in a rectangular enclosure with a 60 ˚C heated vertical surface (right edge). Source: [5].

Optical determinations of SoC in PCM can also be accomplished using more compact equipment, such as a light source and illuminance sensor placed at opposite sides of a PCM enclosure to measure light transmission [6]. This technique, as well as the photographic technique described above, rely on a sharp contrast between either the colour or transmittance of the two PCM phases. Normally, the liquid phase will present as transparent while the solid phase presents as opaque (for crystalline solids especially).

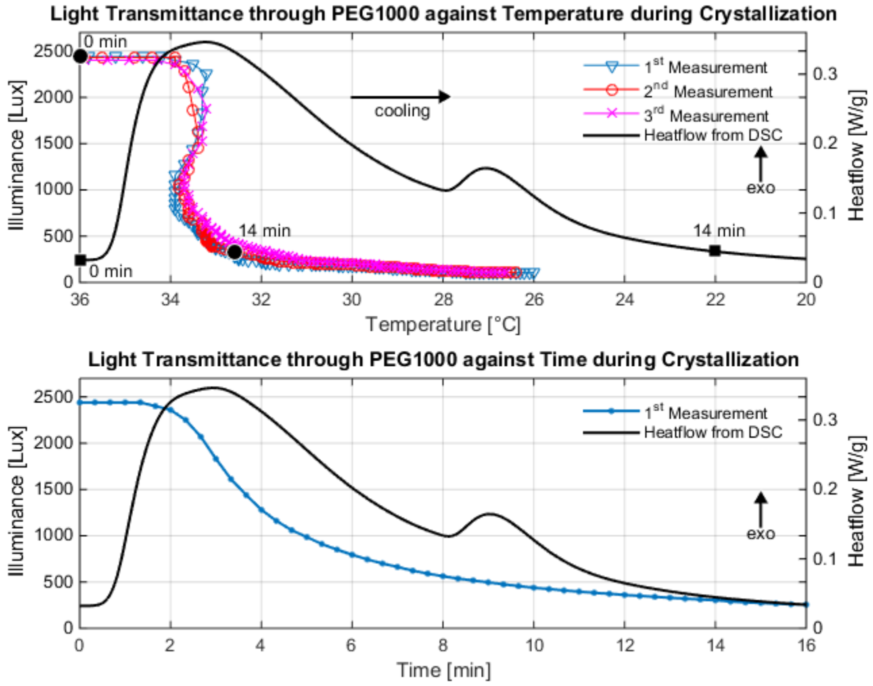


Figure 5-8. Visible light transmission measured through a sample of PEG 1000 undergoing solidification from the melt. Source: [6].

Figure 5-8 illustrates the observed step change in PCM transmittance in a solidifying sample of PEG 1000. While this technique has been shown to provide a strong, possibly linear response of light transmittance to PCM phase fraction, ∂, it suffers significantly from many barriers to practical deployment. These include issues with progressive fouling of vessel surfaces, the requirement for at least transparent sight glass openings in the vessel walls, line-of-sight between the source and sensor that is unobstructed by internal vessel features (e.g., HX surfaces, temperature probes), limited depth of PCM to allow sufficient light transmission, local SoC determination only, etc. Just as with the photographic method, this method also lacks the ability to determine the sensible heat contents of the individual phases.

5.5.1.4 Ohmic/Capacitive (Material Level)

For common PCM composed either of ionic compounds or polar organic compounds, it is expected that a step change in ohmic resistance should be observed between the solid and liquid phases due to their differences in charge mobility under the effect of external electric fields. For non-polar organic compounds, it is expected that a step change in capacitance should be observed. Such as with the optical techniques, ohmic/capacitive techniques are unable to ascertain the sensible heat contents of the liquid and solid phases but are intended to directly monitor the evolution of the local phase fraction, ∂, with reduced measurement hysteresis.

An individual PCM's material response to electric stimuli should be first ascertained to determine suitability for either ohmic or capacitive SoC determinations as well as under what conditions to obtain the largest contrast between phases. For instance, Figure 5-9 illustrates how a paraffinic PCM's ohmic response compares to that of a salt hydrate PCM. In the case of the paraffin, it was found to exhibit high ohmic resistance in both phases with very little contrast, whereas the ionic conductivity in the liquid phase of the salt hydrate increased the bulk conductivity by two orders of magnitude [7]. On the other hand, the capacitance of the paraffin, while still not exhibiting such high phase change contrast (12% diff. for RT 54HC [7]), can be at least configured practicably to generate a sufficiently strong sensor signal as opposed to what could be observed for electrical conductivity.

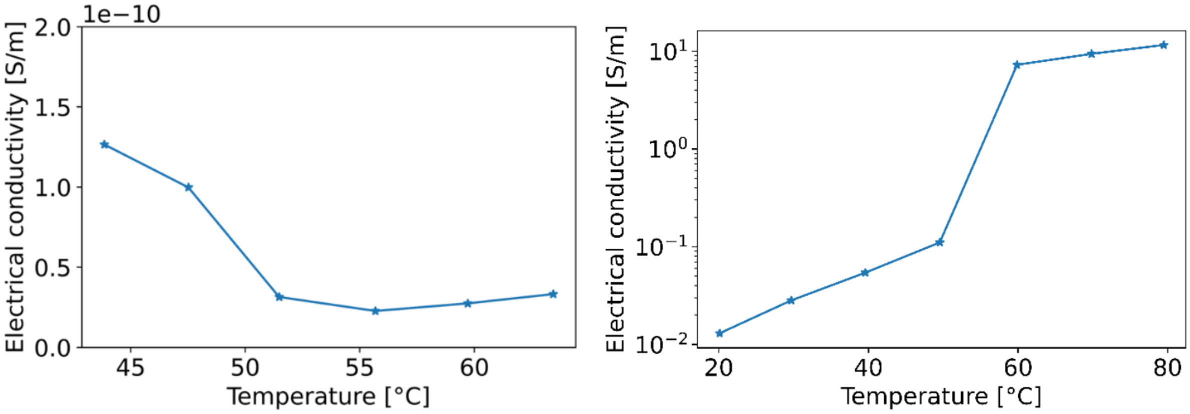


Figure 5-9. (left) Solid and liquid phase electrical conductivity measurements of Rubitherm RT 54HC paraffin mixture PCM (54 °C nominal melting temperature); (right) Solid and liquid phase electrical conductivity measurements of stoichiometric sodium acetate trihydrate ($NaC_2H_3O_2 \cdot 3H_2O$) salt hydrate PCM (58 °C peritectic transition temperature). Source: [7].

For practical implementation with PCM TES systems, capacitance measurements of organic PCM might prove useful in closely monitoring ∂ for SoC determination in thinly encapsulated PCM as the measurement cell is highly sensitive to distance separating the parallel plate electrodes. For PCM such as salt hydrates that exhibit good electrical conductivity in the liquid phase but poor conductivity in the solid phase, measurement cells for conductance/resistance are not so sensitive to electrode spacing. Also, it is presently unclear how this method would respond to the presence of metallic structures in the PCM enclosure, e.g., heat exchangers, vessel walls, sheathed temperature probes. One possibility for ease of implementation of ohmic SoC determination would be to calibrate a commonly available electrical conductivity flow meter for SoC measurement of salt hydrate phase change slurries or water-ice slurries with electrolytes dissolved in the liquid phase.

5.5.1.5 Flow Cell Measurements (Component Level): Optical, Acoustic, Ohmic

While optical, acoustic, and ohmic SoC techniques might prove difficult to implement calibrated in static PCM at the component level, they can be more easily integrated into flow cell apparatuses for PCM slurries. PCM slurries, at least anywhere a flow stream is present, must keep solidification fractions sufficiently low (e.g., < 50% mass) so as to remain fluidized for proper conveyance. As such, it is relatively simple to conceive a SoC measurement flow cell using either acoustic or electromagnetic wave techniques as it can be made compact and not be affected by heat exchanger and other equipment.

In fact, commercial equipment for each method can be readily purchased, although unlikely factory-calibrated to a particular PCM for SoC determination. Examples of off-the-shelf sensors are ultrasonic flow sensors (acoustic – SoC could be calibrated to either acoustic density or time-of-flight), electromagnetic flow sensors (ohmic – often used to measure aqueous solution concentration in flow) and turbidity sensors (optical – also already employed to measure concentration of suspended solids). Flow cell densometry, however, would prove challenging as typical equipment used for flow measurements of density do not operate well in the presence of suspended solids (e.g., Coriolis flow meters or rotameter (velocity head) coupled with a flow velocity sensor).

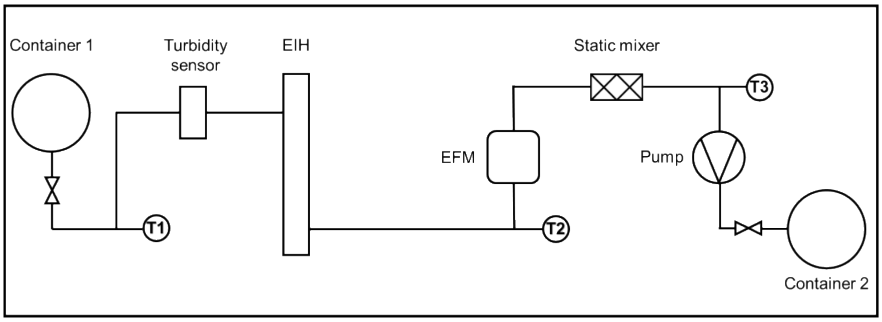


Figure 5-10. Flow diagram of the SoC-turbidity calibration test bench for $K_2HPO_4 \cdot 6H_2O$ pumped slurry by Schmit et al. (Schmit, et al., 2018). A prepared slurry was loaded into container 1 then transferred to container 2 via the turbidity sensor and temperature sensor T1, electrically heated (EIH) to full melting and slight superheating of the liquid phase, with volumetric flow rate (EFM) measured at temperature T2, with a final fully mixed flow measurement at T3. The solid fraction was determined via flow calorimetry between T3 and T1 at the flowrate measured and known fluid density $\rho = f(T)$. Source Schmit et al. [9].

Schmit et al. [8]-[9] have successfully demonstrated lab calibration of a conventional turbidity sensor[4] to a slurry of $K_2HPO_4 \cdot 6H_2O$ prepared from its stoichiometric liquid solution (Figure 5-10). For calibration (Figure 5-11), the transmission technique turbidity sensor's factory calibrated reference fluid output of concentration unit (*CU*) was correlated to the solid fraction in the stream (reducing with time due to ambient heat gain, T_{trns} = 14.3 °C for $K_2HPO_4 \cdot 6H_2O(s)$ [8]. The solid fraction in the stream was determined dynamically using flow-based calorimetry for known ΔH_{trns}, C_p of the liquid phase, and liquid phase density and volumetric flowrate measured via electromagnetic flow sensor. As seen in Figure 5-11, correlation of *CU* to %mass $K_2HPO_4 \cdot 6H_2O(s)$ was overall linear and a good match, but

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[4] Note that turbidity sensors are designed as either sensitive to very dilute suspensions (scattering technique) or for more concentrated suspensions (transmission technique) and should be selected accordingly for the anticipated concentration and size of suspended solids.

difficulties were encountered when it was ascertained that the $K_2HPO_4{\cdot}3H_2O(s)$ species was present in the feed, which presumably altered the optical response due to both its different optical properties and crystal size ($K_2HPO_4{\cdot}6H_2O(s)$ forms uniformly small crystals, <1 mm diameter, due to slow crystal growth rate). While CU was suspected to be over-represented when $K_2HPO_4{\cdot}3H_2O(s)$ crystals were present, it would also underestimate the feed solid fraction as $K_2HPO_4{\cdot}3H_2O(s)$ has a more elevated T_{trns} (~47 °C [8]) and would therefore not dissolve completely in the calibration test bench by Schmit et al. [9].

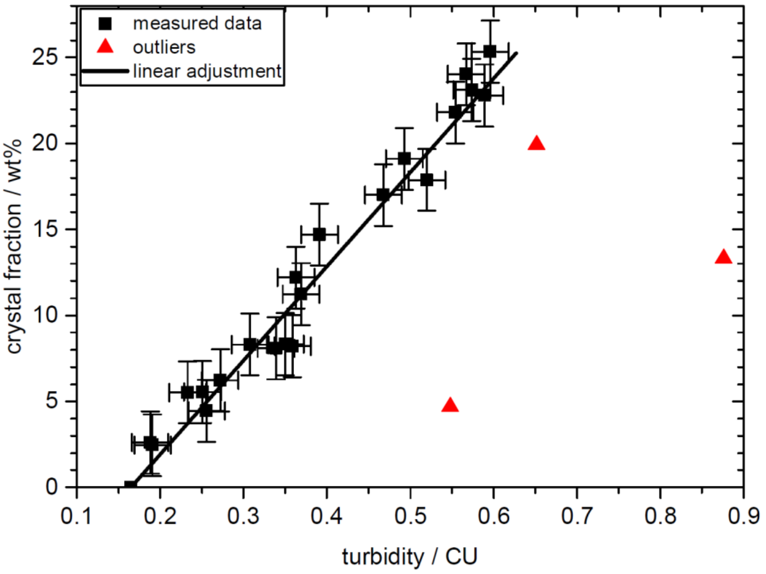
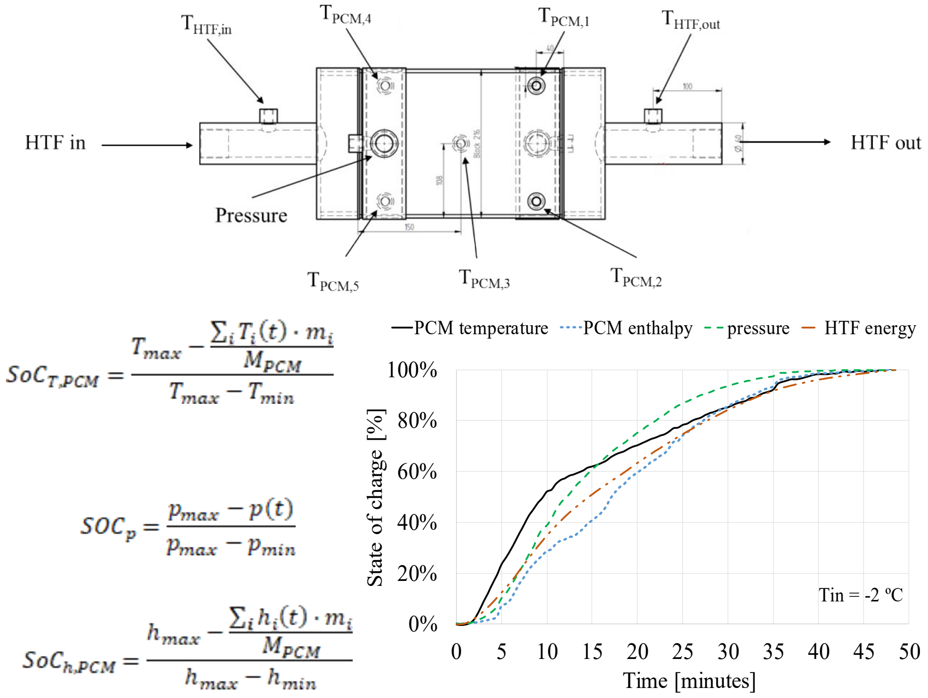


Figure 5-11. Linear calibration plot of solid fraction of $K_2HPO_4{\cdot}6H_2O$ to transmission technique turbidity measurement of concentration units (CU) factory calibrated to a reference fluid. Noted outliers were identified as suspected contamination by $K_2HPO_4{\cdot}3H_2O(s)$ in the slurry. Source: [9].

5.5.1.6 Control Volume (Component Level)

The control volume technique constitutes the method whereby most other SoC determination techniques are evaluated and calibrated (see Figure 5-12) and is fundamentally useful in black box evaluations of PCM TES. It is a fundamentally simple and robust technique from which the cumulative heat content of system can be measured using Eq. (6.12) and requires a fixed number of sensors for TES of any volume: 1x mass flow rate measurement of the HTF, 1x temperature difference measurement of the HTF inlet and outlet, 1x measurement of the PCM internal temperature in relation to external heat loss and 1x ambient temperature measurement or a surface heat flux measurement in their stead.



$$SoC_{T,PCM} = \frac{T_{max} - \frac{\sum_i T_i(t) \cdot m_i}{M_{PCM}}}{T_{max} - T_{min}}$$

$$SOC_p = \frac{p_{max} - p(t)}{p_{max} - p_{min}}$$

$$SoC_{h,PCM} = \frac{h_{max} - \frac{\sum_i h_i(t) \cdot m_i}{M_{PCM}}}{h_{max} - h_{min}}$$

Figure 5-12. Experimental PCM enclosure instrumented for the comparison of control volume SoC determination (labelled “HTF energy” in the SoC chart) to both volume-integrated temperature field (and enthalpy-weighted volume integral, $SoC_{t,PCM}$ and $SoC_{h,PCM}$ equations and labelled “PCM temperature” and “PCM enthalpy” in the SoC chart) and PCM cavity pressure (equation labelled SoC_p and “pressure” in the SoC chart). Source: (Gasia 2018).

$$SoC \;=\; \frac{\int(\dot{m}c_\mathrm{p}\Delta T_\mathrm{HTF} - UA_\mathrm{loss}\Delta T_\mathrm{amb})dt}{E_\mathrm{max}} \times 100\% \tag{6.12}$$

However, this technique does not rely on state-based determinations of phase fraction distribution or heat content of the PCM within a TES, but relies instead on a numerically integrated, pseudo-steady state series of heat transfer measurements and heat loss modelling, therefore accumulating uncertainty both with the number and duration of time intervals used for data sampling. In practical terms, this necessitates reaching a predefined, uniform, end-state at which SoC is known with certainty from state-based determinations (e.g., complete charge/discharge) and to re-initiate numerical integration of transient SoC determination only when departing once again from this uniform and certain state in order to zero the baseline transient uncertainty of the SoC determination.

As this technique is most useful to calibrate other state-based SoC techniques that are not subject to cumulative uncertainties, it is advisable to use only high accuracy temperature probes (e.g., platinum resistance temperature probes or special limit thermocouples), high accuracy thermopiles to measure HTF inlet and outlet temperature differences, and high accuracy flow meters that can readily determine mass flow rate independently of the HTF temperature. The latter is most important for the determination of SoC in smaller, lab scale PCM TES whereby small HTF flow rates and ΔT are observed. These are likely less important to cumulative uncertainties in larger PCM TES (MWh and MW scale) whereby the HTF conditions are more easily measured with greater certainty. However, which larger volumes of HTF in the TES HX when working with large PCM TES, care must also be taken to account for the portion of sensible thermal energy accumulated within the HTF in the PCM TES control volume boundaries [10].

Separately from the trappings of determining the HTF contributions to Eq. (6.12), the heat loss characteristics of the TES vessel must also be well characterized in the value of UA_loss and the basis at which ΔT_amb is determined. This is normally done by evaluating the internal temperature and sensible-only heat content of the PCM in the vessel under static-loss conditions only (zero HTF flow).

5.5.1.7 Temperature Field Mapping (Component Level)

This technique is fundamentally the simplest in its conception but can be the most costly to implement in larger TES vessels and to obtain SoC determinations with greater resolution in both space and time due to the large number of temperature sensors required. It can be regarded as a real-life implementation of the Stefan transient PCM problem, in which the phase fraction is determined from the relative amount of the domain occupied by either superheated liquid (in heating mode) or supercooled solid (in cooling mode).

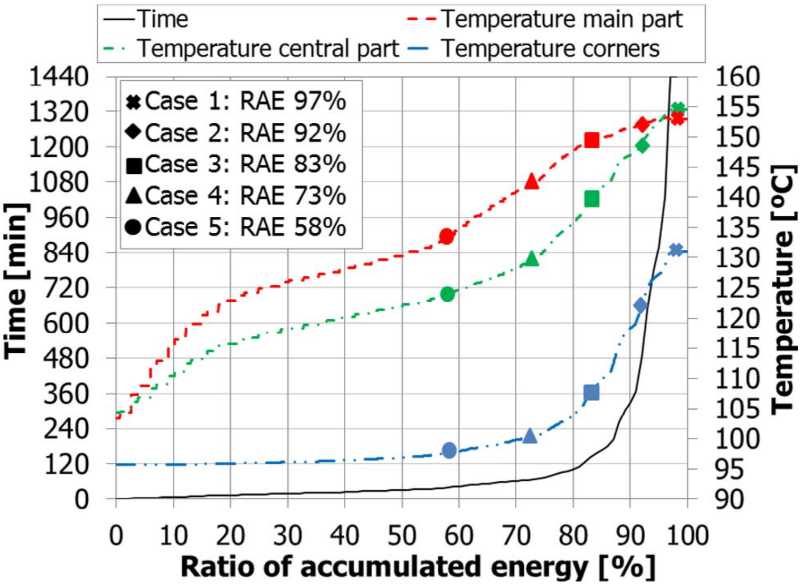


Figure 5-13. Temperature profiles at different positions inside a PCM container during melting phase. Source: (Zsembinszki 2020).

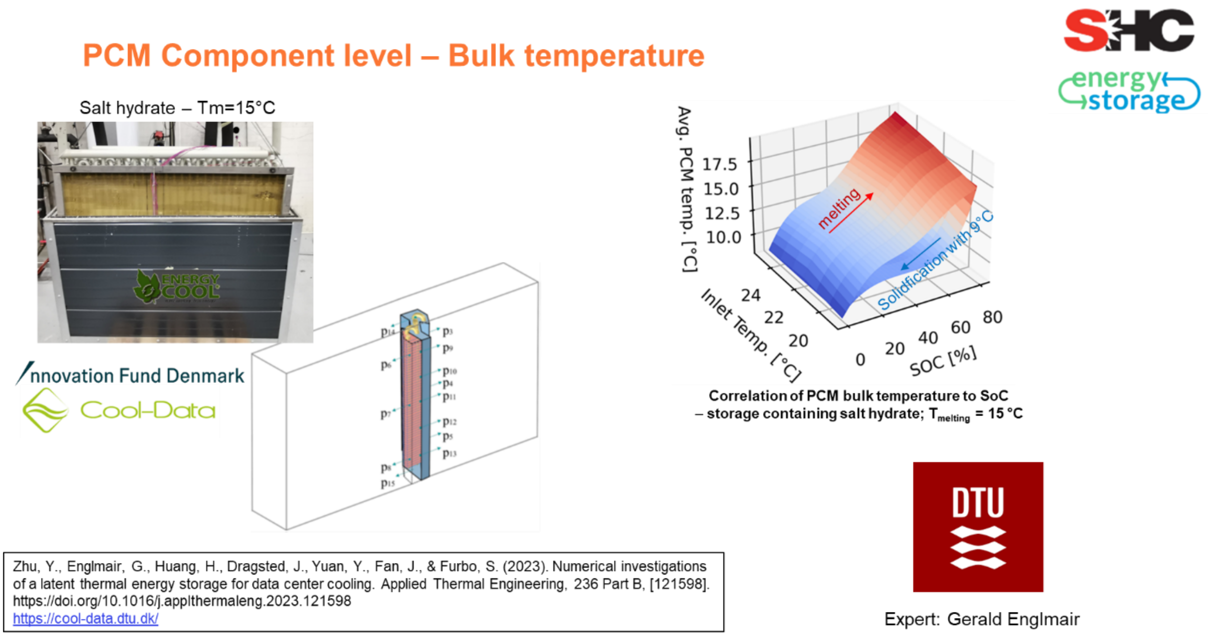
As with the Stefan problem, identifying the position of the phase boundary is the key to determining the phase distribution. To accomplish this, a spatially discretized grid of the TES vessel is devised, and temperature probes are inserted in each of these discretization nodes. This can be reduced to 1D or 2D discretization rather than a full 3D and can take advantage of axial symmetry for the PCM's transient temperature profile depending on the particulars of the geometry of the PCM domain inside the TES vessel and dominant heat exchange processes (conduction only or with convection).

The basis for SoC determination can be therefore reduced to a general equation for ∂ in the form of Eq. (6.13). Other approaches may be similarly formulated for improved correlation, e.g. $SoC_{T,PCM}$ and $SoC_{h,PCM}$ in Figure 5-12, of which $SoC_{h,PCM}$ exhibited the most favourable response at low SoC.

$$\partial = \begin{cases} \dfrac{\iiint bool(T > T_{trns})\,dV}{V_{total}} \times 100\% \\ 1 - \dfrac{\iiint bool(T < T_{trns})\,dV}{V_{total}} \times 100\% \end{cases} \qquad (6.13)$$

Figure 5-13 illustrates how individual temperature probes correlate poorly to SoC determined by the control volume method, whereas spatially integrated temperature fields, such as in Eq. (6.13), drastically improve correlation, as seen in Figure 5-12. However, as noted in Figure 5-14, such calibrations of average TES temperature can exhibit both hysteresis and shifts due to either charging, discharging, partial charge/discharge, and HTF conditions. Therefore, this technique benefits from thorough calibration of all anticipated operating conditions.

This method can work reliably during both complete and partial charge/discharge operations as the technique can always distinguish between phases either by their superheating or supercooling in reference to a phase front that is defined as a temperature gradient discontinuity within the PCM domain. In practical terms, this would mean that the phase front is situated somewhere between adjacent nodes where $T = T_{\mathrm{trns}}$ on one side and either $T < T_{\mathrm{trns}}$ or $T > T_{\mathrm{trns}}$ on the other side.



PCM Component level – Bulk temperature

Salt hydrate – Tm=15°C

Innovation Fund Denmark

Cool-Data

Correlation of PCM bulk temperature to SoC – storage containing salt hydrate; T_{melting} = 15 °C

Zhu, Y., Englmair, G., Huang, H., Dragsted, J., Yuan, Y., Fan, J., & Furbo, S. (2023). Numerical investigations of a latent thermal energy storage for data center cooling. Applied Thermal Engineering, 236 Part B, [121598]. https://doi.org/10.1016/j.applthermaleng.2023.121598
https://cool-data.dtu.dk/

Expert: Gerald Englmair

Figure 5-14. Example of PCM TES temperature field mapping of SoC, calibrated to fixed HTF inlet temperature/ flow rate. Source: [11].

As can be seen in Eq. (6.13), uncertainty in determining ∂ is affected equally by the temperature probe uncertainty to determine that $T \neq T_{\mathrm{trns}}$ and the spatial discretization of the PCM domain as the phase front constitutes a 3D surface rather than a volume. Therefore, finer discretizations more closely approximates the phase front and can better track its movements in time, whereas coarser discretizations result in sluggish transient response of determining ∂ as well as underestimation of the superheated/supercooled fractions as a larger portion of the domain is deemed ambiguously at the phase transition equilibrium condition. However, a promising compromise between coarse and fine spatial grids of temperature probes is to calibrate a transient energy model of the particular TES to only a few strategically placed probes and use this in real time to augment the spatial resolution using interpolation (Figure 5-15) [12]. This latter technique can be described as a reduction of parameters approach to temperature field mapping SoC.

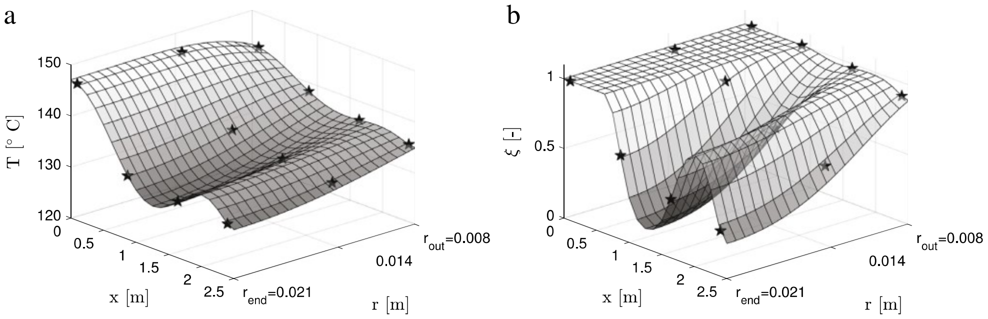
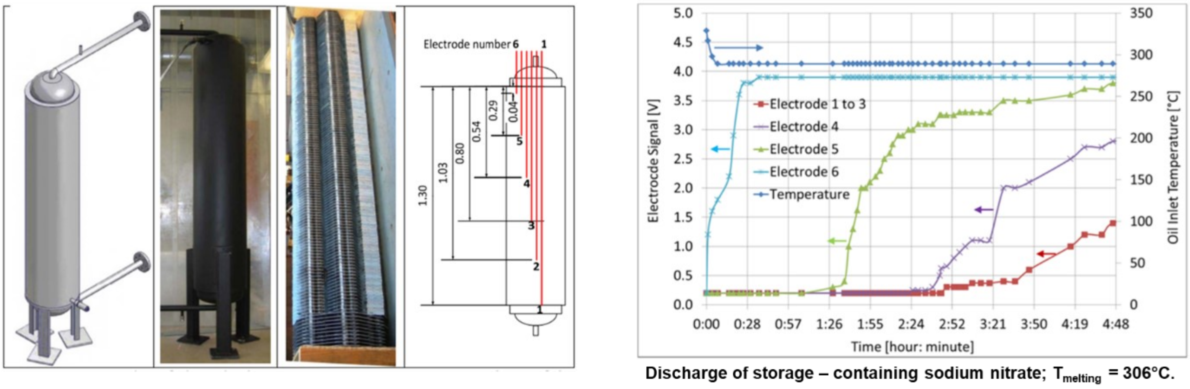


Figure 5-15. Example of calibrated PCM TES energy model interpolations of a local temperature field $T(r, x)$ (a) and corresponding local phase fraction field $\xi(r, x)$ (b) at some transient operating state of the TES. T and ξ at * denote collocation points of temperature probes. Source: [12].

5.5.1.8 Ohmic Resistance Field Mapping (Component Level)

Similarly to temperature field mapping, spatially discretized grid of ohmic resistance probes can be utilized to determine the PCM phase fraction (Figure 5-16). Just as was shown for individual temperature probes in Figure 5-13, individual electrodes in the PCM bulk do not correlate well to SoC but would instead benefit from spatial integration similar to that of Eq. (6.13). However, unlike with temperature field mapping which can be correlated to the relative enthalpy of the pure solid and liquid phases, ohmic resistance measurement provides a signal mainly of the phase fraction, and so provides SoC determination in only a narrow temperature range to T_{trns}.



Discharge of storage – containing sodium nitrate; $T_{melting}$ = 306°C.

Figure 5-16. (left) Molten salt PCM enclosure with vertically distributed electrodes; (right) transient voltage profiles from vertically distributed electrodes during PCM solidification. Source: [13].

While not reported in the literature, it is possible that one strength of ohmic resistance field mapping in comparison to temperature field mapping could be its reduced hysteresis during charge/discharge operations, as ohmic resistance directly measures the local phase fraction, which temperature probes cannot.

5.5.1.9 Cover Gas Pressure Measurement (Component Level)

Measurements of the cover gas pressure in the space above the PCM in a fixed volume TES holds promise in determining the bulk, average, phase fraction, and overall SoC (Figure 5-12) using only one pressure cell and one temperature probe (used to compensate the temperature effect on cover gas volume).

Naturally, the cover gas above a PCM in a fixed volume TES acts as a direct analogue to the bulk volume expansion/contraction of the PCM [14] and can be determined via either ideal gas approximations or more rigorous, real gas models of state. For practical considerations, the effect of PCM vapour pressure must be accounted in the volumetric determination of the cover gas, especially when using salt hydrate PCM and when operating PCM TES at higher degrees of PCM liquid superheating. Other effects, such as cavity formation inside the PCM solid, may lead to increased uncertainty in correlating the cover gas volume with the bulk PCM volume, arising as hysteresis between charging and discharging operations (Figure 5-17).

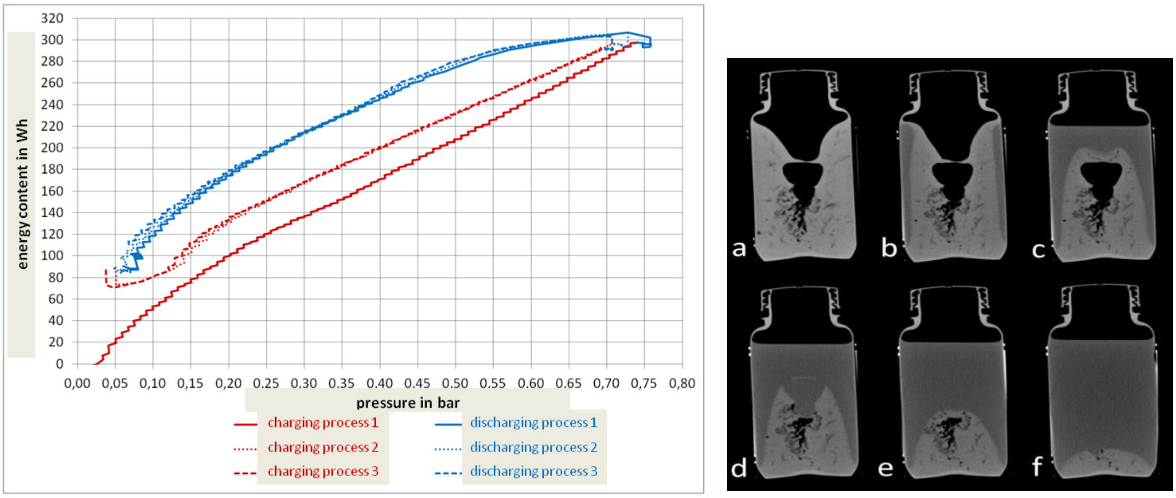


Figure 5-17. (left) PCM cavity pressure profiles during sequential melting (red) and solidification (blue) cycles; (right) CT scan cross section images of the PCM during melting (a to f). Source: [2].

5.5.1.10 Binary Mixture Solubility (Component Level)

As described in Eqs. (6.3) and (6.4) in Section 5.4.3.1, the SoC of binary PCM operating both within the liquidus dome and in the superheated liquid region above it can be described accurately using temperature alone. This technique has been developed and deployed in pre-commercial field prototype PCM CTES by Louis Desgrosseilliers at Neothermal Energy Storage Inc. in Canada [15] at TRL 7. The PCM in question is a 1:1 molar mixture of sodium acetate trihydrate (SAT, 136 g/mol, $NaC_2H_3O_2{\cdot}3H_2O$) and DI water, corresponding therefore to an average CTES sodium acetate (82 g/mol) mass fraction of $w_0 = 0.532$. The SAT compound corresponds to $w_{A,c} = 0.603$.

Using both the detailed binary phase equilibrium data for water-sodium acetate anhydride in Figure 5-20 and detailed thermodynamic modelling described in both [16] and [17], the technique used by Neothermal results in a system of equations (Eqs. (6.14)-(6.19)) able to generate the continuous relationship correlating the PCM's Δh to T in the range -18 ˚C < $T \leq$ 105 ˚C in Figure 5-18. Such a relationship can be implemented either as a set of equations for each of the three states represented (phase change, superheated liquid, supercooled liquid) or as a set of three Δh vs. T look-up tables.

$$H_{SAT(aq)}(T) = 1.56\left(T - T_{ref}\right)\frac{\mathrm{kJ}}{\mathrm{kg\ K}} + \frac{4.27}{2}\times 10^{-3}\left(T^2 - T_{ref}^2\right)\frac{\mathrm{kJ}}{\mathrm{kg\ K^2}} + 284\,\frac{\mathrm{kJ}}{\mathrm{kg}} \tag{6.14}$$

$$H_{SAT(s)}(T) = 0.811\left(T - T_{ref}\right)\frac{\mathrm{kJ}}{\mathrm{kg\ K}} + \frac{4.06}{2}\times 10^{-3}\left(T^2 - T_{ref}^2\right)\frac{\mathrm{kJ}}{\mathrm{kg\ K^2}} \tag{6.15}$$

$$H_w(T) = 4.18\frac{\mathrm{kJ}}{\mathrm{kg\ K}}\left(T - T_{ref}\right) \tag{6.16}$$

$$H(T) = w_w H_w(T) + (1 - w_w - w_s)H_{SAT(aq)}(T) + w_s H_{SAT(s)}(T) \tag{6.17}$$

$$T_{liq} = 1368.4w_{SA}^3 - 2412w_{SA}^2 + 1459.9w_{SA} - 244.3 \tag{6.18}$$

$$w_s = \frac{0.532 - w_{SA,liq}}{0.603 - w_{SA,liq}} \tag{6.19}$$

Where subscripts SA, SAT, s, liq, and w refer to quantities belonging to anhydrous sodium acetate, sodium acetate trihydrate, SAT solid phase, saturated liquid phase, and excess liquid water only (water not belonging to SAT's water of hydration), respectively. Note that Eqs. (6.18) and (6.19) apply only for $0.233 \leq w_{SA,liq} \leq 0.580$ and that $w_s = 0$ for both the superheated and supercooled liquid states. While the superheated liquid state can be easily ascertained from the current PCM temperature, the presence of the supercooled liquid state vs. the phase change equilibrium state for $T \leq 55$ ˚C can be ascertained only knowing the PCM's nucleation history (either triggered or autonucleation-induced). Consequently, this technique is especially useful in representing the SoC of supercooling binary, heat of dissolution PCM.

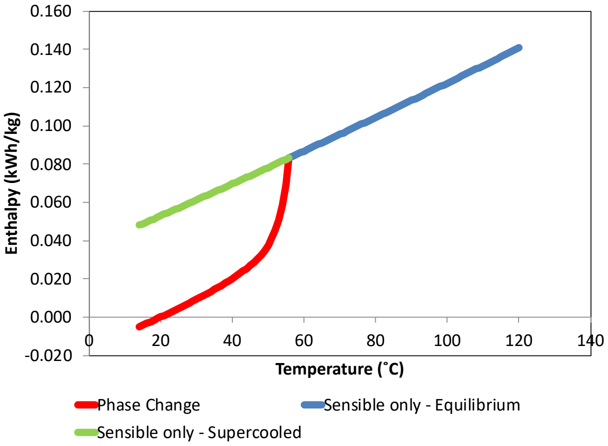


Figure 5-18. Δ*h* vs. *T* profile for $w_0 = 0.532$ sodium acetate and water binary PCM in three separate states: 1) superheated liquid (sensible only - equilibrium), 2) phase change, and 3) supercooled/supersaturated liquid (sensible only - supercooled). Reproduced with permission from © Neothermal.

Applications of this technique can be performed using very few temperature sensors submerged in the PCM. Neothermal has utilized as few as one sensor to approximate bulk PCM SoC in CTES vessels containing 30-60 kg of PCM, with the sensor situated at the bottom of the CTES vessel and positioned farthest away from the heat exchanger surfaces. While the approach of using only one sensor ignores both temperature and concentration gradients that develop within the PCM CTES during operation, it has been found to be an adequate proxy for bulk SoC for PCM CTES both with slow dynamic response (pseudo steady-state assumption) and small heat diffusion path length from the heat exchange surface into the full depth of the PCM (lumped capacitance assumption). Such an approach would be suitable to coarsely determine the bulk average PCM CTES SoC (e.g., SoC = {0%, 25%, 50%, 75%, 100%}). Figure 5-19 illustrates the comparison between the single temperature probe approach used by Neothermal in field CTES residential HVAC prototype systems during charging operations (electric resistance heat source) and an analytical model of lumped capacitance, constant heat input rate and constant UA static heat loss. Only minor differences arose due to lumped capacitance model not representing the higher salt concentration local to the temperature probe at the bottom of the CTES vessel that developed and stabilized in the field CTES over repeated cycles (resulting in higher liquidus temperatures, ≤58˚C rather than ≤55˚C), as well as due to the pseudo-steady state model neglecting the heat transfer fluid circuit's high temperature limit control heater on/off cycling by modelling the joule heat input source as remaining always constant.

When using only one temperature sensor to determine SoC using this technique, it must be noted that sound engineering judgement must be exercised in order to select the most appropriate location of the probe. This will also depend on the intended electronic control actions triggered by SoC signals. For instance, the rational for placing a lone temperature sensor at the bottom of a PCM CTES vessel farthest away from heat exchanger surfaces is to determine the end-of-charge state of the CTES with certainty. However, once the PCM is solidified, the ability to accurately determine the end-of-discharge would require additional control system calibration due to the CTES typically favouring residual charge to remain at higher elevations if the heat transfer fluid path in the heat exchanger is arranged counter-current to the bottom-up positive temperature gradient in the PCM. Additionally, a second sensor can be included at a higher elevation as a low-cost solution to accurately determining both the CTES end-of-charge and end-of-discharge states.

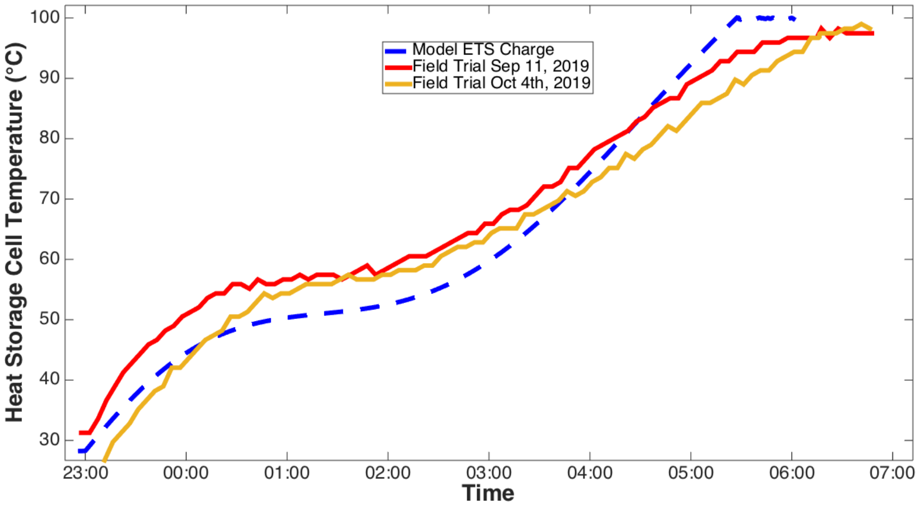


Figure 5-19. Comparison between lumped capacitance, constant heat input rate and constant UA static heat loss model and Neothermal PCM CTES prototype HVAC system field data using only a single temperature probe situated at the bottom of a 30 kg PCM CTES vessel [15]. Reproduced with permission from © Neothermal.

Certainly, this method can be applied also using an array of temperature sensors able to provide a spatially averaged value of the PCM CTES SoC. In these instances, knowledge of the PCM volume allocations and local concentration in proximity to each probe will be required to correctly allocate mass-weightings to the bulk average PCM SoC. Fortunately for PCM CTES systems that utilize supercooling and triggered nucleation, the pre/post nucleation temperature at each probe location can be used to analytically infer the local concentration of the active phase changing PCM component using Eqs. (6.14)-(6.19) to solve $\Delta h_{pre} = \Delta h_{post}$, as nucleation from a supercooled medium occurs very quickly and can thus be treated as instantaneous and therefore, isenthalpic.

The accuracy of the bulk material response as it relates to determining SoC using this method is dependent on the steepness of the Δh vs. T slope in the phase change region nearing T_{trns}[5], temperature probe uncertainty, the uncertainty of the thermodynamic properties used in Eqs. (6.14)-(6.16), and the uncertainty in either measuring the loaded mass of PCM in the CTES or calculating the local concentration using the inference technique described in the paragraph above for pre/post nucleation events form a supercooled liquid state. Generally, the temperature probes represent the largest of these uncertainties, which is further enhanced by the propagation of model uncertainty in the steep slope of the phase change region Δh vs. T profile. For the SAT + water PCM

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[5] The steepness of this slope is affected most strongly by both the magnitude of Δh_{trns} and w_0 as well as the degree of flatness of the slope of T_{liq} as it approaches $w_{A,c}$.

CTES used by Neothermal (w_0 = 0.532), quantifying SoC in the range 20 ˚C ≤ T ≤ 100 ˚C using thermocouple probes with +/- 1.0 ˚C uncertainty results in ≤ 1% uncertainty in SoC for 20 ˚C ≤ T ≤ 40 ˚C and 55 ˚C < T ≤ 100 ˚C and ≤ 10% uncertainty in SoC for 40 ˚C ≤ T ≤ 55 ˚C.

This technique is suitable for any bulk quantity of binary, liquidus PCM > 0.1 kg, with the number of temperature probes required a function only of the engineering requirements of the PCM CTES (bulk-average SoC accuracy, end-of-charge and end-of-discharge detection, supercooling threshold detection, etc). Careful engineering judgement must also be applied in the selection of the temperature probe materials of construction for fitness of service (temperature, pressure, corrosion), style (thermowell, sheathed probe, encapsulated probe), underlying physics (RTD, thermistor, thermocouple), and measurement uncertainty.

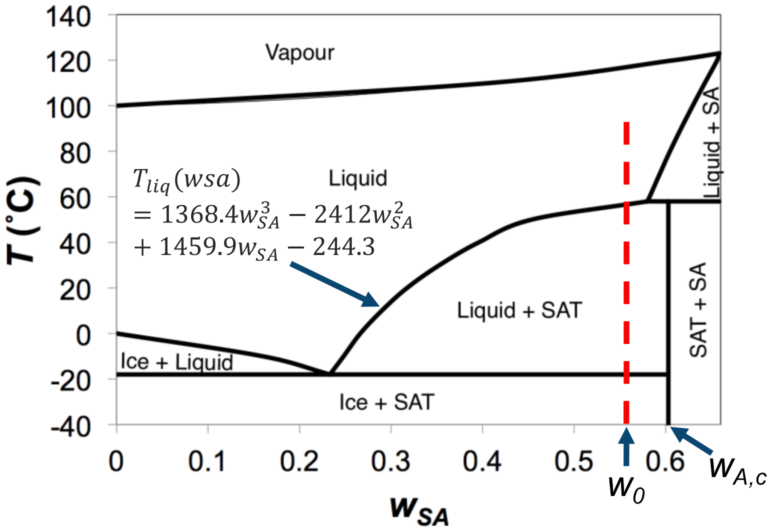


Figure 5-20. Partial binary phase equilibrium diagram for water and sodium acetate (SA), forming the coordination compound sodium acetate trihydrate (SAT) at w_{SA} = 0.603 ($w_{A,c}$). A binary PCM representative of the thermal balance in Eq. (6.3) can be represented by a PCM system with a total mixture mass fraction denoted by w0. Data from: (Green, 1908).

5.5.2 Thermochemical Energy Storage

The lack of linear relationships between temperature and enthalpy of thermochemical materials means that state of charge determination methods require different approaches. As a result, therehas been a significant number of research groups working to develop a SoC determination method for TCM storage systems. The most popular type of TCM that are being researched are water vapour sorption materials like zeolites or salt hydrates and as such there exist some methods to determine SoC for ammoniacates and absorption systems. In the following sections the primary methods of SoC determination for absorption systems are briefly discussed. Table 5-3 and Table 5-4 give an overview of the groups that have worked on developing these different methods.

Table 5-3: TCM SoC Experimental principles and the institutes that apply them.

Method	Institutes
Mass measurement	AEE INTEC, FHOÖ, LBNL, CNR-ITAE
Volume measurement	HSLU, NRCan, TNO
Enthalpy balance	Swansea, FHOÖ, NRCan, CNR, TNO
Temperature and vapour pressure	TNO, UBir,
Electric capacity	FHOÖ, Swansea
Spectroscopic measurement	TUW

Table 5-4: List of contributing institutions and their abbreviations.

Institute	Full name	Location
AEE INTEC	AEE Institute for sustainable technologies	Gleisdorf, Austria
Swansea	University of Swansea	Swansea, United Kingdom
UBir	University of Birmingham	Birmingham, United Kingdom
HSLU	University of applied sciences, Lucerne	Lucerne, Switzerland
TNO	Netherlands Organisation for Applied Scientific Research	The Hague, Netherlands
FHOÖ	University of applied sciences Upper Austria	Wels, Austria
TUW	Technical University Vienna	Vienna, Austria
NRCan	Natural Resources Canada CanmetENERGY-Ottawa	Ottawa, Canada
CNR-ITAE	Consiglio Nazionale delle Richerche - Institute for Advanced Energy Technologies	Messina, Italy
LBNL	Lawrence Berkeley National Laboratory	Berkeley, USA

5.5.2.1 Mass measurement

The uptake of sorbate can be determined by weighing the container for the sorbate or the storage with the storage material, or both. This way, the uptake of sorbate by the sorption material can be tracked and the state of charge calculated using the total mass of desorbed material and the enthalpy curve of the material. The design of the mass measuring system must ensure that no other forces than gravity apply to the balance. The primary source of an external force that could affect measurements is the thermal expansion during heating or cooling of components that are connected both to the parts on the balance and to the floor. This source of error does not apply when the material chamber can be disconnected, making it possible to weigh the sorbate before and after the experiment. However, this method of measurement does not give insight into the development of the SoC, nor will it likely be applicable to commercial systems.

5.5.2.2 Liquid volume measurements

Monitoring the changes in the level of water inside a TCM storage can be used to directly measure how much water has been absorbed or desorbed from a known reference starting point. The reference measurement produces the relation between the amount of water in the container and the average state of charge of the active material in the system while considering possible residual water or water vapour in other parts of the system. The reference curve can be used to calculate the current water load to determine the SoC.

The water level can be measured either by using a float, or measuring the pressure at the bottom of the vessel and using a pre-determined relation between pressure and water level.

It is possible to determine the water load of a TCM by using predetermined isotherm curves of vapour pressure vs. water load. The maximum and minimum values of water load can be compared to the current water load to determine the SoC. Using this method, if there is residual water or water vapour in different parts (e.g. piping) of the storage system it can cause inaccuracy in determining the SoC. Additional knowledge of the amounts of residual water and/or water vapour will help to increase the accuracy of the SoC determination.

Figure 5-21. Demonstration set-up of a sodium hydroxide closed absorption system at EMPA, Switzerland.

Volume measurement for SoC determination can also be used in absorption systems, as in these types of systems both charged and discharged storage material are liquids. Aqueous sodium hydroxide heat storage system, an example as shown in Figure 5-21, is designed as a closed system consisting of a heat and mass exchanger with two tanks containing the charged and discharged sodium hydroxide and water. The volume can be determined by measuring the liquid level in the tank containing the concentrated sorbent which can directly be used to indicate the state of charge.

5.5.2.3 Enthalpy balance measurement

One method of determining state of charge is to consider a control volume around the TES where heat added to the control volume leads to a higher state of charge, and heat removal leads to a lower SoC. The measurement of the heat flow is commonly calculated by measuring the volumetric or mass flow rate and temperature difference of inlet and outlet of the heat transfer fluid. The accuracy of this method of SoC determination depends on the reference state of charge and on the heat losses of the TES. Determining an accurate reference state of charge requires a system control strategy that ensures the TES returns to a minimal SoC. This is typically accomplished by removing heat from the TES over a long timeframe, often until the outlet temperature change is below a minimum threshold. To account for challenges introduced by heat losses from the TES, the heat loss rate usually must be pre-determined, typically as a function of the temperature. The effect of the heat losses on the SoC then can be calculated if the temperature history of the TES is known.

5.5.2.4 Temperature and vapour pressure

The relation between temperature and vapour pressure of a sorption material can be used to determine the SoC of a storage. This relation is an equilibrium-state property, which means that it can only be used if all storage material in the storage volume is at equilibrium. This method can be challenging to use since it cannot be used at times of charging of discharging. Additionally, the time needed to arrive at an equilibrium state and the relationship between temperature and vapour pressure (*p*-*T* diagrams) must be known.

5.5.2.5 Capacitive sensor (material level)

In sorption materials, the SoC is directly related to the amount of sorbate that is taken up by the sorbent. If the relative amount of sorbate in a volume of material can be determined, the amount of material taken up can be calculated and the SoC determined.

If the sorption material is a dielectric material, the uptake of sorbate will change the dielectric properties (the permittivity) which can be measured with the capacitive method.

For the adsorption of water in zeolite, this method has been applied by several institutes:

The Applied University of Upper Austria has determined the relative permittivity of three zeolites as a function of the relative water content of the zeolite as shown in Figure 5-22. A clear consistent dependence of the permittivity on the water content can be determined.

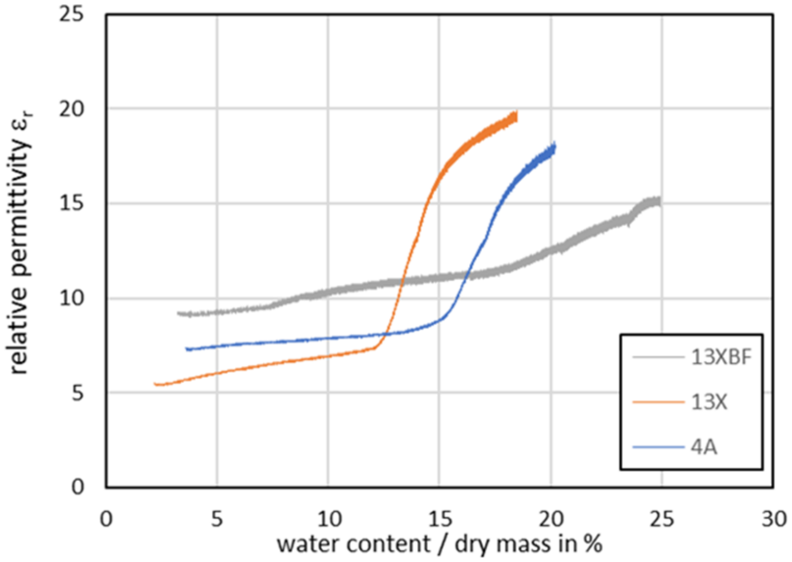


Figure 5-22. The relative permittivity as a function of the relative water content of three different zeolites.

This method has been developed and tested for an open sorption rotating reactor. The capacitance sensor consists of two small parallel plates of aluminum which forms a capacitor as shown in Figure 5-23. The capacitance of the device is determined by the amount of water around the plates. The resonance frequency in an oscillatory circuit depends on the capacitance which relates to the water content of the material.

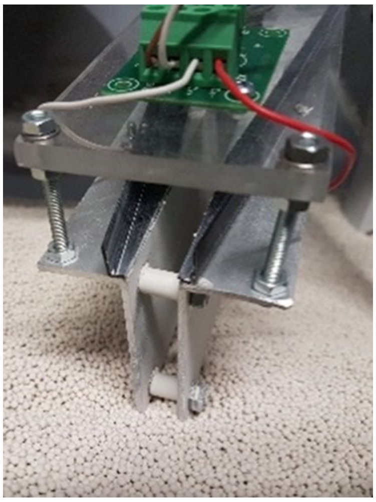


Figure 5-23. A capacity sensor which consists of two parallel aluminum plates. Resonant frequencies are near 200 kHz.

Water content is the most significant variable for frequencies on the order of 200 kHz. When higher frequencies on the order of 2 MHz are used, capacitance becomes strongly dependent on temperature. This requires a separate temperature measurement to determine water content. This effect is particularly relevant for cylindrical capacitance sensors as shown in Figure 5-24.

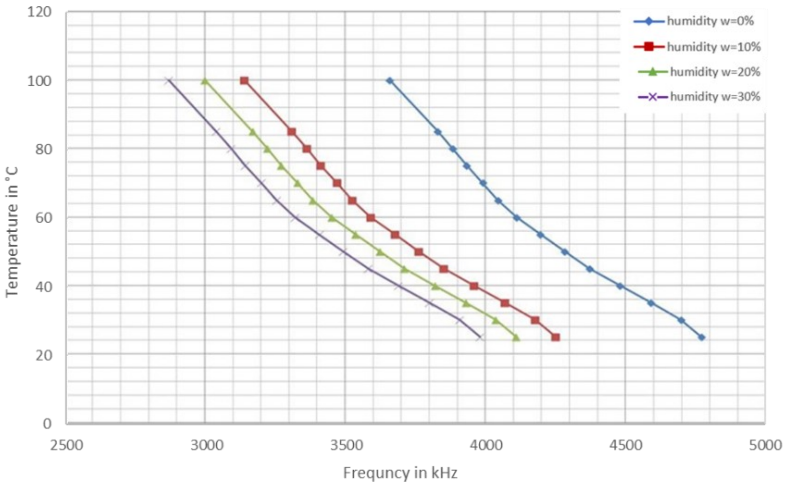


Figure 5-24. Resonance frequencies of zeolite 13XBF determined for different humidity levels and temperatures.

5.5.2.6 Measurement of light absorption spectra

Copper salts such as copper chloride and copper sulphate $CuSO_4$ absorb ammonia when undergoing an enthalpy change which causes the material to change in colour from white to blue. By measuring the reflectance of the material in the blue part of the spectrum the state of charge of the salt can be identified. An example of the change in spectra between uncharged and charged salt is shown in Figure 5-25. These spectra have been determined by in situ monitoring the diffuse reflection of a copper chloride powder sample using a UV-VIS-NIR spectrometer. A flow of inert gas and ammonia as well as temperature and pressure control of the sample is required.

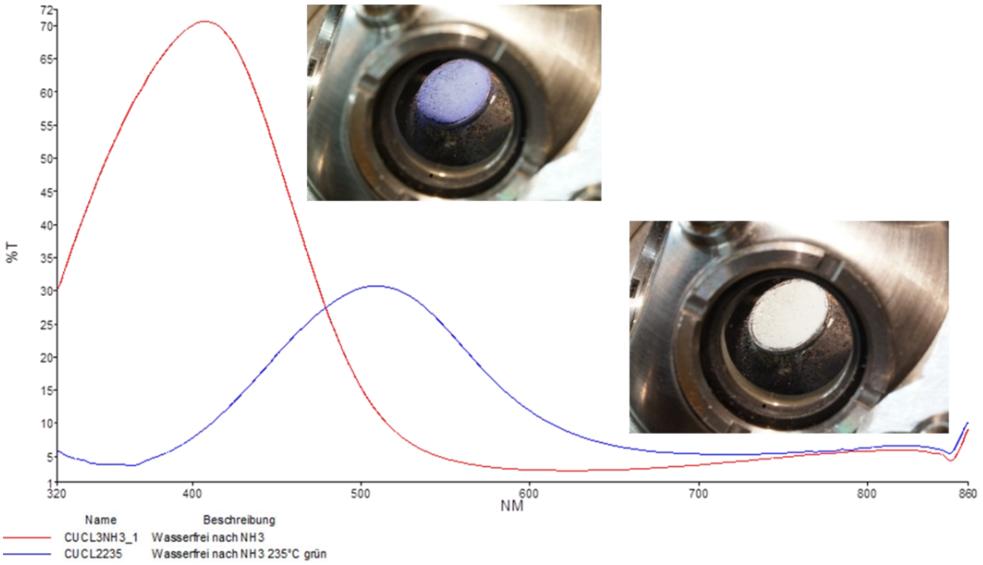


Figure 5-25. Spectral comparison of solid $CuCl_2$ (blue line) and solid $CuCl_2 \cdot xNH_3$ (red line) Measured in diffuse reflectance with a Perkin-Elmer Lambda 900 UV-vis-NIR spectrometer.

5.6 System Application

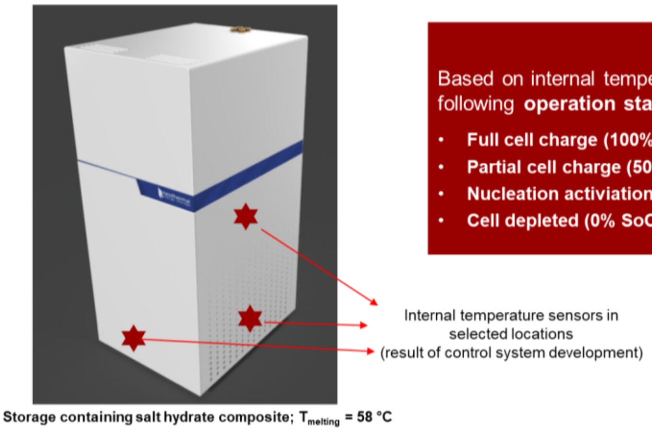
This activity aimed to summarize the state of knowledge on material bulk response (first level - Material) linked system control requirements (third level).

As outlined by expert pitch presentations, direct interaction of material bulk response (e.g. local temperature measurements in characteristic storage locations) with the control system can be found in prototype systems. Case descriptions were collected - including information on the calibrated correlation of material bulk response with external (e.g. heat flux) measurements. In this context, the following key question was addressed: *What are the main (limiting) threshold values regarding system functionality?*

A description of four examples (a-d) of material bulk response to system controls can be found here:

a) Local PCM temperature measurements interacting with heating system controls

Neothermal runs its PCM storage based on local measurements of the PCM (Sodium Acetate Trihydrate). The exact sensor placement of internal sensors as well as temperature threshold values are a result of experimental development and calibration of the controls with the aim to provide a more efficient heating systems in domestic households. Figure 5-26 gives an overview description of the setup.



Storage containing salt hydrate composite; $T_{melting}$ = 58 °C

Based on internal temperature distribution, the following **operation states** are determined:

- **Full cell charge (100% SoC)**
- **Partial cell charge (50-100% SoC)**
- **Nucleation activiation required (≤ 50%)**
- **Cell depleted (0% SoC)**

Utilizing stable supercooling of Sodium Acetate Trihydrate

Source: Neothermal energy storage Inc.; Further information available at https://neothermal.ca/

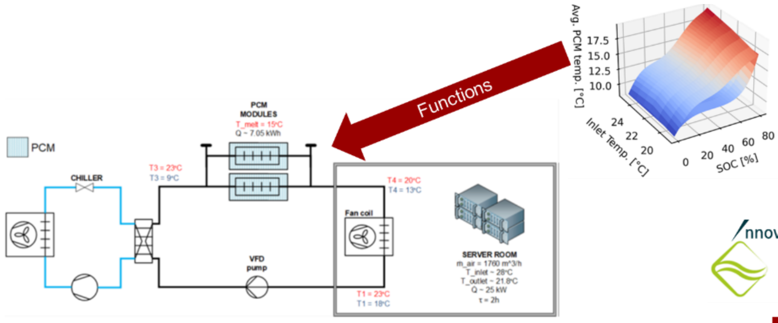
neothermal energy storage

Expert: Louis Desgrosseillers

Figure 5-26. Neothermal Energy Storag Inc: PCM heat storage control based on SoC determination.

b) PCM bulk temperature measurements for development of a “virtual storage”

In the “Cool-Data” research project at DTU, the development of PCM bulk temperature measurements was measured during various charge and discharge cycles - variation flow rates and temperatures of the heat transfer fluid. The data was then applied to form a data-driven PCM storage model in Python. Interlinked to a Modelica model of a server room cooling system, the data-driven storage model served for identifying optimal system configuration and controls. Figure 5-27 illustrates the chosen approach – further information can be found in the mentioned publication.



Server room cooling model to develop a predictive system control algorithm

Zhu, Y., Englmair, G., Huang, H., Dragsted, J., Yuan, Y., Fan, J., & Furbo, S. (2023). Numerical investigations of a latent thermal energy storage for data center cooling. Applied Thermal Engineering, 236 Part B, [121598]. https://doi.org/10.1016/j.applthermaleng.2023.121598
https://cool-data.dtu.dk/

Innovation Fund Denmark
Cool-Data

DTU

Expert: Gerald Englmair

Figure 5-27. Technical University of Denmark: Application of data-driven PCM cold storage model for system optimization.

c) SoC determination enabling ancillary services

Latent Thermal Energy Storage with Phase Change Materials can serve as an asset for flexible heating & cooling supply for buildings as well as for industry. State-of-charge (SoC) detection, i.e., a determination of the remaining capacity available in a thermal energy storage, is crucial for optimized storage operation schedulers and allow a precise thermal power control. Thus, the integration of instant and reliable technique for determining the SoC and a precise TPC in a model predictive control (MPC) system would pave the way for optimal operation of grids coupling different energy sectors – including power-to-heat and waste heat utilization from industry. Figure 5-28 illustrates the interaction of both thermal end electrical grids via a heat storage-heat pump unit.

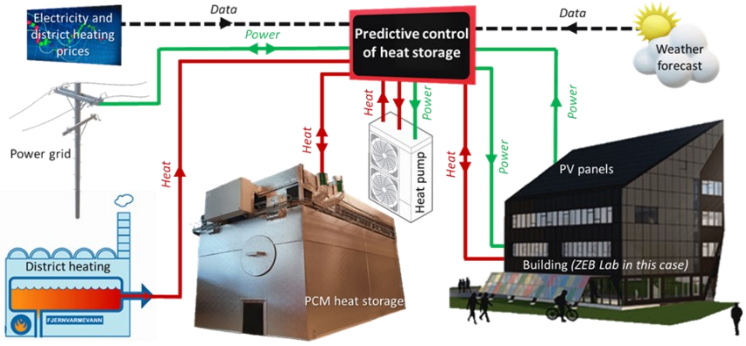


Figure 5-28. SINTEF Energy: Illustration of PCM heat storage implementation for more flexible operation of thermal and electrical grids Source: https://www.sintef.no/en/projects/2021/presav-prediktive-styringsstrategier-til-aktiv-varmelagring-i-zeb-laboratoriet/.

d) Operation of solar heating and cooling system with latent heat storage

At DTU, a segmented heat storage prototype with four flat PCM units, containing 150 L of different SAT composites each and a 735 L water tank was built. Stable supercooling of SAT was utilized. Functionality tests with an evacuated tubular collector array proved combined short and long-term heat storage by PCM units. The prototype was implemented in a solar combi-system with 22.4 m^2 (aperture) evacuated tubular collectors. It was demonstrated with SH and DHW demand patterns of a 130 m^2 Passive House in Danish climate. A strategy for charging and discharging of water tank and PCM units was developed. Automated operation was realized by a monitoring system and a control program. Local PCM temperature measurements served for system controls.

Englmair, G., Moser, C., Furbo, S., Dannemand, M., & Fan, J. (2018). Design and functionality of a segmented heat-storage prototype utilizing stable supercooling of sodium acetate trihydrate in a solar heating system. APPLIED ENERGY, 221, 522-534. https://doi.org/10.1016/j.apenergy.2018.03.124

Englmair, G., Moser, C., Schranzhofer, H., Fan, J., & Furbo, S. (2019). A solar combi-system utilizing stable supercooling of sodium acetate trihydrate for heat storage: Numerical performance investigation. APPLIED ENERGY, 242, 1108-1120. https://doi.org/10.1016/j.apenergy.2019.03.125

At ZAE Bayern, local PCM temperature measurements were utilized for control of a solar heating and cooling systems utilizing an absorption chiller and latent heat storage. Tracking the temperature of PCM in identified (experiment) location as input parameter for the system controller. For further information:

Helm M., Hagel K. Hiebler S. Schweigler C., „Solar heating and cooling with absorption chiller and latent heat storage", part of book: "Thermally driven heat pumps for heating and cooling", Ed. Annett Kühn, Universitätsverlag TU Berlin, 2013. ISBN 978-3-7983-2596-8.

5.7 Conclusions

State of charge determination utilizes measurement techniques of material bulk response. While measurement techniques are subject to material science, state of charge is a component level property (analogy: electrical battery). In flexible heating and cooling systems "thermal batteries" are needed: Thermal Energy Storage with instantaneous State of Charge determination.

The SoC of a thermal energy storage system is not just about the interaction between material and the component. Rather, how they work together incorporated in an actual storage system has to be considered. Ignoring this could lead to inaccurate assessments of the SoC.

And: At the storage system level, the interaction between CTES material and component(s) might manifest differently. Meaning that this interaction can be influenced and potentially altered at the system level by the boundary conditions of the application.

5.7.1 Measurement techniques and their application in storage prototypes:

Related to PCM applications, results of the experts' survey indicate that the combination of bulk temperature and heat flux measurement is the most common used techniques in the laboratory applications.

Novel techniques (independent from heat flux measurement – e.g. chamber pressure, electrical resistance, etc.) aim to track the overall phase fraction of the PCM bulk in a storage container.

Experimental data is typically used for developing digital twins for system simulation (context: system controls) and/or to validate numerical models for heat transfer optimization (e.g. ANSYS fluent – CFD).

Innovation projects with industrial partners is needed to develop practical, reliable sensor solutions considering application needs – modular SoC detection solutions (independent from a specific application/ storage geometry) are aimed.

TCM: Common: a) Sorbate content of sorption material; b) Mass of reactants in closed vessels.

Novel techniques (non-intrusive) are important for components & high temperature storage solutions – also since internal temperature measurements do not reflect the available capacity of TCM during charging/ discharging.

Measurement techniques were mainly tested in different small-scale setups (lab environment) in conjunction with material characterization. A few component-level (demonstrators) examples have been received.

Results from ongoing research projects are not published yet and should be analyzed in a future task period.

5.7.2 System application - potential:

Storage integration into (digitalized) energy systems require interaction with advanced (predictive) controls. Reliable SoC determination is based on material bulk response instead of heat flux measurements.

SoC determination and derived thermal power contributes to flexibility (ancillary) services of heating and cooling systems as well as increase of supply security (e.g. server room cooling, industrial processes) – context: increased share of renewables in for both, electricity and heat supply.

Would it be possible to economically feasible control as storage without SoC determination?

Improved ancillary serves with increased supply reliability and/or reduction of backup generation capacity. Link: Task 41 on “Economics of Energy Storage.

Interdisciplinary, applied research is needed to bridge material science and system engineering.

5.8 References

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6 Subtask D: Stability of PCM and TCM

6.1 Introduction and Objectives

6.1.1 Investigating CTES material stability

What is meant by CTES material stability? A general definition could be: A CTES material is stable if its relevant properties (e. g. melting/reaction enthalpy and temperature, chemical composition, etc.) remain unchanged within a certain limit (compared to the initial state) during and after testing. Testing can refer to both laboratory tests and monitoring of the CTES material within an actual storage system.

Therefore, to talk about CTES material stability, it is necessary to know or investigate the processes that lead to a CTES material no longer being stable. In the context of this Task, these processes are referred to as degradation mechanisms.

Different degradation mechanisms are to be considered when studying CTES material stability. For example, chemical degradation of organic PCM at high temperatures (Figure 6-1, left [1]) or breaking up zeolite pellets by hydrothermal aging (Figure 6-1, right [2]).

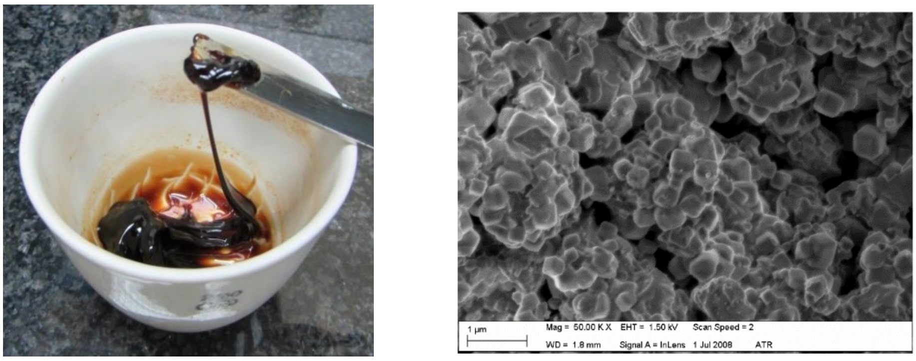


Figure 6-1: Examples for degradation of PCM (left: thermal decomposition of D-mannitol, a sugar alcohol [1]) and TCM (right: breaking up zeolite pellets by hydrothermal aging [2]).

In the previous Annex 33, one topic was testing PCM under application conditions. This included an inventory of properties of PCM that change comparing lab-scale experiments with tests under application conditions, and a paper on experimental devices and techniques to investigate degradation of PCM [3]. Both deliverables pointed to the relevance of investigating the stability of PCM. It became obvious that the stability of PCM, as a key requirement for a successful development and commercialisation of latent heat thermal energy storage systems, strongly depends on the material (class) and the applied testing conditions. This means that no general statement of the type "Material xy is stable." or "Material xy is not stable." can be made without reporting the specific testing conditions.

The state of scientific literature with respect to the stability of PCM can be illustrated with three representative papers. The first paper is exemplary for many similar publications: a review paper on tested CTES materials (in this case PCM) and applied experimental methods. Ferrer et al. [4] reported on thermally cycled PCM of different material classes (including organic and inorganic materials). They prepared extensive tables with data for initial (before cycling) and final (after cycling) material properties and indicated the applied test method. In addition, they listed the experimental devices including information on the manufacturer and device type used by different authors.

The second paper proposes a methodology for a step-by-step validation of CTES materials, exemplary applied to a sugar alcohol used as PCM. With validation, Bayón and Rojas [5] mean testing and verifying the long-term stability and long-term performance of a material. They state that “no testing protocol or guideline exists up to now for validating storage media, so that authors apply their own criteria, not only for designing testing procedures but also for predicting the material behaviour under long-term operation." Their proposed "methodology consists of different stages that include PCM characterization, preliminary assessment tests, and accelerated life testing." Overall, their method has a strong focus on considering application conditions (called "service conditions") when testing the stability. To perform accelerated tests – which are expected to provide a faster assessment of the stability of a material – it is crucial to, first, know the relevant degradation factors (e.g. high-temperature, oxygen atmosphere, etc.) and, second, perform "tests under increasing stress level of degradation factors" (e.g. higher temperatures than those to which the CTES material is normally exposed). As an example, they choose D-mannitol, a sugar alcohol, to illustrate their methodology. Among others, they evaluate "lifetime relationship diagrams for the thermal degradation of D-mannitol" showing the reduction in melting enthalpy obtained after exposure to different static temperatures (between 170 and 210 °C).

In the third paper, Mehling [6] presents a systematic approach to investigate property degradation of PCM. He emphasizes that "as different applications impose different conditions [...], testing should be tailored to the individual case". According to his method, "first the basic functions and related properties that might be subject to testing, e.g., with a specific application in mind" are to be identified. Following this, the method proposes an "approach to find the degradation effects and underlying mechanisms to allow tailoring and optimizing test procedures". The paper demonstrates the approach for the function of heat storage of PCM.

Overall, these three papers span the current state of research into the stability of PCM. Similar papers can be found for TCM. There is a lot of data available, often with little background information on the experimental boundary conditions of testing. At the same time, there are suggestions for a structured approach to investigating stability, taking into account the specific application.

Based on the outlined state of literature and the work from the previous Annex 33, the Task 40 experts have derived the following objectives for Subtask D.

6.1.2 Objectives

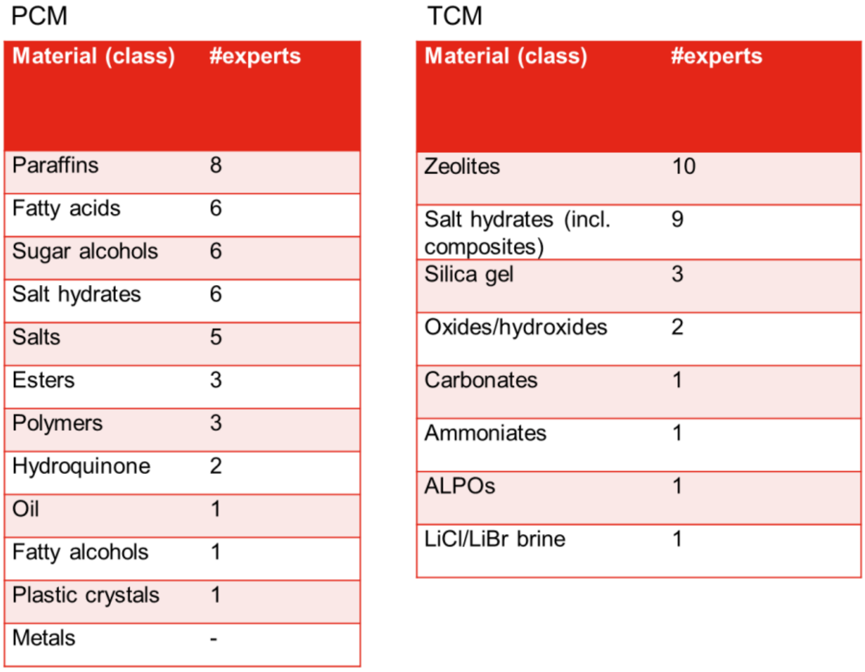
The main goal of Subtask D was to come to a better understanding of the stability of PCM and TCM and, thereby, derive recommendations for an application-oriented stability testing. Previous works and the state of literature lack of (I) sorting and differentiating the relevant degradation mechanisms, (II) showing which test methods are suitable for determining the respective degradation, and (III) making (material class-specific) recommendations for accelerating the measurements.

The two objectives to work towards this goal were:

1. Mapping degradation mechanisms for CTES material classes
2. Come up with recommendations for stability testing
   a. …based on simple experiments
   b. …to faster investigate stability by accelerating degradation

6.2 Overview of experience with CTES material stability among the Task experts

To work on the two objectives, the existing expertise of the Task participants regarding CTES material stability was first queried. Figure 6-2 lists the number of Task experts with expertise on stability studies for different PCM and TCM material classes.



PCM

Material (class)	#experts
Paraffins	8
Fatty acids	6
Sugar alcohols	6
Salt hydrates	6
Salts	5
Esters	3
Polymers	3
Hydroquinone	2
Oil	1
Fatty alcohols	1
Plastic crystals	1
Metals	-

TCM

Material (class)	#experts
Zeolites	10
Salt hydrates (incl. composites)	9
Silica gel	3
Oxides/hydroxides	2
Carbonates	1
Ammoniates	1
ALPOs	1
LiCl/LiBr brine	1

Figure 6-2: Number of experts within Task 40 with expertise on stability studies for different PCM and TCM material classes.

In the case of PCM, paraffins, fatty acids, sugar alcohols, and salt hydrates/salts are the material classes with the most experience in the Task group. Among TCM, zeolites and salt hydrates (incl. composites) were most extensively studied. Figure 6-2 shows that the Task group has plenty of R&D experience regarding CTES material stability.

Table 6-1 lists the Task experts with experience on CTES material stability testing. Along with the investigated material (classes), the applied experimental test methods including their specifications are reported. This list summarizes the basis for the work on the Subtask D objectives. It becomes obvious that stability testing methods are strongly connected with the nature of the investigated CTES material (class). Table 6-1 does not reflect the complete status of the experimental investigation of CTES material stability, but it does illustrate very well the broad range of investigation methods that are used.

Table 6-1: Task experts with experience on CTES material stability testing; investigated PCM and TCM; applied testing devices and experimental conditions (sorted alphabetically by country).

Name	Organisation	PCM	TCM	Testing device, boundary conditions
Gayaneh Issayan, Bernhard Zettl	Univ. of Applied Science Upper Austria		• Zeolites • Salt hydrates • Natural zeolite composites	• Closed system: 5 mbar/20–130 °C • Open system: 20–250 °C, up to 70 cycles https://doi.org/10.2991/ahe.k.220301.011
Peter Weinberger	TU Vienna, Austria		• Ammoniates • Carbonates	
Wim van Helden	AEE Intec, Austria		• Zeolites	
Reda Djebbar, Lia Kouchachvili, Dylan Bardy	NRCan, Canada		• Natural zeolites-based salt hydrate composites • Biomass-based composites	• TGA/DSC with humidity generator: 25–250 °C; 1–17 mbar water vapour pressure • Kg-scale closed type lab test bench: 25–160 °C; up to 25 mbar water vapour pressure
Handan Tezel	Univ. of Ottawa, Canada		• Silica gel + salt hydrates • Vermiculite + salt hydrates • Flax shives + salt hydrates • Zeolites	
Dominic Groulx	Dalhousie Univ., Canada	• Fatty acids (mostly dodecanoic acid) • Paraffins		• Cycling setup that can be used for PCM with melting temperatures between 20 and 70 °C that do not supercool by a large amount. • High temperature testing by putting small amounts of PCM in the thermal chamber (temperature up to 200 °C) and leaving them there for weeks or a few months possible.
Alireza Afshari, Evdoxia Paroutoglu, Allesandro Maccarini	Aalborg Univ., Denmark	• Paraffins • Fatty acids • Inorganic salt hydrates • Renewable oils		• DSC, Optical Microscopy, and SEM. • Manual thermal cycling of PCM through 200 thermal cycles equivalent to 6 months of lifetime. • The thermal cycles were set in the range -30 to +80 °C with a scanning rate of 1.5 K/min in a dynamic mode. The mass of each sample was 3 to 6 mg.

Name	Organisation	PCM	TCM	Testing device, boundary conditions
Gerald Englmair, Jianhua Fan	DTU, Denmark	• Salt hydrates		
Nolwenn Le Pierrès, Michel Ondarts, Jonathan Outin, Elise Berut	Univ. Savoie Mont Blanc, France		• Zeolites • Zeolites + salt hydrates • Activated carbon + salt hydrates • Silica + PEG + salt hydrates	
Grégory Largiller	CEA, France	• Nitrate salts • Sugar alcohol • Fatty alcohol • plastic crystals	• Zeolites	• DSC: 12 ml, 20–275 °C, under static air • DSC: 850 µl, -40–140 °C, under static or flowing air or N_2, controlled RH. • TGA coupled DSC: large range of volumes, 5–500 °C, under static or flowing air or N_2, controlled RH • LFA: on powders or bulk samples (10 mm or 12.4 mm diameter)
Franziska Klünder, Stefan Gschwander	Fraunhofer ISE, Germany	• Sugar alcohols • Paraffins • Fatty acids • Polymers		• Cycling test rig (-40–200 °C) • Climate chamber (-40–180 °C) • DSC
Christoph Rathgeber	ZAE Bayern, Germany	• Salt hydrates	• Zeolites • LiBr and LiCl brine	• Two thermal cycling test rigs for PCM • Hydrothermal stability cycling test rigs for sorption materials
Emanuela Mastronardo	Univ. of Messina, Italy		• Salt hydrates • Hydroxides • Oxides	• TGA • Dynamic water sorption analyser • DSC

Name	Organisation	PCM	TCM	Testing device, boundary conditions
Ruud Cuypers	TNO, Netherlands		• Salt hydrates • 'Stabilized' salt hydrates (i.e. salt hydrates in a matrix, or salt hydrates with additives for better cycling behavior)	• Boundary conditions are use in the built environment, for heating and/or domestic hot water. • Two concepts: the vacuum concept (working mainly with Na_2S) and the 'closed loop' concept (working with K_2CO_3). • Thermal charging (up to 80–100 °C by e.g. flat plate or vacuum tube collectors) or electrical charging (up to roughly 130 °C in a pressurized system). • Testing consists of materials testing (pT-meter, sorption analysis, DTA, outgassing tests, accelerated cycling tests), testing in components ("1-kg setup" including a mock-up heat exchanger and the possibility to change temperatures of desorption/evaporation/condensation), and module testing (in a 'real life' setup at the scale of several 100's of kg's).
Henk Huinink	TU Eindhoven, Netherlands		• Salt hydrates	
Alenka Ristić	NIC, Slovenia		• APOs • Zeolites • $CaCl_2$-PHTS/FeKIL2/γ-alumina • MOFs	• Hydrothermal stability cycling test for sorption materials • Dynamic gravimetric water sorption analyzers: IGA-100 and IGAsorp-XT sorption gravimetrical analysers (Hiden Isochema Ltd., Warrington, UK)
Rocio Bayón	CIEMAT, Spain	• Paraffins • Salts • Hydroquinone • Sugar alcohols		

Name	Organisation	PCM	TCM	Testing device, boundary conditions
Inés Fernández, Camila Barreneche	Univ. of Barcelona, Spain	• Paraffin • Salts • Salt hydrates • Fatty acids • Fatty esters • Fatty eutectics • Sugar alcohols • Nano-enhanced PCM	• $MgSO_4 \cdot 6H_2O$ • $Na_2S \cdot xH_2O$ • $CaCl_2 \cdot 6H_2O$ • Zeolite • Silica gel • Natural hydrated salts	• Test: thermal cycler (low and high T) • Characterization: XRD, FT-IR, Gas Chromatography, HPLC, NMR-H, NMR-C
Gabriel Zsembinszki, Emiliano Borri, Luisa F. Cabeza, David Verez	Univ. of Lleida, Spain	• Sugar alcohols • Paraffins • Salt hydrates • Fatty acids • Polymers • Salts • Esters • Hydroquinone		• DSC 3+ Mettler Toledo, -50–500 °C • INECC-30/300 Intelec compact climatic chamber, from -50–500 °C • Ristretto CYCL06 thermocycler, 4–105 °C • Unique self-manufactured test box for the thermal cycle of heterogeneous samples (15x15x3 cm), 5–45 °C
Rebecca Ravotti	HSLU, Switzerland	• Esters • Salt hydrates • Paraffins • Fatty acids • Sugar alcohols		• DSC 823e, DSC3+ Mettler Toledo, -60–600°C • TGA/DSC Mettler Toledo RT to 1,000 °C • EasyMax Mettler Toledo, -20–300 °C • Hot Stage built in-house with polarized DinoLite microscope, 5–130 °C • Cycling unit built in-house, RT to 150 °C with optical information (camera) • XRD D2 Phaser Bruker, 5–150 °C, 2theta • ATR-IR • GC-MS for organics only • THB for both liquids (RT to 150 °C) and solids • Densitometer Mettler Toledo (liquids), CT for solid density • Moisture analyser Mettler Toledo and Karl Fischer titrator

Name	Organisation	PCM	TCM	Testing device, boundary conditions
Yulong Ding, Helena Navarro, Anabel Palacios Trujillo	Univ. of Birmingham, UK	• Salt hydrates • Paraffins • Sugar alcohols • Molten salts	• Zeolites • Salt hydrates composites • Silica gel	• PCM: STA, DSC, Cycling furnace and test rigs for larger samples • TCM: STA. Humidity chamber and test rigs for building/waste heat recovery • Boundary conditions STA: -100–900 °C, 0–80% RH under low pressure. • Humidity chamber: RT to 150 °C, 0–99% RH
Jonathon Elvins	Swansea Univ., UK		• Vermiculite + $CaCl_2$ • Vermiculite/perlite + $SrBr_2$ • CaO	
Carolina Costa	Northumbria Univ., UK	• Paraffins • Fatty acids		• Test device under construction

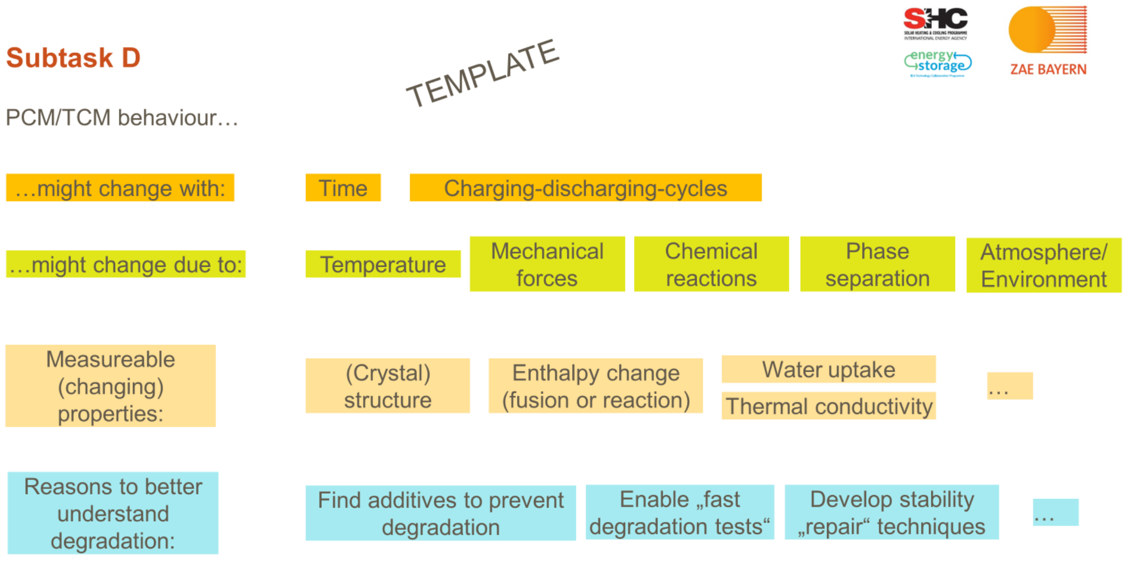
6.3 Mapping of CTES material degradation

6.3.1 Motivation

CTES material degradation mapping should provide an easy-to-read and comprehensive overview that directly shows the relationships between test conditions, degradation mechanisms, and effects on the material and, if tested, the CTES system. In the course of Task 40, several visualization approaches were proposed, discussed, and further refined. Common to all approaches was the ambition to sort and structure discussions on stability, insofar as different questions and perspectives should be included in such a mapping: What are the reasons for degradation? What are the effects of degradation on the material (properties)? How can degradation be identified and quantified? How to accelerate degradation to accelerate the testing?

6.3.2 Visualization approaches

Figure 6-3 is an attempt towards such a structuring. A distinction (lines of different colours) is made between what CTES material behaviour might change with, what it might change due to, measurable properties to assess that change, and reasons to better understand the degradation. This structuring was proposed and discussed at the early expert meetings.



Subtask D

TEMPLATE

ZAE BAYERN

PCM/TCM behaviour…

…might change with: Time | Charging-discharging-cycles

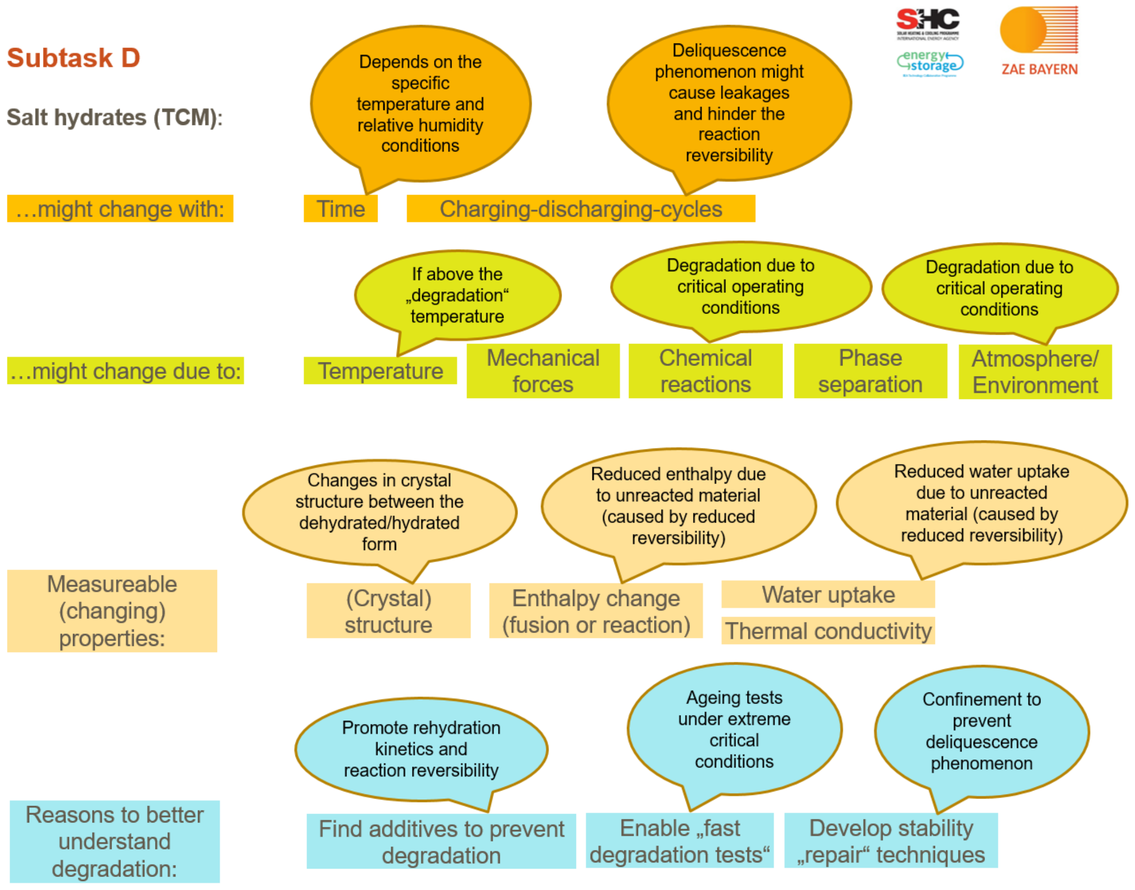
…might change due to: Temperature | Mechanical forces | Chemical reactions | Phase separation | Atmosphere/ Environment

Measureable (changing) properties: (Crystal) structure | Enthalpy change (fusion or reaction) | Water uptake | Thermal conductivity | …

Reasons to better understand degradation: Find additives to prevent degradation | Enable „fast degradation tests“ | Develop stability „repair“ techniques | …

Figure 6-3: First approach to structure CTES material stability.

The template was distributed among the Task experts with CTES material stability knowledge (cf. Table 6-1). Task experts were asked to add their comments to the template to provide an overview of the stability behaviour of the CTES material (class) they have experience with. As an example, show the template filled in for salt hydrates to be used as TCM.



Subtask D

Salt hydrates (TCM):

…might change with: Time | Charging-discharging-cycles

Depends on the specific temperature and relative humidity conditions

Deliquescence phenomenon might cause leakages and hinder the reaction reversibility

…might change due to: Temperature | Mechanical forces | Chemical reactions | Phase separation | Atmosphere/ Environment

If above the „degradation" temperature

Degradation due to critical operating conditions

Degradation due to critical operating conditions

Measureable (changing) properties: (Crystal) structure | Enthalpy change (fusion or reaction) | Water uptake | Thermal conductivity

Changes in crystal structure between the dehydrated/hydrated form

Reduced enthalpy due to unreacted material (caused by reduced reversibility)

Reduced water uptake due to unreacted material (caused by reduced reversibility)

Reasons to better understand degradation: Find additives to prevent degradation | Enable „fast degradation tests" | Develop stability „repair" techniques

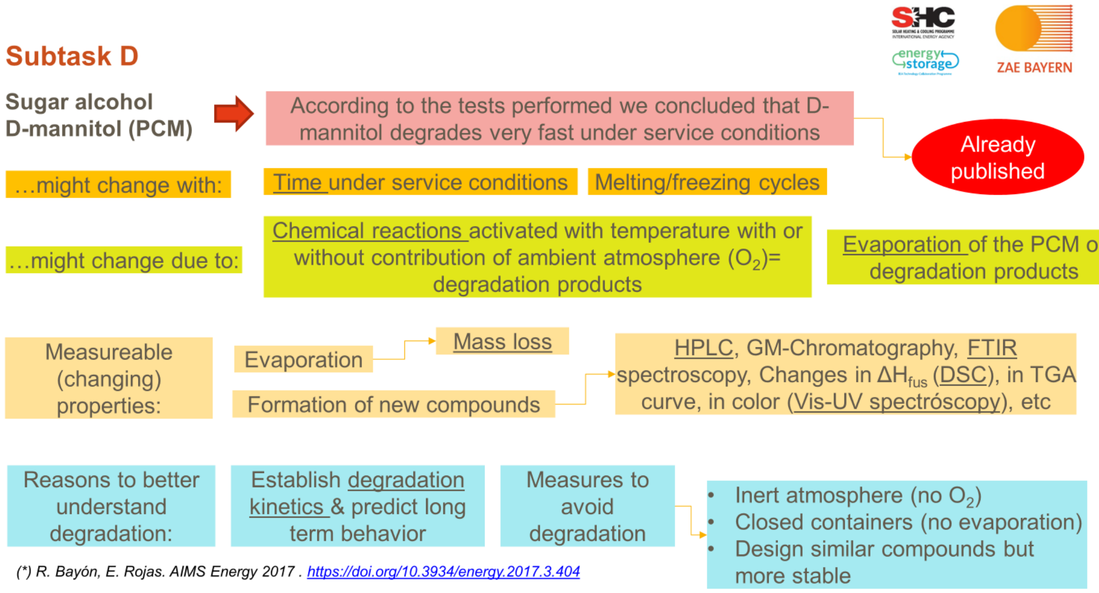
Promote rehydration kinetics and reaction reversibility

Ageing tests under extreme critical conditions

Confinement to prevent deliquescence phenomenon

Figure 6-4: First approach to structure CTES material stability filled in for salt hydrates as TCM (source: Univ. Messina).

A modification of this presentation type was proposed by Rocio Bayón of CIEMAT, Spain (Figure 6-5).



Subtask D

Sugar alcohol D-mannitol (PCM)

According to the tests performed we concluded that D-mannitol degrades very fast under service conditions

Already published

…might change with: Time under service conditions | Melting/freezing cycles

…might change due to: Chemical reactions activated with temperature with or without contribution of ambient atmosphere (O_2)= degradation products | Evaporation of the PCM or degradation products

Measureable (changing) properties: Evaporation → Mass loss | Formation of new compounds → HPLC, GM-Chromatography, FTIR spectroscopy, Changes in ΔH_{fus} (DSC), in TGA curve, in color (Vis-UV spectróscopy), etc

Reasons to better understand degradation: Establish degradation kinetics & predict long term behavior | Measures to avoid degradation

- Inert atmosphere (no O_2)
- Closed containers (no evaporation)
- Design similar compounds but more stable

(*) R. Bayón, E. Rojas. AIMS Energy 2017 . https://doi.org/10.3934/energy.2017.3.404

Figure 6-5: Second approach to structure CTES material stability filled in for D-mannitol as PCM (source: CIEMAT).

It adapts the presentation type specifically to the selected material class, links the relevant degradation mechanisms to appropriate experimental investigation methods, adds a conclusion on stability according to the investigation conditions applied and refers to a corresponding publication (if available).

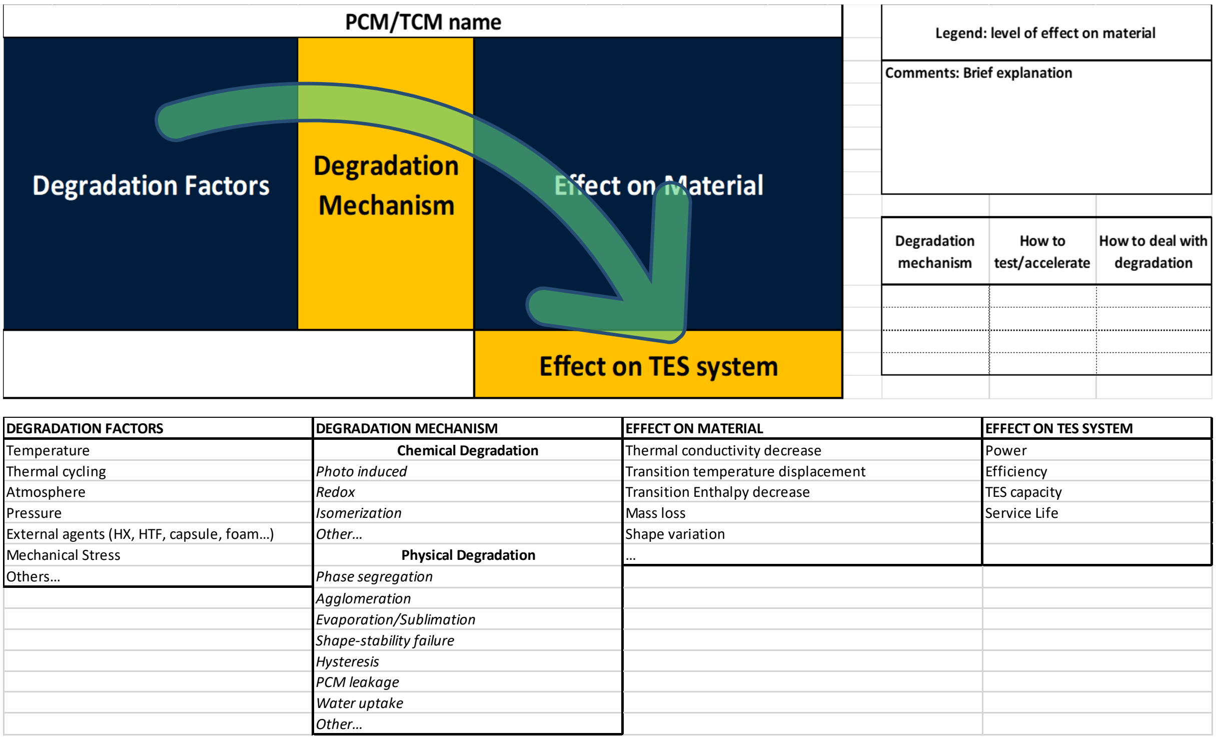
Received examples for the first and second approach to visualize CTES material stability are collected in the Appendix (section 8.1) of this final report.

A third type of presentation was developed by Ángel Serrano of CIC energiGUNE, Spain. This approach connects the degradation mechanisms (e.g. phase separation, corrosion, polymorphism) with their effect on the CTES material (e.g. change in transition enthalpy or thermal conductivity) and the performance on system level (e.g. change in power or capacity). The degradation mechanisms are in turn specified in more detail by their dependence on application conditions, in this approach called "degradation factors" (e.g. temperature, thermal cycling, atmosphere, etc.).

The template shown in Figure 6-6 is divided into a table with

a) Degradation factors
b) Degradation mechanisms
c) Effect on the material
d) Effect on the TES system

In addition, the template provides a box to leave a brief summary comment, along with a table that gathers information on how to test/ accelerate the selected degradation mechanisms and how to deal with this degradation.



Legend: level of effect on material

Comments: Brief explanation

Degradation mechanism	How to test/accelerate	How to deal with degradation

DEGRADATION FACTORS	DEGRADATION MECHANISM	EFFECT ON MATERIAL	EFFECT ON TES SYSTEM
Temperature	**Chemical Degradation**	Thermal conductivity decrease	Power
Thermal cycling	*Photo induced*	Transition temperature displacement	Efficiency
Atmosphere	*Redox*	Transition Enthalpy decrease	TES capacity
Pressure	*Isomerization*	Mass loss	Service Life
External agents (HX, HTF, capsule, foam…)	*Other…*	Shape variation	
Mechanical Stress	**Physical Degradation**	…	
Others…	*Phase segregation*		
	Agglomeration		
	Evaporation/Sublimation		
	Shape-stability failure		
	Hysteresis		
	PCM leakage		
	Water uptake		
	Other…		

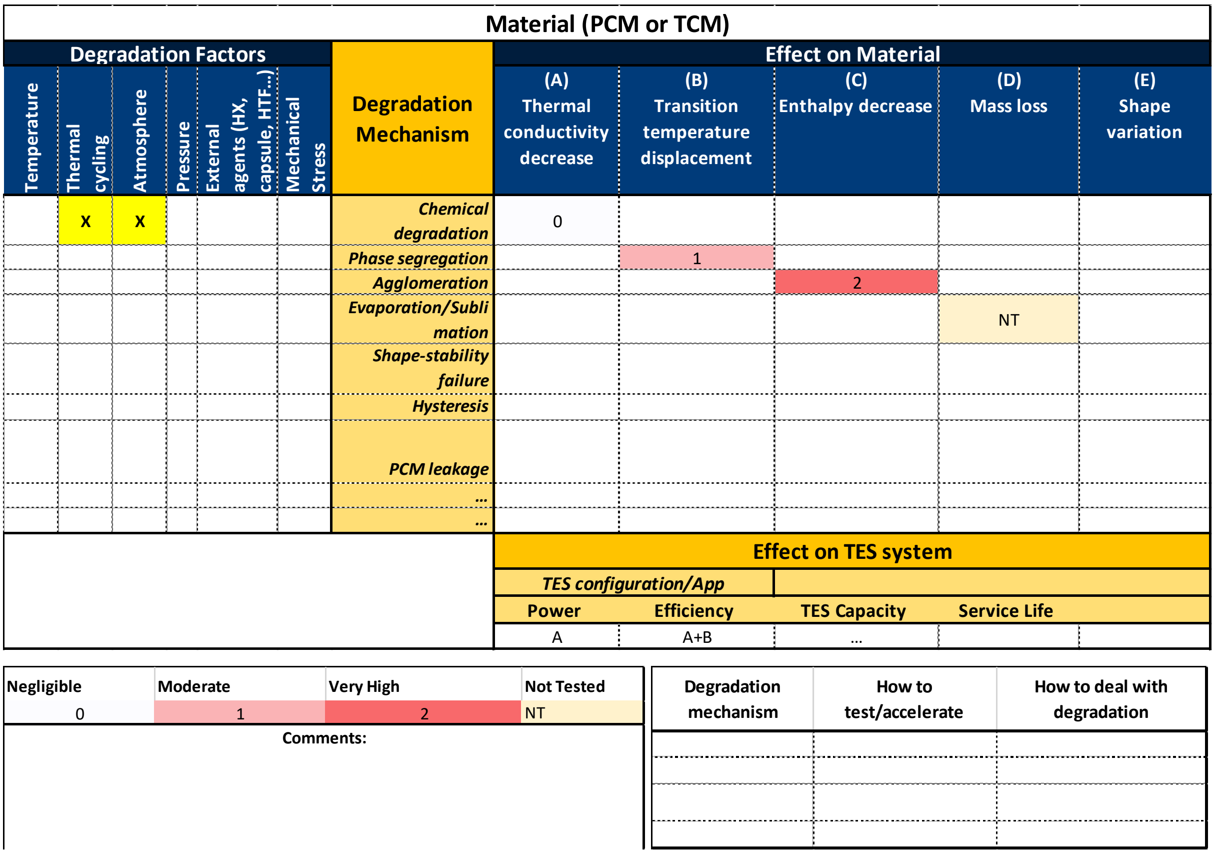
Figure 6-6: Explanation of the third approach's template to structure CTES material stability.

The backbone of the document is the table with degradation mechanisms. Therefore, experts first indicate those degradation mechanisms that affect the material based on their experience. Second, an "X" marks those degradation factors that trigger the degradation mechanism. Third, the effect of this degradation mechanism on the PCM/TCM material is rated as 0 (negligible), 1 (moderate), 2 (very high), or NT (not tested).

The effect on the TES system typically depends on various factors, such as the TES system configuration or the application. In the template, the effect on the TES system is indicated through letters A, B, etc., which correspond to the different "Effects on Material".

Finally, experts may add a brief summary of the stability of the investigated CTES material, testing options for the degradation mechanisms, and proposals for dealing with the degradation (if possible and known).

The actual template that was shared with the Task experts is Excel-based. A screenshot of the template is given in Figure 6-7.



Material (PCM or TCM)

Degradation Factors						Degradation Mechanism	Effect on Material				
Temperature	Thermal cycling	Atmosphere	Pressure	External agents (HX, capsule, HTF...)	Mechanical Stress		(A) Thermal conductivity decrease	(B) Transition temperature displacement	(C) Enthalpy decrease	(D) Mass loss	(E) Shape variation
	X	X				*Chemical degradation*	0				
						Phase segregation		1			
						Agglomeration			2		
						Evaporation/Sublimation				NT	
						Shape-stability failure					
						Hysteresis					
						PCM leakage					
						...					
						...					

Effect on TES system				
TES configuration/App				
Power	Efficiency	TES Capacity	Service Life	
A	A+B	...		

Negligible	Moderate	Very High	Not Tested
0	1	2	NT

Comments:

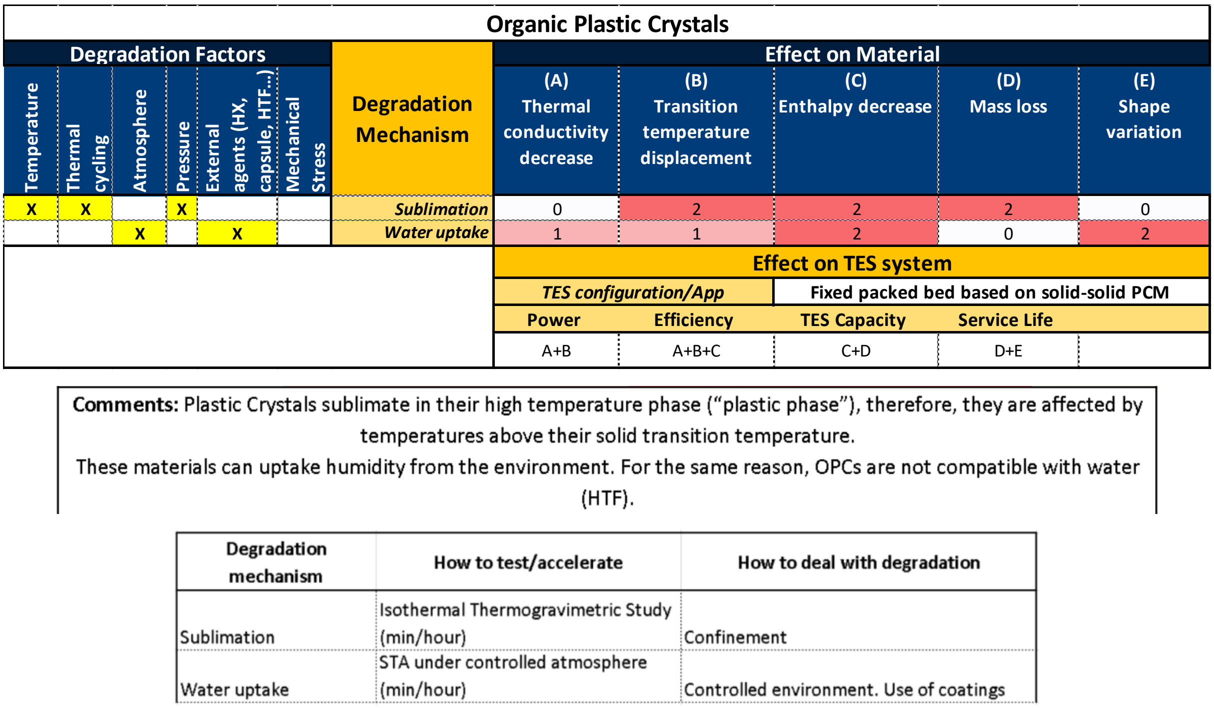
Degradation mechanism	How to test/accelerate	How to deal with degradation

Figure 6-7: Third approach’s template to structure CTES material stability.

6.3.3 Examples and results

In the following, the received examples of the third and final approach (cf. Figure 6-6 and Figure 6-7) to map CTES material degradation are given. The subsection headings contain the name of the CTES material or material class and if it is used as PCM or TCM. The sources of information are indicated in the figures’ captions. The effect of a degradation mechanism on the material is rated as 0 (negligible), 1 (moderate), 2 (very high), or NT (not tested).

6.3.3.1 Organic plastic crystals (PCM)



Organic Plastic Crystals

Degradation Factors: Temperature	Thermal cycling	Atmosphere	Pressure	External agents (HX, capsule, HTF...)	Mechanical Stress	Degradation Mechanism	Effect on Material: (A) Thermal conductivity decrease	(B) Transition temperature displacement	(C) Enthalpy decrease	(D) Mass loss	(E) Shape variation
X	X		X			*Sublimation*	0	2	2	2	0
		X		X		*Water uptake*	1	1	2	0	2

Effect on TES system

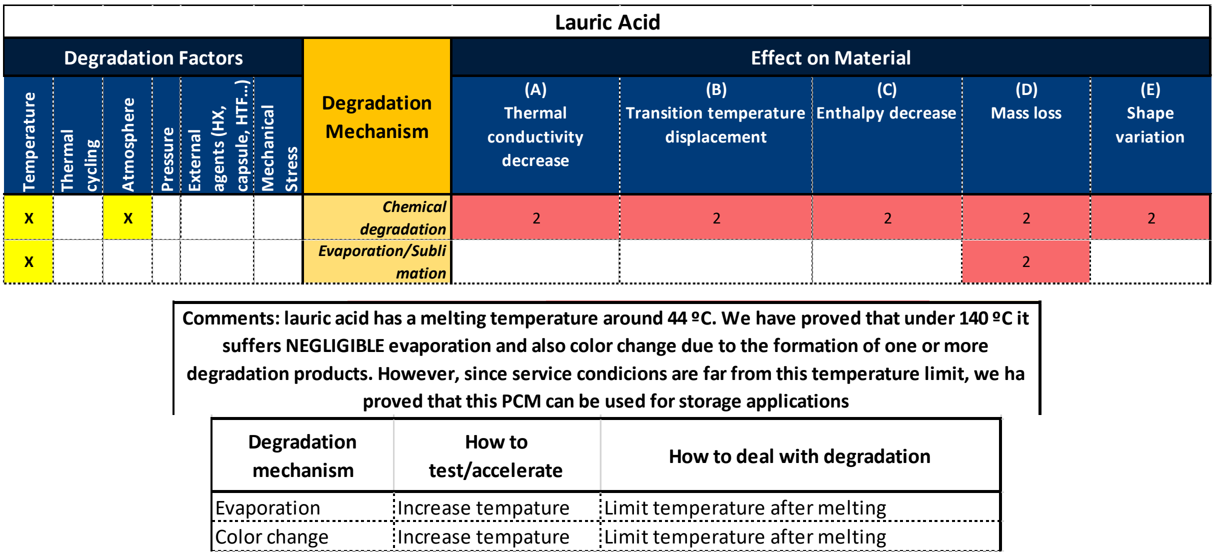
TES configuration/App	Fixed packed bed based on solid-solid PCM			
Power	**Efficiency**	**TES Capacity**	**Service Life**	
A+B	A+B+C	C+D	D+E	

Comments: Plastic Crystals sublimate in their high temperature phase ("plastic phase"), therefore, they are affected by temperatures above their solid transition temperature.
These materials can uptake humidity from the environment. For the same reason, OPCs are not compatible with water (HTF).

Degradation mechanism	How to test/accelerate	How to deal with degradation
Sublimation	Isothermal Thermogravimetric Study (min/hour)	Confinement
Water uptake	STA under controlled atmosphere (min/hour)	Controlled environment. Use of coatings

Figure 6-8: Degradation mapping of organic plastic crystals (by Ángel Serrano, CIC energiGUNE).

6.3.3.2 Lauric acid (PCM)



Lauric Acid

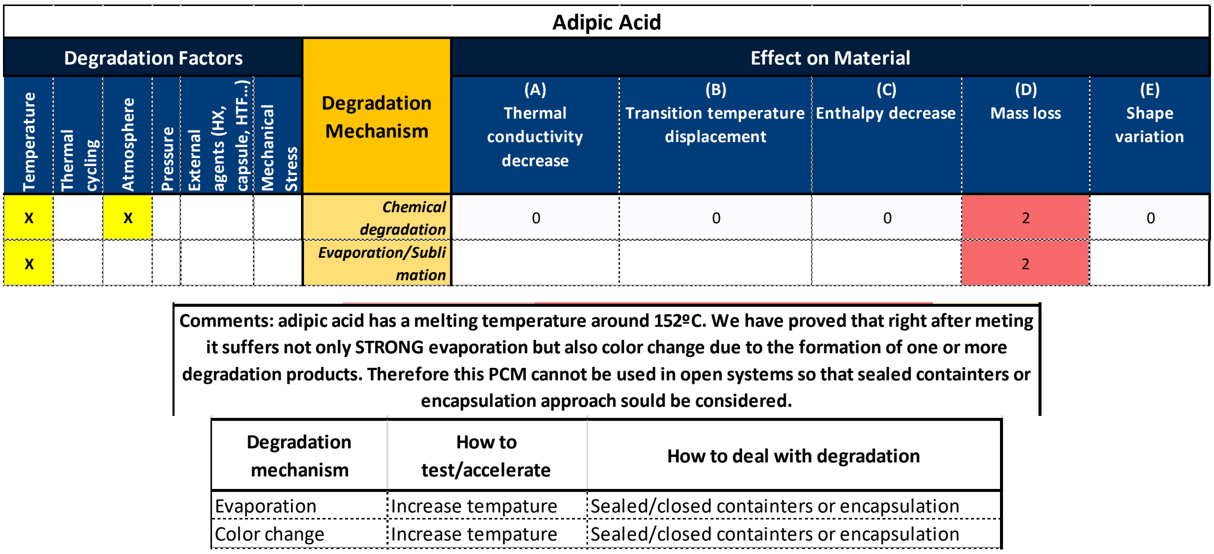
Degradation Factors: Temperature	Thermal cycling	Atmosphere	Pressure	External agents (HX, capsule, HTF...)	Mechanical Stress	Degradation Mechanism	Effect on Material: (A) Thermal conductivity decrease	(B) Transition temperature displacement	(C) Enthalpy decrease	(D) Mass loss	(E) Shape variation
X		X				*Chemical degradation*	2	2	2	2	2
X						*Evaporation/Sublimation*				2	

Comments: lauric acid has a melting temperature around 44 ºC. We have proved that under 140 ºC it suffers NEGLIGIBLE evaporation and also color change due to the formation of one or more degradation products. However, since service condicions are far from this temperature limit, we ha proved that this PCM can be used for storage applications

Degradation mechanism	How to test/accelerate	How to deal with degradation
Evaporation	Increase tempature	Limit temperature after melting
Color change	Increase tempature	Limit temperature after melting

Figure 6-9: Degradation mapping of lauric acid (by Rocio Bayón, CIEMAT).

6.3.3.3 Adipic acid (PCM)



Adipic Acid

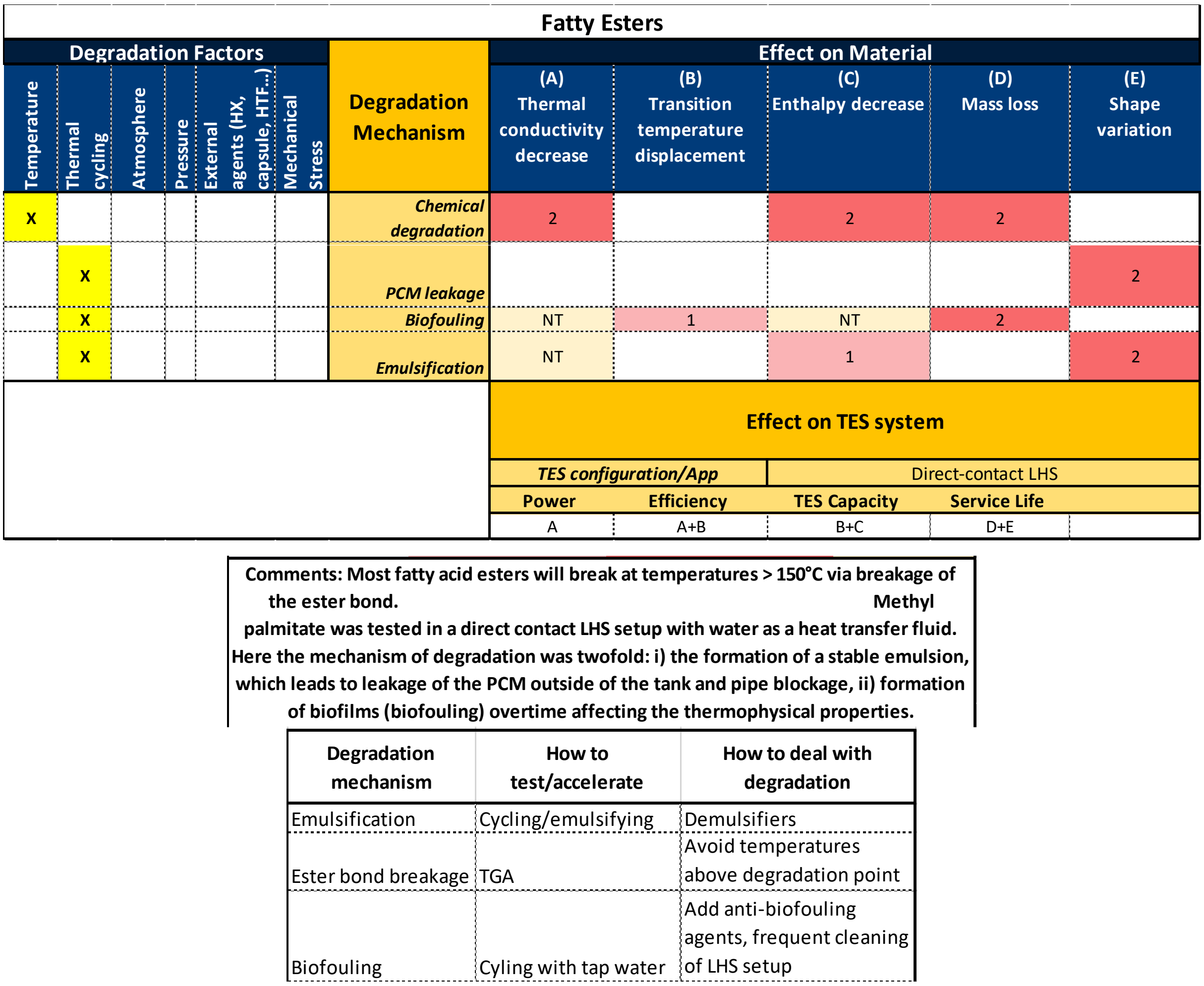
Degradation Factors						Degradation Mechanism	Effect on Material				
Temperature	Thermal cycling	Atmosphere	Pressure	External agents (HX, capsule, HTF...)	Mechanical Stress		(A) Thermal conductivity decrease	(B) Transition temperature displacement	(C) Enthalpy decrease	(D) Mass loss	(E) Shape variation
X		X				*Chemical degradation*	0	0	0	2	0
X						*Evaporation/Sublimation*				2	

Comments: adipic acid has a melting temperature around 152ºC. We have proved that right after meting it suffers not only STRONG evaporation but also color change due to the formation of one or more degradation products. Therefore this PCM cannot be used in open systems so that sealed containters or encapsulation approach sould be considered.

Degradation mechanism	How to test/accelerate	How to deal with degradation
Evaporation	Increase tempature	Sealed/closed containters or encapsulation
Color change	Increase tempature	Sealed/closed containters or encapsulation

Figure 6-10: Degradation mapping of adipic acid (by Rocio Bayón, CIEMAT).

6.3.3.4 Fatty esters (PCM)



Fatty Esters

Degradation Factors						Degradation Mechanism	Effect on Material				
Temperature	Thermal cycling	Atmosphere	Pressure	External agents (HX, capsule, HTF...)	Mechanical Stress		(A) Thermal conductivity decrease	(B) Transition temperature displacement	(C) Enthalpy decrease	(D) Mass loss	(E) Shape variation
X						*Chemical degradation*	2		2	2	
	X					*PCM leakage*					2
	X					*Biofouling*	NT	1	NT	2	
	X					*Emulsification*	NT		1		2

Effect on TES system

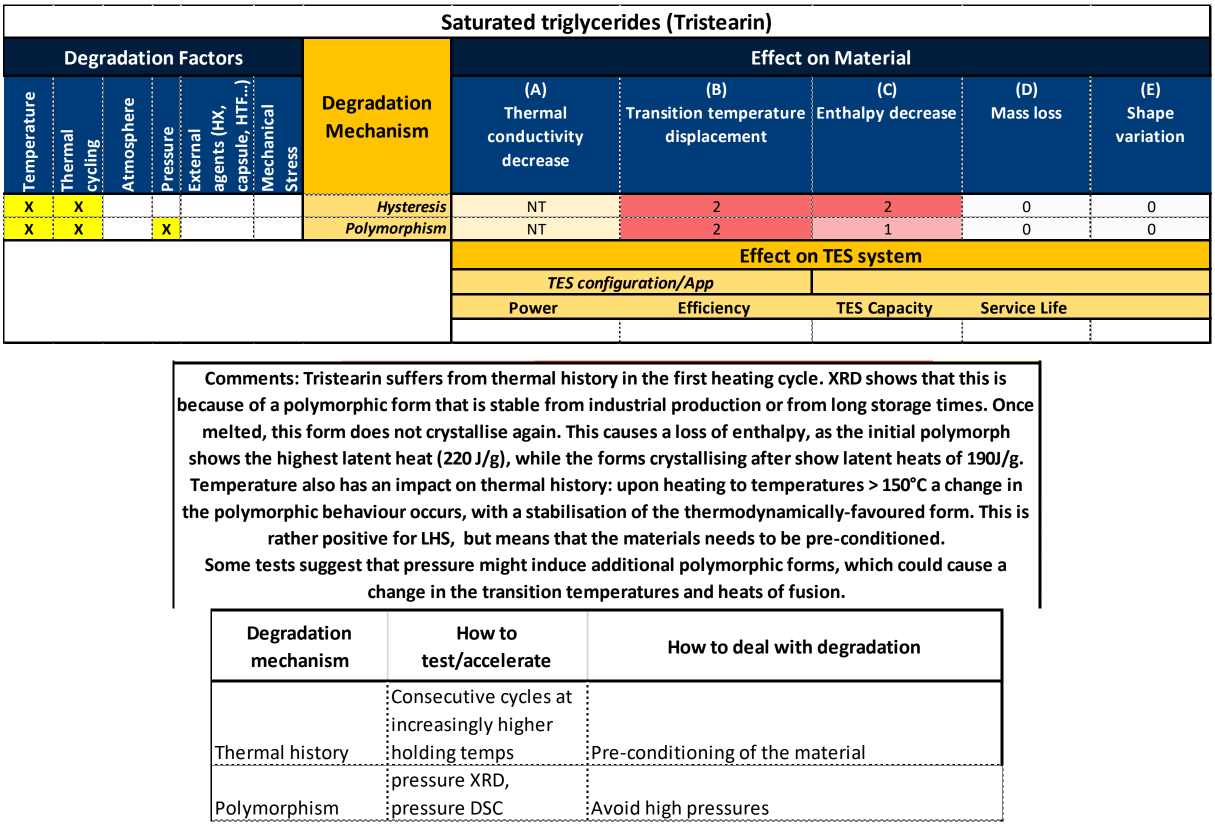
TES configuration/App	Direct-contact LHS			
Power	**Efficiency**	**TES Capacity**	**Service Life**	
A	A+B	B+C	D+E	

Comments: Most fatty acid esters will break at temperatures > 150°C via breakage of the ester bond. Methyl palmitate was tested in a direct contact LHS setup with water as a heat transfer fluid. Here the mechanism of degradation was twofold: i) the formation of a stable emulsion, which leads to leakage of the PCM outside of the tank and pipe blockage, ii) formation of biofilms (biofouling) overtime affecting the thermophysical properties.

Degradation mechanism	How to test/accelerate	How to deal with degradation
Emulsification	Cycling/emulsifying	Demulsifiers
Ester bond breakage	TGA	Avoid temperatures above degradation point
Biofouling	Cyling with tap water	Add anti-biofouling agents, frequent cleaning of LHS setup

Figure 6-11: Degradation mapping of fatty esters (by Rebecca Ravotti, HSLU).

6.3.3.5 Saturated triglycerides (PCM)



Saturated triglycerides (Tristearin)

Degradation Factors						Degradation Mechanism	Effect on Material				
Temperature	Thermal cycling	Atmosphere	Pressure	External agents (HX, capsule, HTF..)	Mechanical Stress		(A) Thermal conductivity decrease	(B) Transition temperature displacement	(C) Enthalpy decrease	(D) Mass loss	(E) Shape variation
X	X					*Hysteresis*	NT	2	2	0	0
X	X		X			*Polymorphism*	NT	2	1	0	0
							Effect on TES system				
							TES configuration/App				
							Power	Efficiency	TES Capacity	Service Life	

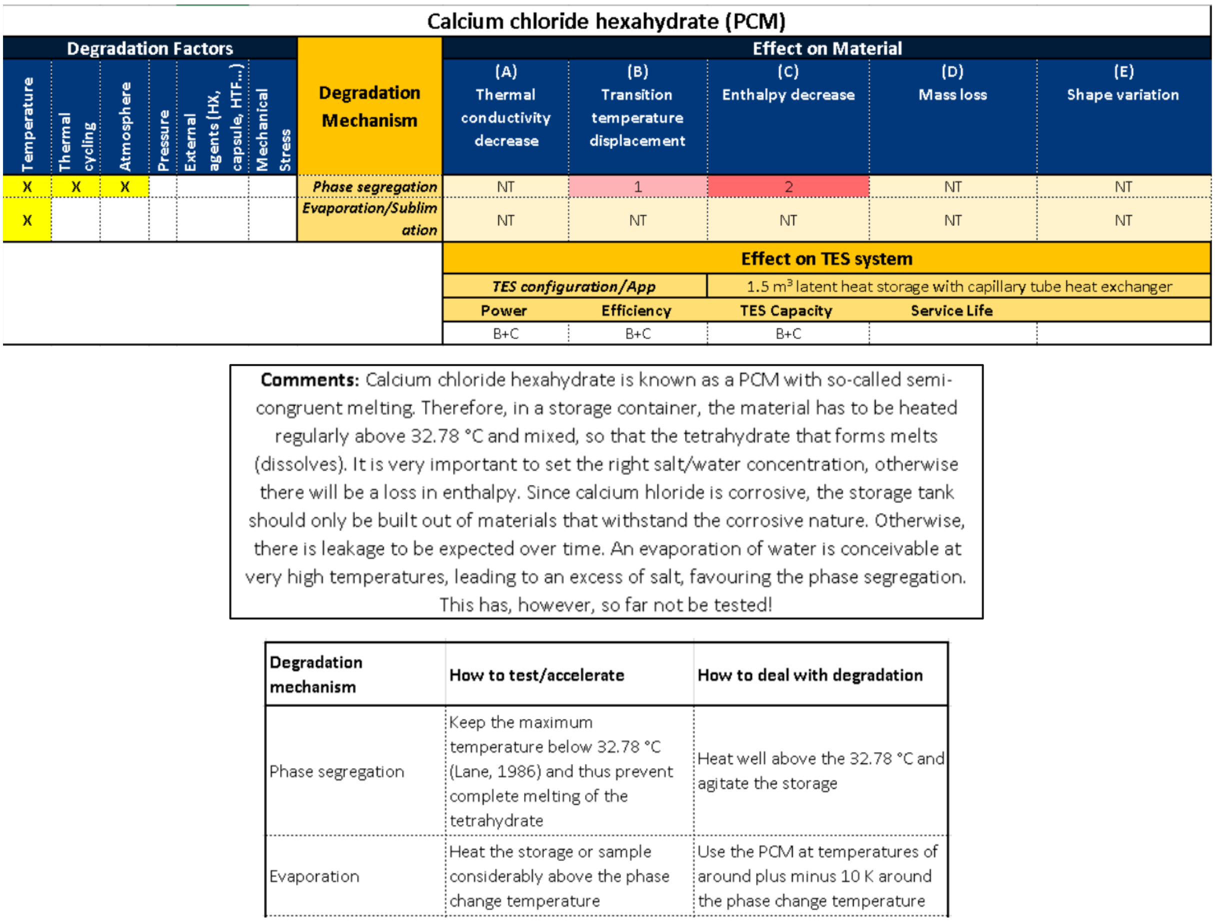
Comments: Tristearin suffers from thermal history in the first heating cycle. XRD shows that this is because of a polymorphic form that is stable from industrial production or from long storage times. Once melted, this form does not crystallise again. This causes a loss of enthalpy, as the initial polymorph shows the highest latent heat (220 J/g), while the forms crystallising after show latent heats of 190J/g. Temperature also has an impact on thermal history: upon heating to temperatures > 150°C a change in the polymorphic behaviour occurs, with a stabilisation of the thermodynamically-favoured form. This is rather positive for LHS, but means that the materials needs to be pre-conditioned.

Some tests suggest that pressure might induce additional polymorphic forms, which could cause a change in the transition temperatures and heats of fusion.

Degradation mechanism	How to test/accelerate	How to deal with degradation
Thermal history	Consecutive cycles at increasingly higher holding temps	Pre-conditioning of the material
Polymorphism	pressure XRD, pressure DSC	Avoid high pressures

Figure 6-12: Degradation mapping of saturated triglycerides (by Rebecca Ravotti, HSLU).

6.3.3.6 Calcium chloride hexahydrate (PCM)



Calcium chloride hexahydrate (PCM)

Degradation Factors							Effect on Material				
Temperature	Thermal cycling	Atmosphere	Pressure	External agents (HX, capsule, HTF...)	Mechanical Stress	Degradation Mechanism	(A) Thermal conductivity decrease	(B) Transition temperature displacement	(C) Enthalpy decrease	(D) Mass loss	(E) Shape variation
X	X	X				*Phase segregation*	NT	1	2	NT	NT
X						*Evaporation/Sublimation*	NT	NT	NT	NT	NT

Effect on TES system

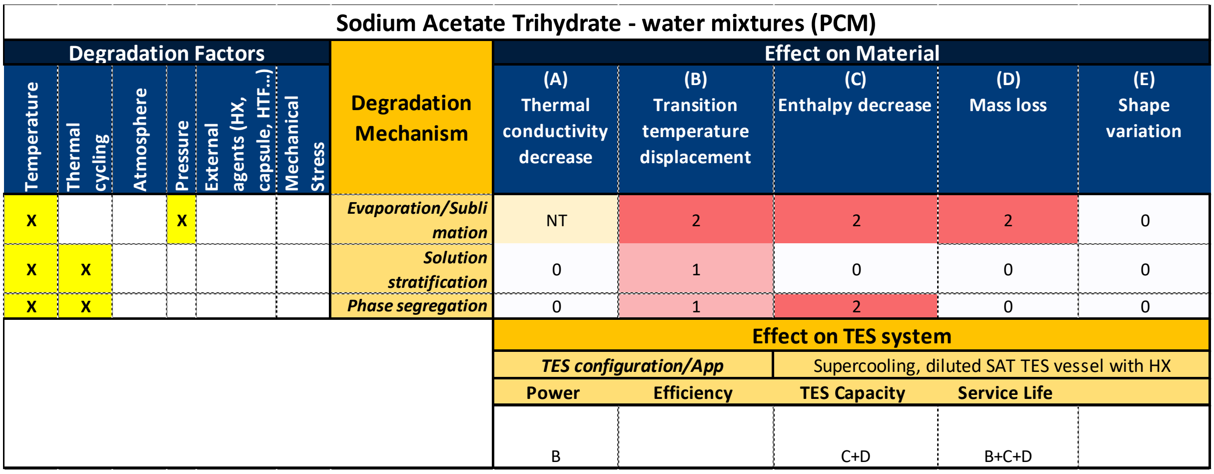
TES configuration/App	1.5 m³ latent heat storage with capillary tube heat exchanger			
Power	**Efficiency**	**TES Capacity**	**Service Life**	
B+C	B+C	B+C		

Comments: Calcium chloride hexahydrate is known as a PCM with so-called semi-congruent melting. Therefore, in a storage container, the material has to be heated regularly above 32.78 °C and mixed, so that the tetrahydrate that forms melts (dissolves). It is very important to set the right salt/water concentration, otherwise there will be a loss in enthalpy. Since calcium hloride is corrosive, the storage tank should only be built out of materials that withstand the corrosive nature. Otherwise, there is leakage to be expected over time. An evaporation of water is conceivable at very high temperatures, leading to an excess of salt, favouring the phase segregation. This has, however, so far not be tested!

Degradation mechanism	How to test/accelerate	How to deal with degradation
Phase segregation	Keep the maximum temperature below 32.78 °C (Lane, 1986) and thus prevent complete melting of the tetrahydrate	Heat well above the 32.78 °C and agitate the storage
Evaporation	Heat the storage or sample considerably above the phase change temperature	Use the PCM at temperatures of around plus minus 10 K around the phase change temperature

Figure 6-13: Degradation mapping of calcium chloride hexahydrate (by Henri Schmit, ZAE Bayern).

6.3.3.7 Sodium acetate trihydrate – water mixtures (PCM)



Sodium Acetate Trihydrate - water mixtures (PCM)

Degradation Factors						Degradation Mechanism	Effect on Material				
Temperature	**Thermal cycling**	**Atmosphere**	**Pressure**	**External agents (HX, capsule, HTF...)**	**Mechanical Stress**		**(A) Thermal conductivity decrease**	**(B) Transition temperature displacement**	**(C) Enthalpy decrease**	**(D) Mass loss**	**(E) Shape variation**
X			X			*Evaporation/Sublimation*	NT	2	2	2	0
X	X					*Solution stratification*	0	1	0	0	0
X	X					*Phase segregation*	0	1	2	0	0

Effect on TES system				
TES configuration/App		Supercooling, diluted SAT TES vessel with HX		
Power	**Efficiency**	**TES Capacity**	**Service Life**	
B		C+D	B+C+D	

Comments:

1- Sodium acetate trihydrate (SAT) - water as well as other salt hydrate compounds suffer most greatly from improper management of water vapour loss as this will permanently alter the mixture composition and, thus, its binary equilibrium phase change characteristics. Due to the high molar ratio of water to anhydrous salt, saturated water vapour pressure above the solutions remains high and is therefore liable to vapour loss at temperatures > 60 degC if not properly managed.

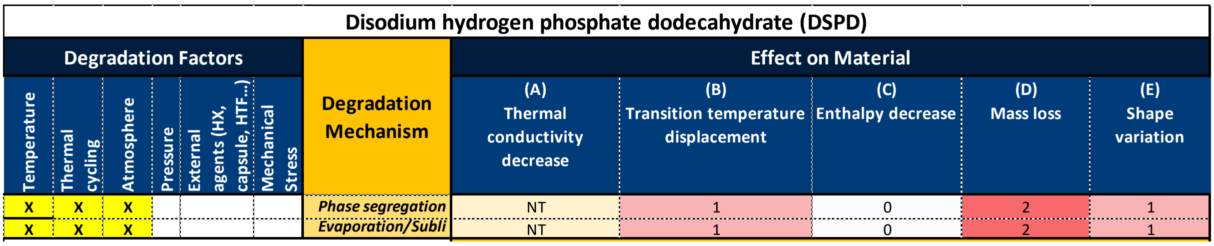
2- When using salt hydrate-water mixtures without thickeners, a vertical concentration gradient will innevitably arise, but will stabilize with time, not affecting the total available enthalpy, but redistributing it to the zones of higher salt concentration. Height of the vessel and the intensity of the heat flux giving rise to internal convection will each impact the concentration distribution over long term operation of the TES. Note that a more dilute salt hydrate-water mixture will result in more severe solution stratification, so may not be suitable for use in tall vessels as the available area for heat transfer during phase change will be limited only to the bottom of the vessel as well as significantly alter the local solubility/Tsat of the salt solution. More concentrated mixtures are overall more resistant to these shifts in Tsat.

3 - Phase segregation, i.e., formation of anhydrous salt, for incongruent salt systems can be avoided with sufficiently elevated and lengthy heat soak during the charge phase to ensure complete dissolution of the salt and allow for potentially slow dynamics of this dissolution (mass diffusion at the interface of anhydrous salt-aqueous solution)

Degradation mechanism	How to deal with degradation
evaporation (loss of water vapour)	Closed vessel with or without expansion tank maintained at > 0 atm_g. When using an external expansion tank, ensure that tube/hose run and expansion tank connection are arranged/oriented to permit reflux of condensed water vapour to the PCM vessel. Extra water, even in very minute quantities, is recommended to ensure slightly greater than the stoichiometric ratio of water to SA needed to form the desired hydrate compound. Also, vented vessels are prone to inducing heterogeneous nucleation in salt hydrate solutions that are intended to supercool due to both dehydration of salt at the liquid-vapour interface, but also from particulate contaminant transfer from ambient air
Solution stratification	Increased heat transfer intensity during charging phase may improve mixing and shift concentrated salt stratum towards the top of the vessel, but a stable concentration gradient in the liquid phase will develop over the long term but this should not decrease available enthalpy if there is no anhydride formation nor loss of water vapour. Available enthalpy becomes redistributed to the more concentrated strata, affecting mainly the heat transfer by way of affecting the temperature field along the height of the HX during phase change processes, favouring lower portions over higher ones. Select vessel height appropriately for the salt hydrate-water average concentration and typical heat flux. Increased height will both aide internal convection, but also intensify stratification, therefore not alone a means of improving solution mixing. If heat flux is insufficent, it is advised to reduce vessel height and increase width-depth instead.
Phase segregation	Superheating treatment is necessary to ensure complete dissolution of SA-water mixture on every cycle where solidification of SAT occurs (with or without supercooling/triggered nucleation).

Figure 6-14: Degradation mapping of SAT-water mixtures (by Louis Desgrosseilliers, SPF).

6.3.3.8 Disodium hydrogen phosphate dodecahydrate (PCM)



Disodium hydrogen phosphate dodecahydrate (DSPD)											
Degradation Factors						**Degradation Mechanism**	**Effect on Material**				
Temperature	**Thermal cycling**	**Atmosphere**	**Pressure**	**External agents (HX, capsule, HTF...)**	**Mechanical Stress**		**(A) Thermal conductivity decrease**	**(B) Transition temperature displacement**	**(C) Enthalpy decrease**	**(D) Mass loss**	**(E) Shape variation**
X	X	X				*Phase segregation*	NT	1	0	2	1
X	X	X				*Evaporation/Subli*	NT	1	0	2	1

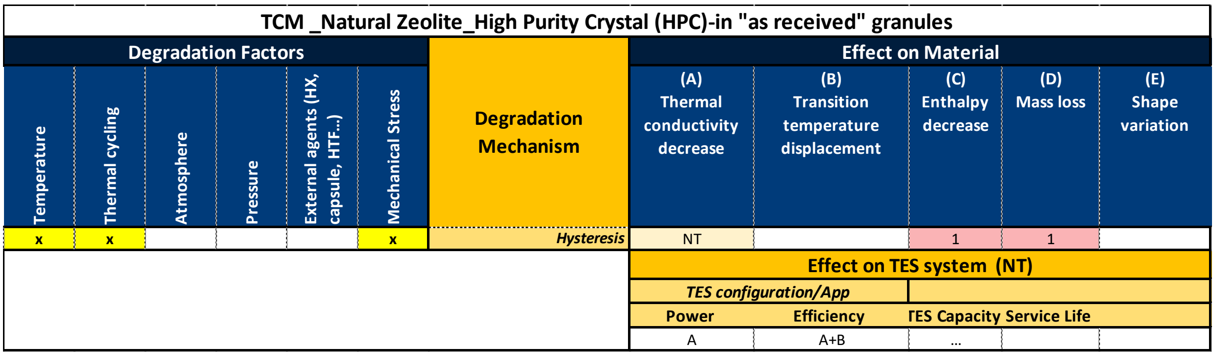
Comments: DSPD shows a strong tendency to dehydrate at compositions of 10 and 28 wt% DSP in water. The effect is stronger the more free water is available (i.e. at 10 wt% composition). XRD and XCT tests suggest that the dodecahydrate form (melting point = 32°C) is not stable, and thus it tends to dehydrate into the heptahydrate (melting point = 45°C) over time. Therefore, the dodecahydrate is not stable enough to be used as PCM.

Our studies also suggest that the dodecahydrate can occur in two different polymorphs, which are however very similar in terms of crystalline structure and occur concomitantly at the same time. Therefore, polymorphism does not affect the TES system in this case.

Degradation mechanism	How to test/accelerate	How to deal with degradation
Evaporation	Cycling, TGA isotherm	Work under controlled humidity, sealed container
Change hydration state	Cycling, isothermal tests (DSC)	Work under controlled humidity, sealed container

Figure 6-15: Degradation mapping of disodium hydrogen phosphate dodecahydrate (by Rebecca Ravotti, HSLU).

6.3.3.9 Zeolite (TCM)



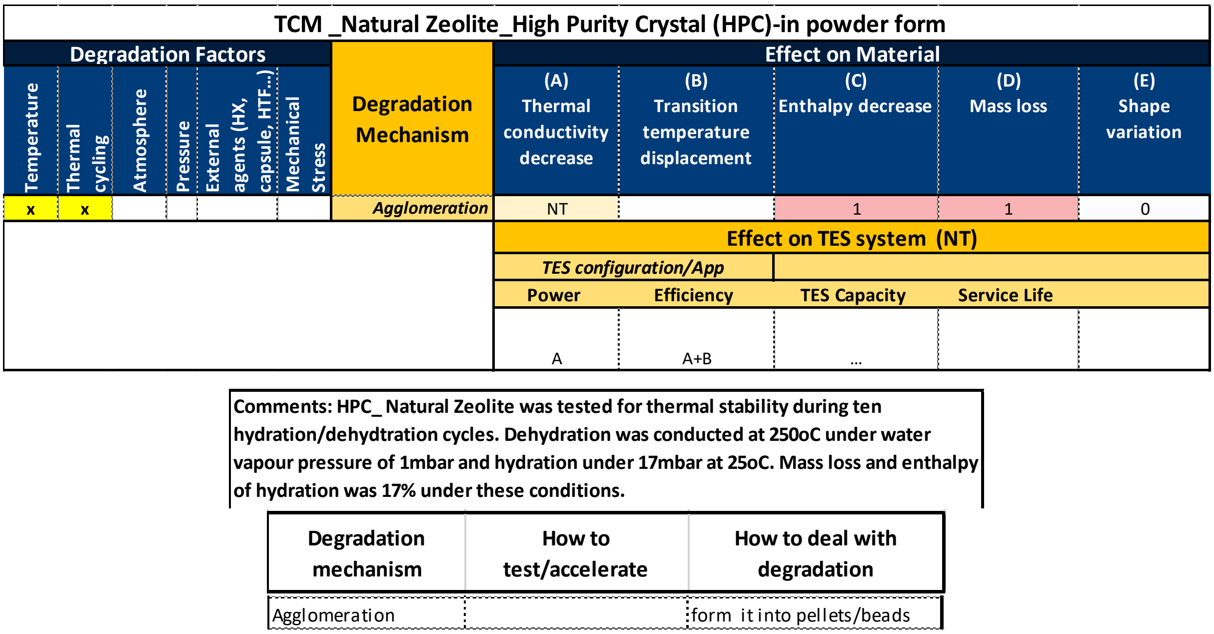
TCM _Natural Zeolite_High Purity Crystal (HPC)-in "as received" granules											
Degradation Factors						**Degradation Mechanism**	**Effect on Material**				
Temperature	**Thermal cycling**	**Atmosphere**	**Pressure**	**External agents (HX, capsule, HTF...)**	**Mechanical Stress**		**(A) Thermal conductivity decrease**	**(B) Transition temperature displacement**	**(C) Enthalpy decrease**	**(D) Mass loss**	**(E) Shape variation**
x	x				x	*Hysteresis*	NT		1	1	

Effect on TES system (NT)				
TES configuration/App				
Power	**Efficiency**	**TES Capacity Service Life**		
A	A+B	...		

Comments: Pellets of the HPC_ Natural Zeolite was tested for thermal stability during ten hydration/dehydtration cycles. Dehydration was conducted at 250oC under water vapour pressure of 1mbar and hydration under 17mbar at 25oC. Mass loss and enthalpy of hydration was ~20% under these conditions. The shape of the pellets has not change and after 4 cycles the mass loss was only 7%.

Degradation mechanism	How to test/accelerate	How to deal with degradation
Hysteresis		optimize the hydration/dehydration comditions

Figure 6-16: Degradation mapping of zeolite pellets (by Lia Kouchachvili, CanmetENERGY).



TCM _Natural Zeolite_High Purity Crystal (HPC)-in powder form

Degradation Factors						Degradation Mechanism	Effect on Material				
Temperature	Thermal cycling	Atmosphere	Pressure	External agents (HX, capsule, HTF...)	Mechanical Stress		(A) Thermal conductivity decrease	(B) Transition temperature displacement	(C) Enthalpy decrease	(D) Mass loss	(E) Shape variation
x	x					*Agglomeration*	NT		1	1	0

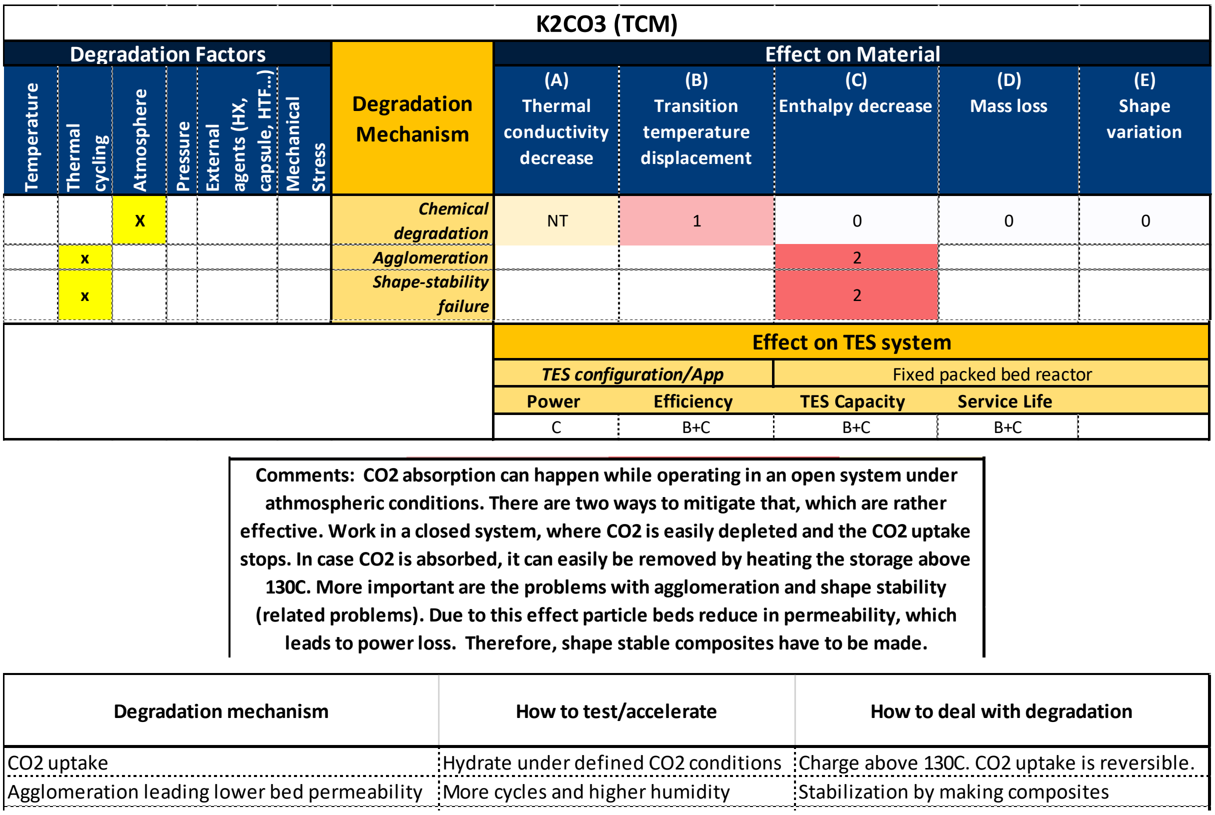
Effect on TES system (NT)				
TES configuration/App				
Power	Efficiency	TES Capacity	Service Life	
A	A+B	...		

Comments: HPC_ Natural Zeolite was tested for thermal stability during ten hydration/dehydtration cycles. Dehydration was conducted at 250oC under water vapour pressure of 1mbar and hydration under 17mbar at 25oC. Mass loss and enthalpy of hydration was 17% under these conditions.

Degradation mechanism	How to test/accelerate	How to deal with degradation
Agglomeration		form it into pellets/beads

Figure 6-17: Degradation mapping of zeolite powder (by Lia Kouchachvili, CanmetENERGY).

6.3.3.10 Potassium carbonate (TCM)



K2CO3 (TCM)

Degradation Factors						Degradation Mechanism	Effect on Material				
Temperature	Thermal cycling	Atmosphere	Pressure	External agents (HX, capsule, HTF...)	Mechanical Stress		(A) Thermal conductivity decrease	(B) Transition temperature displacement	(C) Enthalpy decrease	(D) Mass loss	(E) Shape variation
		X				*Chemical degradation*	NT	1	0	0	0
	x					*Agglomeration*			2		
	x					*Shape-stability failure*			2		

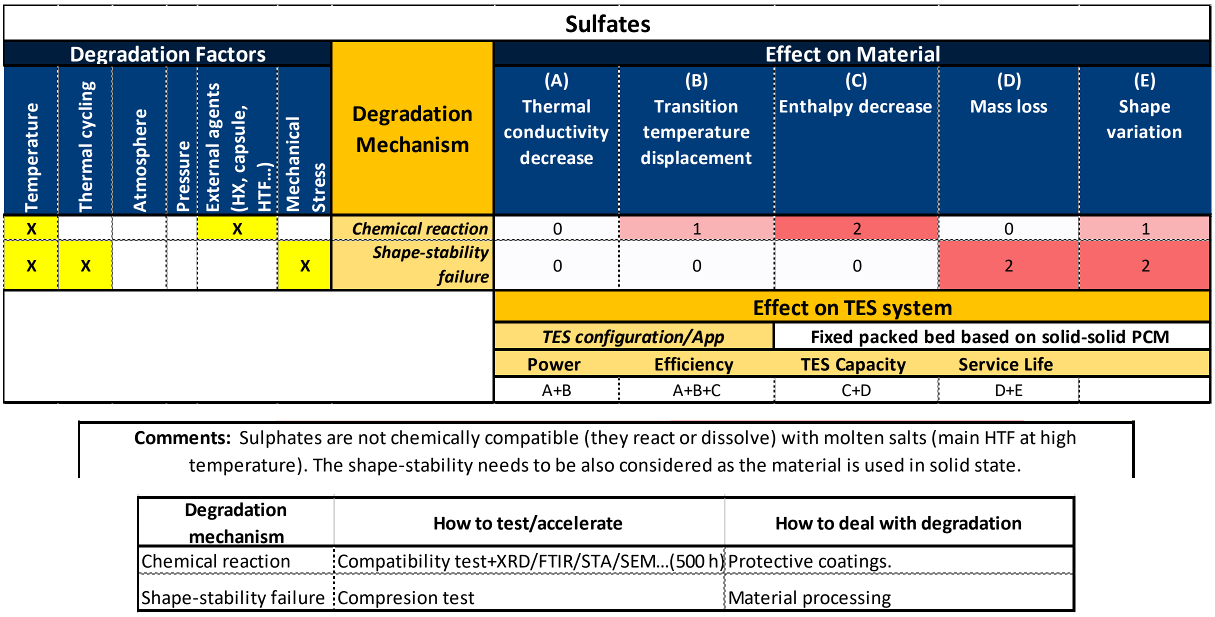
Effect on TES system				
TES configuration/App	Fixed packed bed reactor			
Power	Efficiency	TES Capacity	Service Life	
C	B+C	B+C	B+C	

Comments: CO2 absorption can happen while operating in an open system under athmospheric conditions. There are two ways to mitigate that, which are rather effective. Work in a closed system, where CO2 is easily depleted and the CO2 uptake stops. In case CO2 is absorbed, it can easily be removed by heating the storage above 130C. More important are the problems with agglomeration and shape stability (related problems). Due to this effect particle beds reduce in permeability, which leads to power loss. Therefore, shape stable composites have to be made.

Degradation mechanism	How to test/accelerate	How to deal with degradation
CO2 uptake	Hydrate under defined CO2 conditions	Charge above 130C. CO2 uptake is reversible.
Agglomeration leading lower bed permeability	More cycles and higher humidity	Stabilization by making composites

Figure 6-18: Degradation mapping of potassium carbonate (by Henk Huinink, TU Eindhoven).

6.3.3.11 Sulfates (TCM)



Sulfates

Degradation Factors						Degradation Mechanism	Effect on Material				
Temperature	Thermal cycling	Atmosphere	Pressure	External agents (HX, capsule, HTF...)	Mechanical Stress		(A) Thermal conductivity decrease	(B) Transition temperature displacement	(C) Enthalpy decrease	(D) Mass loss	(E) Shape variation
X				X		*Chemical reaction*	0	1	2	0	1
X	X				X	*Shape-stability failure*	0	0	0	2	2

Effect on TES system

TES configuration/App	Fixed packed bed based on solid-solid PCM		
Power	**Efficiency**	**TES Capacity**	**Service Life**
A+B	A+B+C	C+D	D+E

Comments: Sulphates are not chemically compatible (they react or dissolve) with molten salts (main HTF at high temperature). The shape-stability needs to be also considered as the material is used in solid state.

Degradation mechanism	How to test/accelerate	How to deal with degradation
Chemical reaction	Compatibility test+XRD/FTIR/STA/SEM...(500 h)	Protective coatings.
Shape-stability failure	Compresion test	Material processing

Figure 6-19: Degradation mapping of sulfates (by Ángel Serrano, CIC energiGUNE).

6.3.4 Conclusions

The developed approach to map degradation of CTES materials provides a comprehensive overview of the degradation mechanisms and the corresponding degradation factors which are relevant for a specific material or material class. Such a mapping diagram informs about the effect of different types of degradation on the CTES material and system.

It becomes evident that a certain effect on the material (e.g. a transition temperature displacement) can be caused by different degradation mechanisms (cf. example of SAT-water mixtures in section 6.3.3.7). In the same way, effects on the storage behaviour can usually be attributed to a combination of different effects on the material. In practice, this means that stability tests under application conditions can only be carried out reasonably if there is already an understanding of the dependencies between degradation factors, degradation mechanisms and effects on the CTES material/ system. Such an understanding can be summarized and communicated using the developed degradation mapping diagram.

6.4 Key messages

Key messages of Subtask D are grouped in two categories – key messages on collected data and key messages on deliverables.

The key messages on the collected data are:

- Task 40 experts have comprehensive knowledge on investigating stability and dealing with degradation of CTES materials.
- The developed stability mapping table offers an easy-to-use visualization of CTES material degradation behaviour.
- Experiments to accelerate degradation were collected to accelerate stability investigations.

The key messages on the deliverables are:

- CTES material stability depends on the nature of the material (class) and the operating conditions of the application or laboratory test.
- Understanding CTES stability starting with degradation processes on material level is important to understand a possible performance reduction at component and system level.

In many cases, operating conditions can be selected that allow an application without performance reduction caused by material degradation.

6.5 Outlook

Based on the findings of Subtask D, future research topics could be:

- Development of standardized validation protocols for PCM and TCM stability: Given the lack of widely accepted testing guidelines for validating storage media, a key area for future research would be to create standardized, step-by-step protocols for (long-term) stability prediction and validation.
- Identification and quantification of degradation factors in CTES materials: Further research is needed to identify and quantify the specific degradation mechanisms and factors that affect the stability of PCM and TCM. This could involve developing experimental methods to assess material performance under varying stress levels and environmental conditions, leading to more accurate performance and lifespan predictions.
- Application-specific tailoring of PCM and TCM testing methods: Since different applications impose varying conditions on CTES materials, future research should focus on tailoring testing protocols to specific use cases, for instance high-temperature thermal energy storage. This could include the development of application-specific lifetime prediction models and the exploration of optimized testing methodologies to ensure the reliable performance of materials in real-world scenarios.

6.6 References

[1] W. van Helden, A. Hauer et al. (2020). Material and Component Development for Thermal Energy Storage, *IEA SHC Task 58 / ES Annex 33 Final Report*, available at https://iea-es.org/publications/final-report-annex-33/

[2] J. G. C. Storch (2010). Materialwissenschaftliche Untersuchungen an zeolithischen Adsorbenzien für den Einsatz in offenen Sorptionssystemen zur Wärmespeicherung, Doctoral dissertation, *Technical University Munich*, available at https://mediatum.ub.tum.de/doc/820976/820976.pdf

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7 Subtask E: Effective Component Performance with Innovative Materials

The work in Subtask E on PCM and TCM was carried out in separate groups. Accordingly, the results are also presented separately.

7.1 PCM

7.1.1 Performance indicators

One of the main objectives of the PCM part of Subtask E was to define performance indicators that allow a fair comparison of latent heat thermal energy storage units. This has not been possible so far, as a mere comparison of the average thermal power, for example, is strongly influenced by the initial and boundary conditions during the experiment [1]. Essentially, three methods were developed by the task participants within the task and other projects to minimize these influences and enable a comparable analysis. These methods are briefly presented below and reference is made to further literature where available.

7.1.1.1 $\overline{\dot{C}^{\text{norm}}}/\overline{\dot{Q}^{\text{norm}}}$-plots

Based on previous work done by some participants of the Task [2], the main idea of the approach is to normalize the heat transfer rate $\dot{Q}$ by the volume and a reference temperature difference, calculate a mean value and present the results plotted over a normalized mean value of the capacity flow of the heat transfer fluid in a so-called $\overline{\dot{C}^{\text{norm}}}/\overline{\dot{Q}^{\text{norm}}}$-plot. The definition of the reference temperature difference (for instance the inlet temperature of the heat transfer fluid and the melting temperature of the PCM) and the procedure to calculate the mean of $\dot{Q}$ may have a large effect on the results obtained. A detailed discussion of these aspects can be found in [3] where more than 30 experiments performed by the participants were analyzed. An example of a $\overline{\dot{C}^{\text{norm}}}/\overline{\dot{Q}^{\text{norm}}}$-plot is shown in Figure 7-1.

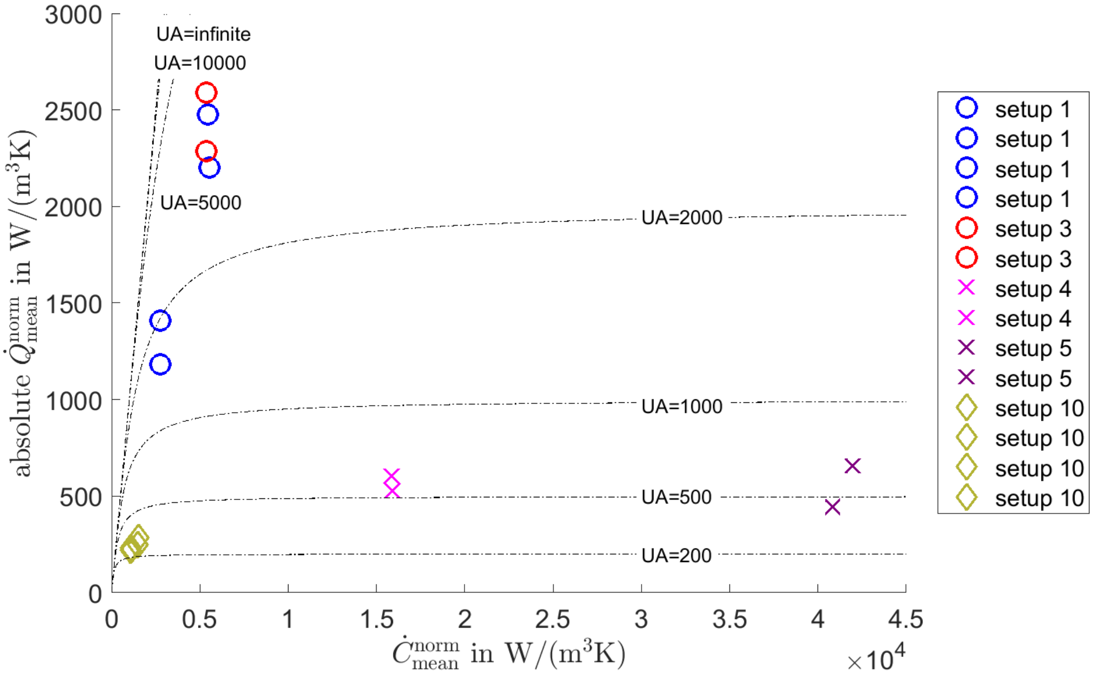

Figure 7-1: Example of a $\overline{\dot{C}^{\mathrm{norm}}}/\overline{\dot{Q}^{\mathrm{norm}}}$-plot for five latent heat thermal energy storage units under different boundary conditions.

7.1.1.2 Three sections approach

One of the greatest difficulties encountered when calculating a mean value of the power of latent heat thermal energy storage units is finding a suitable stop criterion. This is where the "three sections approach" comes in. Tangents are laid through the inflection points that occur in a characteristic discharge power curve of a latent heat thermal energy storage unit. The discharging process is divided into several sections and the end is determined on the basis of their intersections with each other and with the zero line, respectively. The procedure is illustrated in Figure 7-2.

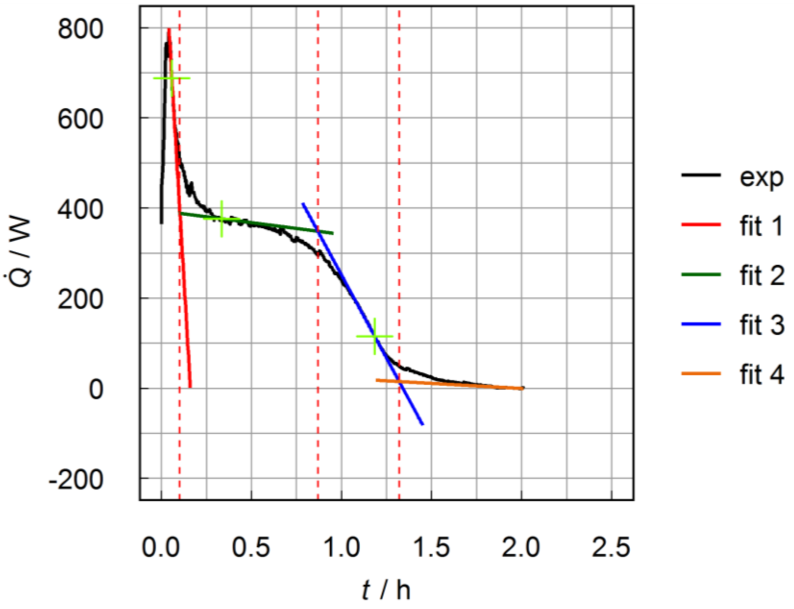

Figure 7-2: Example of the three sections approach shown for the discharging power of a latent heat thermal energy storage unit.

Together with the three sections approach, a comparison with an ideal sensible thermal energy storage unit was also proposed. This also complements the $\overline{\dot{C}^{\mathrm{norm}}}/\overline{\dot{Q}^{\mathrm{norm}}}$-plots well, as in these the UA infinite line (see Figure 7-1) corresponds to an ideal sensible thermal energy storage unit and the plots proposed here and shown in Figure 7-3 give more insight into the actual discharging process.

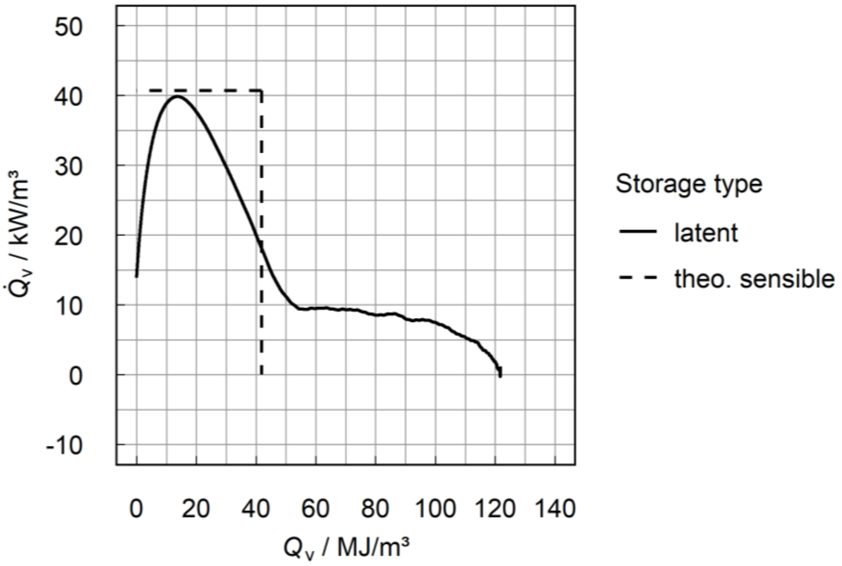

Figure 7-3: Comparison of the discharging power curve of an ideal sensible thermal energy storage unit vs. the discharging power curve of a latent heat thermal energy storage unit.

7.1.1.3 Constant power diagrams

The project VKTES (Development of comparative key figures for thermal energy storage) is funded by the German Federal Ministry for Economic Affairs and Climate Action. The aim of the project is to define key figures for thermal storage systems that will enable the most suitable storage to be selected when planning thermal energy systems. The results will be incorporated into VDI guideline 4657-2, which will be published in 2025. The procedure was presented and discussed within Subtask E during several meetings and has enriched the work of the group.

The procedure for determining the key figures is to be carried out by the manufacturers themselves and should be as simple as possible. The results are to be presented in standardized form on the data sheets of the storages and incorporated into the planning process for thermal energy systems. The procedure is to be applied to all possible types of heat storages (sensible and latent) from the field of building technology.

Depending on the operating conditions, the actual usable heat content of a thermal energy storage can deviate significantly from the theoretical storage capacity calculated from the geometry and material parameters. This can drastically reduce the amount of usable heat, especially at high thermal power rates. The approach developed in the project is intended to take these dependencies into account. It is based on a small number of standardized charging and discharging measurements with a constant volume flow and constant inlet temperature. The resulting power curves are normalized and converted from the time domain to the energy domain. The curves are plotted in such a way that the actual usable heat content of the storage can be determined for specified values for the set thermal power, the temperature and the maximum volume flow.

The method was tested experimentally at several institutes from the project consortium on various sensible and latent heat storages. It was shown that it is well suited for predicting the usable heat content for a variety of operating parameters with sufficient accuracy.

The results from the project will be published in the final report at the *TIB – Leibniz Information Centre for Science and Technology*[6].

7.1.2 Material-component interaction

7.1.2.1 The UA-approach

In addition to simulations and experimental investigations, an analytical method was developed to show the influence of material properties on the performance of latent heat thermal energy storage systems. A simple and illustrative formula (equation 1) was derived which predicts the total discharging time t_{sol} with the help of the UA value, the mass flow rate ($\dot{m}$), the heat capacity (c_{p}) and the inlet temperature (T_{in}) of the heat transfer fluid as well as the energy stored in the storage (Q_{LHTES}) and the melting temperature (T_{m}).

$$t_{\mathrm{sol}} = \left(1 + \frac{UA}{\dot{m} \cdot c_{\mathrm{p}}}\right) \cdot \frac{Q_{\mathrm{LHTES}}}{UA \cdot (T_{\mathrm{m}} - T_{\mathrm{in}})} \tag{1}$$

The UA value is calculated by $UA = 2 \cdot A \cdot \lambda / s$ with the heat transfer surface A, the thermal conductivity λ and the PCM thickness s (s gets half the thickness if the PCM solidifies from two sides).Equation 1 can be further simplified by introducing the number of transfer units (NTU) and the time the PCM at the inlet takes to solidify completely. In this way, equation 2 is obtained.

$$t_{\mathrm{sol}} = (1 + NTU) \cdot t_{\mathrm{sol}}^{\mathrm{init}} \tag{2}$$

The method is currently only valid for plate-type latent heat thermal energy storage units, but a combination with approaches available in the literature for other geometries is conceivable [4][5]. Furthermore, the corresponding publication [6] contains studies on how to include the sensible heat and the thermal resistance of the HTF. A combination with numerical models is also considered.

7.1.3 Experimental characterization

7.1.3.1 Review on existing standards and procedures

There are two standards ASHRAE STANDARD 94.1-2002(RA 2006) “Method of testing active latent heat storage devices based on thermal performance” Regarding the experimental characterization of the thermal performance of latent heat- based TES systems and ANSI/ASHRAE Standard 150-2000 (RA 2004) “Method of Testing the Performance of Cool Storage Systems”. Furthermore, the German participants in the group informed that a German standard was also being prepared to be published by the end of 2024.

Besides the national/international standards which do not completely satisfy the requirements to assess the thermal performance and compare the latent heat storages components from the working group perspective, a survey was collected and the results on the procedures followed by the participants were analysed. The participants listed in the following answered questions about the testing and the measurements procedures to assess the thermal performance.

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[6] https://www.tib.eu/en/

Table 7-1: Participants of the survey on experimental characterization of PCM storage units.

Institutions: participant(s)
CNR ITAE: A. Frazzica, V. Brancato, V. Palomba
Delft University of Technology: Kamel Hooman
Department of Civil and Mechanical Engineering, DTU: Elsabet Nielsen
Department of Civil and Mechanical Engineering, DTU: Jianhua Fan and Gerald Englmair
Fraunhofer ISE: Sebastian Gamisch, Stefan, Gschwander
German Aerospace Center (DLR): Jonas Tombrink, Wolf-Dieter Steinmann
I3a-University of Zaragoza: Monica Delgado, Ana Lazaro
Icam-LTeN (CNRS-Nantes University): Jérôme SOTO
Lab of Applied Multiphase Thermal Engineering – Dalhousie University: Dominic Groulx
Universitat de Lleida: Emiliano Borri, Gabriel Zsembinzski, Luisa F. Cabeza
ZAE Bayern: Simon Pöllinger, Christoph Rathgeber

From the answers received, the following conclusions were depicted:

Operational conditions:

10/11 constant mass flow+constant inlet temperature

8/11 complete melting/solidification tests

10/11 Liquid heat transfer fluid (HTF)

Measurement & sensors:

10/11 HTF inlet/outlet temperatures measured with PT100

Mass flow: Coriolis, magnetic flow meter, pump curve with ΔP measurement

Surface temperature of PCM: thermocouples, Pt100, IR camera

Power estimated from HTF: $\dot{Q} = \dot{m}c(T_{\text{inlet}} - T_{\text{outlet}})$

Energy balance:

Heat losses estimation using steady state testing at different temperatures (only 3 answers received mentioned the evaluation of heat losses)

Thermal performance evaluation:

- Power over time curves

3/11 UA estimation using either phase change temperature/average PCM surface temperature

7.1.3.2 Key points on experimental characterization to be addressed

The working group proposed a draft of experimental procedure attending the most common operation modes: Liquid as heat transfer fluid, constant mass flow and constant inlet temperature of the heat transfer fluid for complete melting/solidification tests.

Objective of the experimental characterization: storage capacity between two temperatures and thermal performance under different conditions, thus the following magnitudes are to be measure.

Table 7-2: Experimental characterization of PCM storage units – magnitudes to be measured.

Magnitude	Most used technique	Recommendation	Additional comments
Heat transfer fluid mas flow	Coriolis, magnetic flow meter, pump curve with ΔP measurement	Direct mass flow measurement	
Heat transfer temperature different between the inlet of the TES system and the outlet.	2xPt100 Thermopile		Representative location when large sections. Existing standard.
TES system volume with insulation			
TES system volume without insulation			

Additional measurements can be considered to complete the characterization.

Table 7-3: Experimental characterization of PCM storage units – additional measurements.

Measurement	Most used technique	Additional comments
Temperature of the storage material or temperature of the HX surface at different location	Thermocouples Pt100 IR camera	to check HX and temperature distribution over time
Pressure drop		hydraulic characterization of the TES system and blocking inside the TES system detection
Ambient temperature	thermocouple	Heat losses estimation

Operation:

Heat losses characterization of the TES system with insulation. Possible approaches:

- Water at different temperatures with no HTF
- HTF at different temperatures
- From steady states at different temperatures

TES system filled with storage material testing:

1) Initial state: steady state at HTF temperature set point ($T_{HTFSp,\ ini}$)*

Conditions to fulfilled the steady sate:

- ✓ Temperature of the HTF at the inlet (T_{inlet}) variation < 1K
- ✓ Temperature of the HTF at the outlet(T_{outlet})variation < 1K

* $T_{HTFSp,\ ini}$>T melting for solidification tests and $T_{HTFSp,\ ini}$>T solidification for melting tests

Performance parameters and results:

1) Capacity parameters were agreed on former task. The evaluation is recommended to provide the parameters: Heat losses included/not included. Insulation included/not included. Integration limits in Power vs time curves.

   Thermal power exchanged is evaluated from experimental data as follows (as the HTF hast no phase change):

$$\dot{Q}(t) = \dot{m}(t) \cdot c_{\mathrm{HTF}} \cdot \Delta T(t) = \dot{m}(t) \cdot c_{\mathrm{HTF}} \cdot (T_{\mathrm{outlet}}(t) - T_{\mathrm{inlet}}(t))$$

   Where $\dot{m}(t)$ is the HTF mass flow (kg/s), c_{HTF} is the specific heat capacity of the HTF in the given temperature range (kJ/(kg·K)).

   Energy storage capacity, ESC_{sys}, between $T_{\mathrm{HTFSp,\,ini}}$ and $T_{\mathrm{HTFSp,\,test}}$ can be estimated as follows:

$$ESC_{\mathrm{sys}} = \int_{T\_\mathrm{HTFSp,ini}}^{T\_\mathrm{HTFSp,test}} \dot{Q}(t) \cdot dt$$

Table 7-4: Definition of energy storage capacity and density.

	definition	units	Theoretical estimation
Energy storage capacity of the system (ESC)	$ESC_{\mathrm{sys}}=ESC_{\mathrm{mat}}+ESC_{\mathrm{comp}}$	kJ or MJ	Temperature range [T_{max}, T_{min}] $ESC_{\mathrm{mat}}=m_{\mathrm{mat}}\cdot\Delta h_{\mathrm{mat}}$ $ESC_{\mathrm{comp}}=m_{\mathrm{comp}}\cdot\Delta h_{\mathrm{comp}}$ Δh: Enthalpy variation within the temperature range
Energy storage density (ESD)	ESD: ESC_{sys}/V $ESD_{\mathrm{without\ ins}}$: $ESC_{\mathrm{sys}}/V_{\mathrm{without\ ins}}$	kJ/m^3 or MJ/m^3	V: Total volume of the heat exchanger, considering insulation and vessel (m^3) $V_{\mathrm{without\ ins}}$: Total volume of the heat exchanger and vessel, but not considering insulation (m^3)

2) Power parameters

As mentioned in the previous section, thermal power exchanged is evaluated from experimental data and the agreement on the minimum recommended data to be provided was:

- Temperature range ($T_{\mathrm{HTFSp,ini}}$ and $T_{\mathrm{HTFSp,test}}$)
- Phase change temperature range of the storage material
- Heat storage material mass (kg)
- ESC_{sys}
- Maximum power, average power
- Power over time curve

7.1.4 References

[1] Groulx, Dominic. "The rate problem in solid-liquid phase change heat transfer: Efforts and questions toward heat exchanger design rules." *Proceedings of the 16th International Heat Transfer Conference (IHTC-16), Beijing, China*. Vol. 16. 2018.

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[4] Alexiades, V., and A. D. Solomon. "Mathematical modeling of melting and freezing processes." (1992).

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7.2 TCM

7.2.1 Introduction

The goal of Subtask E is to optimize the performance of sorption heat storage systems by improving material-component interactions and enabling system comparisons. This is achieved by supporting collaboration in the research community through the establishment of standardized performance metrics for both internal evaluation of individual systems and external comparison between systems. This report provides insight into the standardization developed by Subtask members for system performance with respect to:

- The storage material (internal)
- Other systems (external)

It is widely recognized in the research community that there is a large discrepancy between material and system performance in sorption heat storage [1,2].

7.2.2 Key Achievements

The objective of this Subtask is to develop uniform performance metrics for material-component interaction processes to establish standardized performance metrics that allow consistent evaluation of material-component interactions for different sorption heat storage systems under development.

The achievements of this work are:

- The Development of a standardized absorption curve based performance mapping. This allows system performance to be compared with theoretical material performance. The procedure is published in [3] and further summarized in section 7.2.4.
- The development of a standardized temperature-based test procedure for sorption heat storage in the space heating application. This procedure is published in [4] and summarized in section 7.2.5.
- Based on the standardized temperature-based test procedure, the development of a realistic, application-specific temperature and energy performance table that reflects real operating

conditions for specific applications and provides clear guidance on the expected performance of different system configurations is proposed and summarized in section 7.2.6.

This work is critical given the temperature-dependent performance of sorption materials and systems. Promoting the adoption of this procedure across different processes and demonstrator systems remains a priority.

On this basis, experimental data from various demonstrator systems provided by Subtask participants can be compiled and analyzed to evaluate the interaction between materials and components, highlight key performance characteristics, and identify areas for improvement.

Two surveys were conducted to gather input on system designs and performance evaluation methodologies. The first survey identified a wide variety of system designs, while the second aimed to collect descriptions of component development and testing practices.

The depth of collaboration among the partners was restricted. This is expected due to the nature of this level of research, which involves industrial collaboration and agreement of non-disclosure.

7.2.3 Key performance indicators

The key performance indicators in this work are recognized to be:

- Gross temperature lift (GTL) - [K].

  This is the temperature rise from the low temperature heat source to the high temperature heat sink or vice versa.

- Volumetric energy density - [kWh/m^3].

  This is highly dependent on the test temperature and the definition of the storage volume. So far it is recommended to use the largest volume of sorption material.

- Volumetric charge/discharge power - [W/m^3].

  Power also depends on operating temperatures and is related to energy density.

- Round trip efficiency - [kWh$_{out}$/kWh$_{in}$].

  Due to the low availability (lack) of operational sorption-based thermal energy storage systems, this performance indicator is not yet applicable on the system development scale.

7.2.4 Performance mapping

There is a need for a standardized evaluation of sorption heat storage components and systems with respect to the material performance given by the vapor pressure versus temperature relationship of various concentrations or mass fractions. This standard evaluation will make it possible to quantify development success. As shown in Figure 7-4, deviation from the equilibrium indicates performance loss.

The performance map of the sorption heat storage is based on a good characterization of the sorption material used. An example of such a map is shown in Figure 7-4.

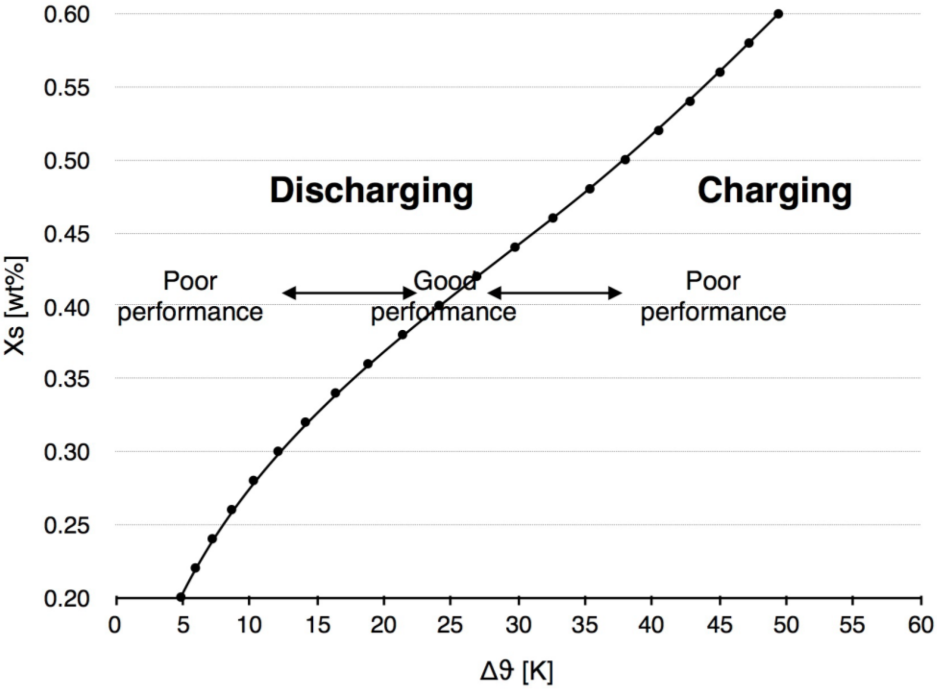

Figure 7-4: Illustration of the mapping procedure, where the x-axis represents the temperature difference between sorbate and sorbent and the y-axis represents the weight percent or mass fraction. Deviation from the theoretical curve indicates loss of system performance.

Key findings in this work are:

- **Non-linear temperature-heat correlation:** There is a non-linear relationship between temperature gain and heat release in all sorption processes. As the sorbent's concentration increases, the temperature gain also increases, but the heat release rate does not linearly follow, leading to potential stagnation in heat transfer, particularly when high-temperature gradients are required.
- **Performance mapping method:** A performance mapping technique is developed using a concentration vs. gross temperature lift diagram, which incorporates the sorbent's equilibrium line and the deviation caused by the non-linear temperature-heat relationship. This mapping helps visualize the operational constraints and the potential performance of the system.
- **Temperature constraints and system operation:** The work emphasizes the importance of operating the system at the minimum necessary temperature rise (gross temperature lift) to optimize heat transfer.
- **Practical implications for building applications:** From this work, it is concluded that sorption heat storage systems could significantly improve energy efficiency in buildings, especially for inter-seasonal heat storage. However, practical implementation requires careful optimization of system parameters to manage the non-linear heat transfer characteristics effectively.

7.2.5 Temperature guideline

There is a need for standardized test conditions for sorption heat storage systems used for long-term thermal energy storage for space heating in buildings. Sorption storage heat storage systems offer the advantage of minimal losses over time compared to traditional thermal storage methods. However, their performance is highly dependent on operating temperatures, which often vary widely and are frequently inconsistently reported in literature. This makes it difficult to compare results between studies.

Key challenges identified are:

- Existing test temperatures for sorption thermal storage systems vary widely and often do not reflect real-world conditions relevant to building applications. This inconsistency can lead to overestimates of performance and hinders the ability to make accurate comparisons between different systems and materials.
- Sorption storage heat storage systems operate on the principle of sorbate release and uptake by a sorbent material. This process is controlled by a temperature swing mechanism where heat is either added or removed to shift the sorption equilibrium. This is dependent on the equilibrium between temperature, pressure and sorbent concentration.

To overcome this problem of incomparable test results from different test methods, a uniform test guideline is proposed. The proposed guideline defines specific static test temperatures that correspond to realistic operating conditions for building applications:

- **Desorption**: Heat source temperatures are set to a maximum of 95 °C input and 92 °C output, which are conditions achievable by solar thermal systems without exceeding practical limits.
- **Condensation**: Heat rejection during charging is performed with water-based heat transfer fluid (HTF) at 30 °C inlet and 35 °C outlet, in line with standard heat pump conditions (EN 14511).
- **Evaporation**: Discharge evaporation takes place at 10 °C inlet and 7 °C outlet, simulating typical low temperature ground heat sources (geothermal heat exchangers) in building environments as defined by the EN 14511 heat pump test standard.
- **Sorption**: Heat absorption also follows the heat pump standard, with HTF temperatures of 30 °C inlet and 35 °C outlet.

This guideline standardizes the evaluation of sorption heat storage systems by ensuring that materials, components, and systems are tested under comparable and realistic conditions. By standardizing test conditions, the guideline facilitates more accurate comparisons of energy density power and temperature gain (gross temperature lift) performance, supporting the advancement of sorption heat storage systems as a viable solution for improving the energy efficiency of buildings.

7.2.6 Realistic application specific performance chart

Based on the test guideline outlined in section 7.2.5, a realistic, application-specific performance chart can be developed. As emphasized, the performance of a sorption heat storage depends on both the heat source and the heat sink during the charge and discharge processes. Therefore, presenting performance data with a simple temperature and energy density graph, as has sometimes been done, does not capture the full complexity of these systems. To facilitate clear and simple communication, especially with non-experts, it is critical to base performance charts on a standardized test guideline.

Figure 7-5 illustrates an application-specific performance chart that follows the proposed temperature test guideline. The graph shows the required desorption input temperature (green) and the absorption output temperature (red), the latter being constant as defined by the test standard, of varying possible systems (varying shapes). The resulting energy density is shown under the conditions specified in the guideline, with the energy density values related to the maximum volume of the sorbent working pair.

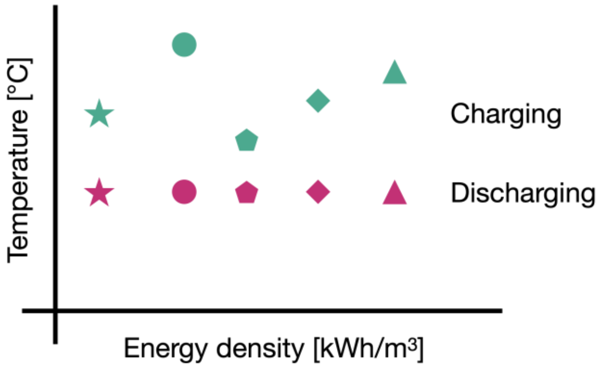

Figure 7-5: Illustration of a realistic application-specific performance chart based on a temperature test guideline. The graph shows the required charge input temperature, the constant discharge output temperature (as defined by the standard), and the specific energy density achieved.

By following the test guideline, this approach allows for the creation of representative and comparable performance charts. However, it should be noted that few results are currently available that follow the defined procedure, highlighting the need for wider adoption of these standardized test methods.

7.2.7 Conclusions

Subtask E has made good progress in advancing the understanding of material-component interactions within sorption heat storage systems. The development of standardized performance indicators, coupled with ongoing analysis of component designs and material properties, is paving the way for more efficient and scalable energy storage solutions. A next step focusing on the establishment of a best practice handbook will provide critical guidance for future development, ensuring that sorption heat storage technologies continue to evolve to meet the demands of diverse heating applications.

For continued success, it is essential to enhance collaboration among task participants, expand the adoption of standardized testing procedures, and address the identified barriers to data sharing and engagement. These efforts will be crucial in achieving the broader goals of Task 40 and supporting the deployment of advanced thermal energy storage technologies worldwide.

7.2.8 Key Messages

1. **Performance Variability**:
    - The performance of thermal energy storage systems is highly dependent on the specific application, necessitating tailored material characterizations and system configurations.
2. **Need for Standardized Testing**:
    - Uniform test schemes are critical for meaningful comparisons of system performance. Despite the establishment of standardized procedures, broader adoption and adherence are needed to facilitate comprehensive evaluations across diverse systems.
3. **Barriers to Progress**:
    - Key barriers include the diversity in system development stages among participants, limited data sharing due to commercial sensitivities, and inconsistent engagement in collaborative efforts. Addressing these challenges is essential for advancing the Subtask objectives and achieving broader impacts.

7.2.9 References

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8 Appendices

8.1 Appendix Subtask A - Software Requirements Document for the new thermal energy storage material database

Adobe Acrobat
Document

8.2 Appendix Subtask D – Stability of PCM and TCM

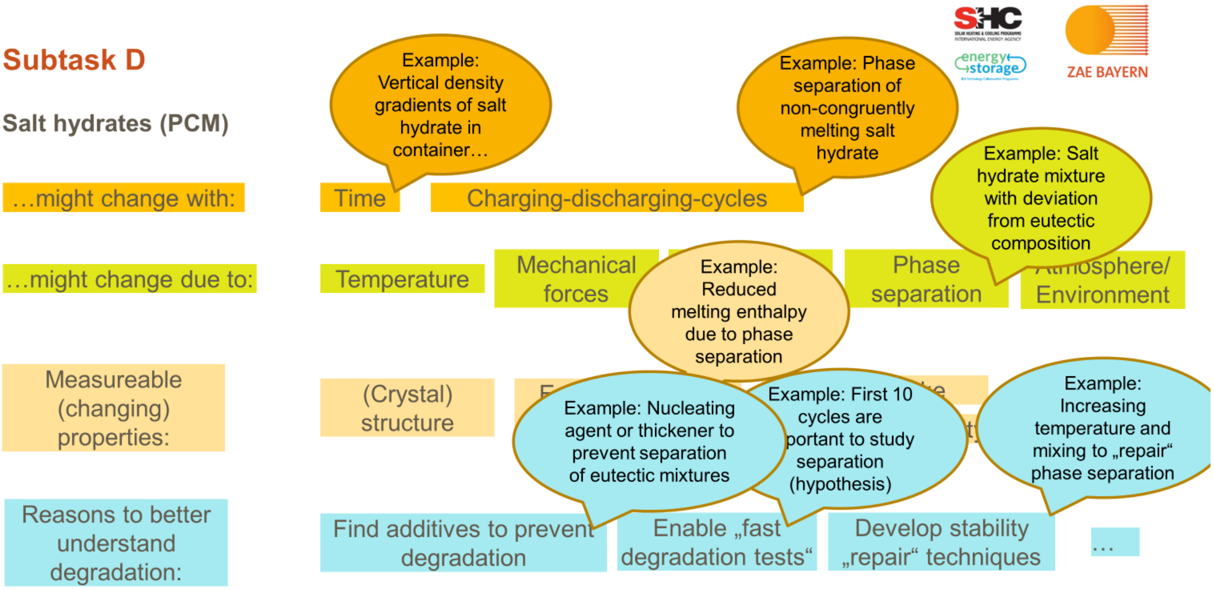


Figure 8-1: First approach to structure CTES material stability filled in for salt hydrates as PCM (source: ZAE Bayern).

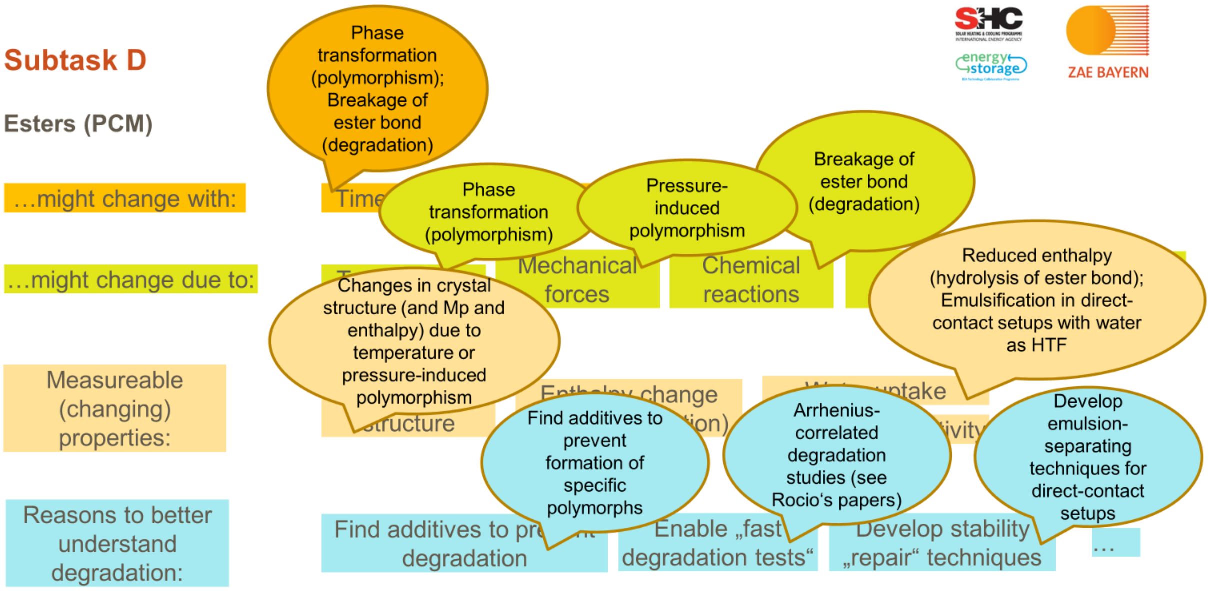
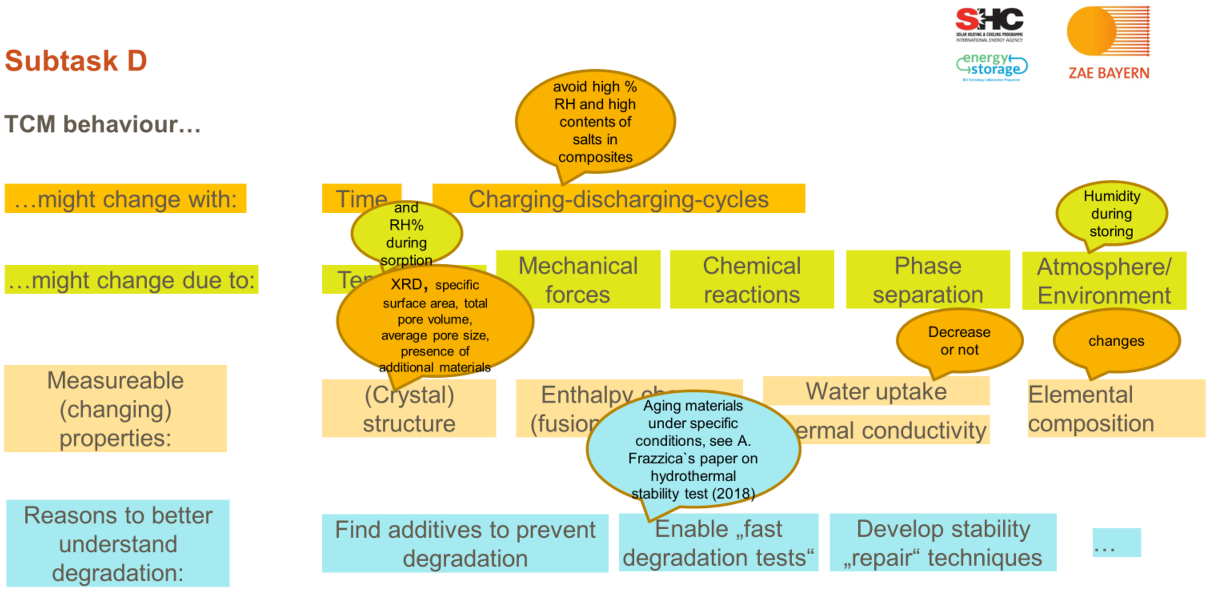


Figure 8-2: First approach to structure CTES material stability filled in for esters as PCM (source: HSLU).



Subtask D

TCM behaviour…

…might change with:

Time

Charging-discharging-cycles

avoid high % RH and high contents of salts in composites

and RH% during sorption

…might change due to:

Te

Mechanical forces

Chemical reactions

Phase separation

Atmosphere/ Environment

Humidity during storing

XRD, specific surface area, total pore volume, average pore size, presence of additional materials

Decrease or not

changes

Measureable (changing) properties:

(Crystal) structure

Enthalpy ch

(fusion

Aging materials under specific conditions, see A. Frazzica`s paper on hydrothermal stability test (2018)

Water uptake

ermal conductivity

Elemental composition

Reasons to better understand degradation:

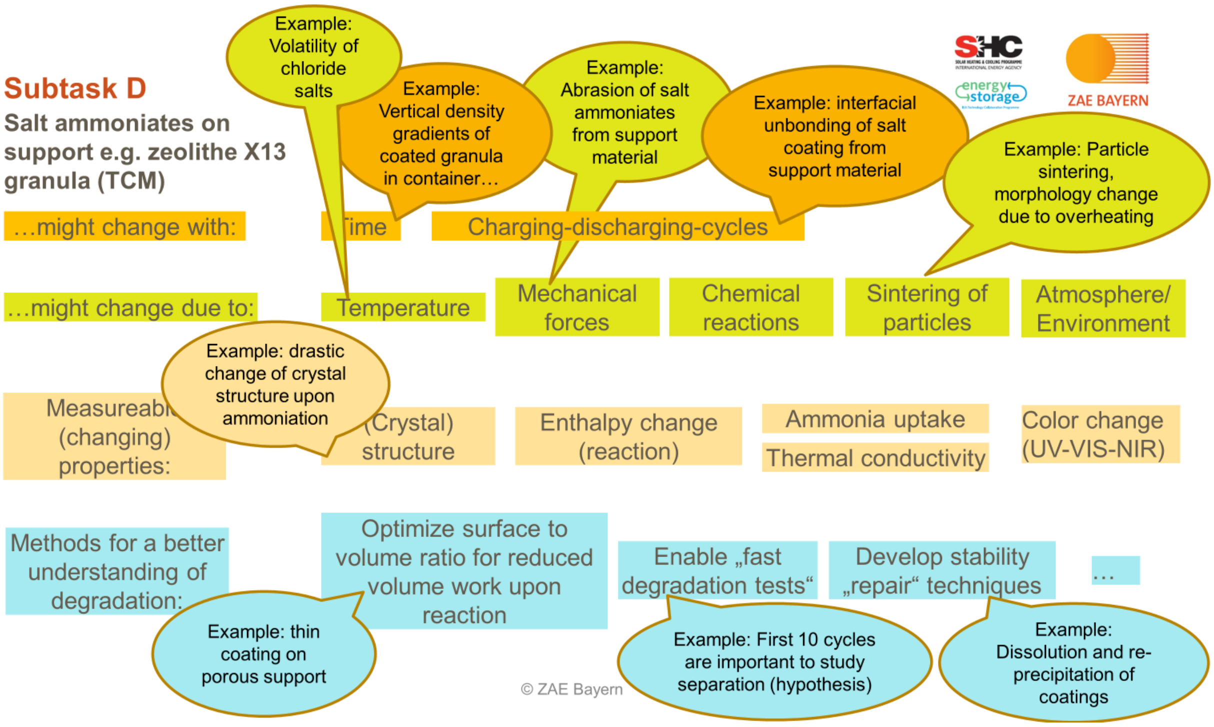
Find additives to prevent degradation

Enable „fast degradation tests“

Develop stability „repair“ techniques

…

Figure 8-3: First approach to structure CTES material stability filled in for TCM (source: NIC).



Subtask D

Salt ammoniates on support e.g. zeolithe X13 granula (TCM)

Example: Volatility of chloride salts

Example: Vertical density gradients of coated granula in container…

Example: Abrasion of salt ammoniates from support material

Example: interfacial unbonding of salt coating from support material

Example: Particle sintering, morphology change due to overheating

…might change with:

ime

Charging-discharging-cycles

…might change due to:

Temperature

Mechanical forces

Chemical reactions

Sintering of particles

Atmosphere/ Environment

Example: drastic change of crystal structure upon ammoniation

Measureabl (changing) properties:

(Crystal) structure

Enthalpy change (reaction)

Ammonia uptake

Thermal conductivity

Color change (UV-VIS-NIR)

Methods for a better understanding of degradation:

Optimize surface to volume ratio for reduced volume work upon reaction

Enable „fast degradation tests“

Develop stability „repair“ techniques

…

Example: thin coating on porous support

Example: First 10 cycles are important to study separation (hypothesis)

Example: Dissolution and re-precipitation of coatings

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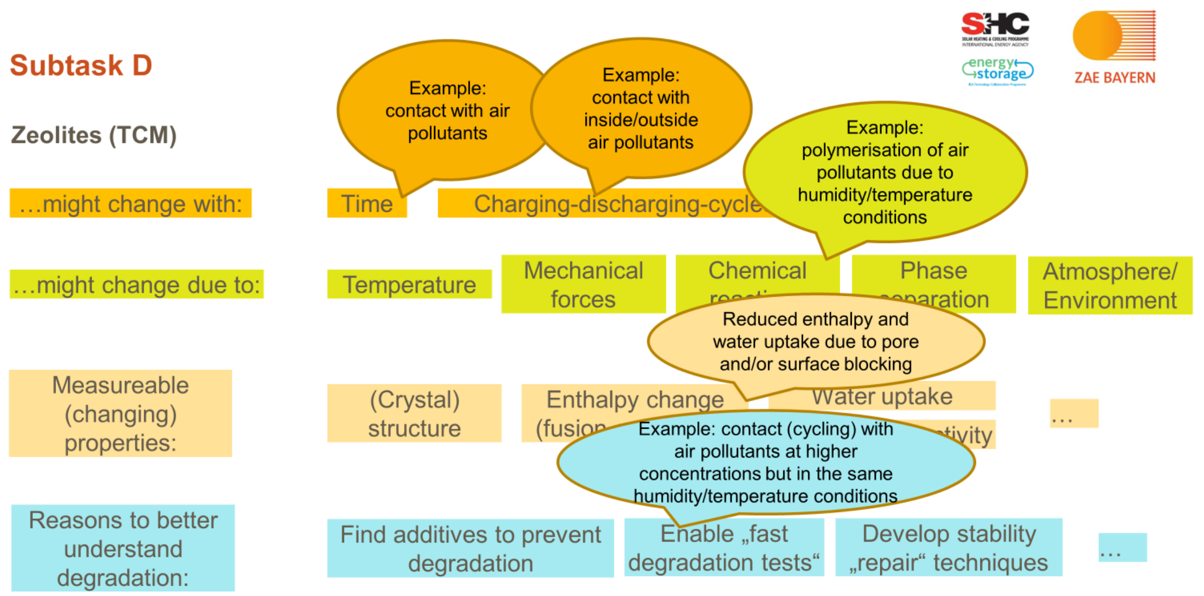
Figure 8-4: First approach to structure CTES material stability filled in for salt ammoniates as TCM (source: TU Vienna).



Subtask D

Zeolites (TCM)

…might change with: | Time | Charging-discharging-cycle

…might change due to: | Temperature | Mechanical forces | Chemical reacti | Phase separation | Atmosphere/ Environment

Measureable (changing) properties: | (Crystal) structure | Enthalpy change (fusion | Water uptake | tivity | …

Reasons to better understand degradation: | Find additives to prevent degradation | Enable „fast degradation tests“ | Develop stability „repair“ techniques | …

Example: contact with air pollutants

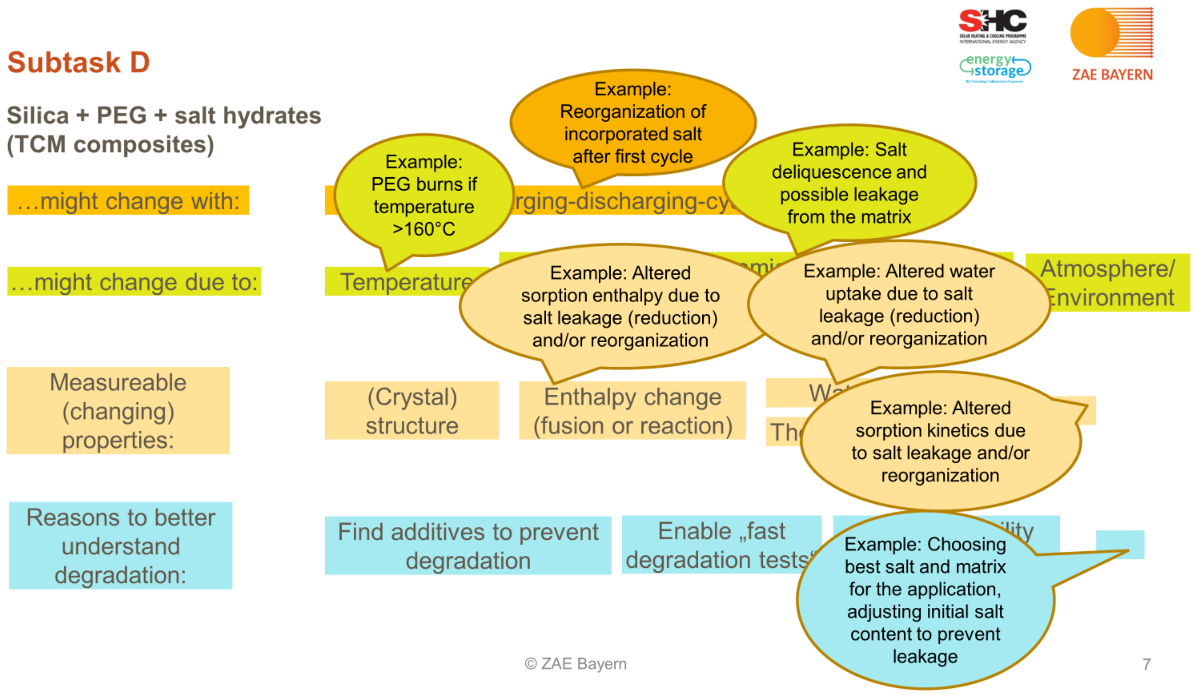
Example: contact with inside/outside air pollutants

Example: polymerisation of air pollutants due to humidity/temperature conditions

Reduced enthalpy and water uptake due to pore and/or surface blocking

Example: contact (cycling) with air pollutants at higher concentrations but in the same humidity/temperature conditions

Figure 8-5: First approach to structure CTES material stability filled in for zeolites as TCM (source: Univ. Savoy Mont Blanc).



Subtask D

Silica + PEG + salt hydrates (TCM composites)

…might change with: | rging-discharging-cy

…might change due to: | Temperature | mi | Atmosphere/ Environment

Measureable (changing) properties: | (Crystal) structure | Enthalpy change (fusion or reaction) | Wa | Th

Reasons to better understand degradation: | Find additives to prevent degradation | Enable „fast degradation tests | lity

Example: Reorganization of incorporated salt after first cycle

Example: PEG burns if temperature >160°C

Example: Salt deliquescence and possible leakage from the matrix

Example: Altered sorption enthalpy due to salt leakage (reduction) and/or reorganization

Example: Altered water uptake due to salt leakage (reduction) and/or reorganization

Example: Altered sorption kinetics due to salt leakage and/or reorganization

Example: Choosing best salt and matrix for the application, adjusting initial salt content to prevent leakage

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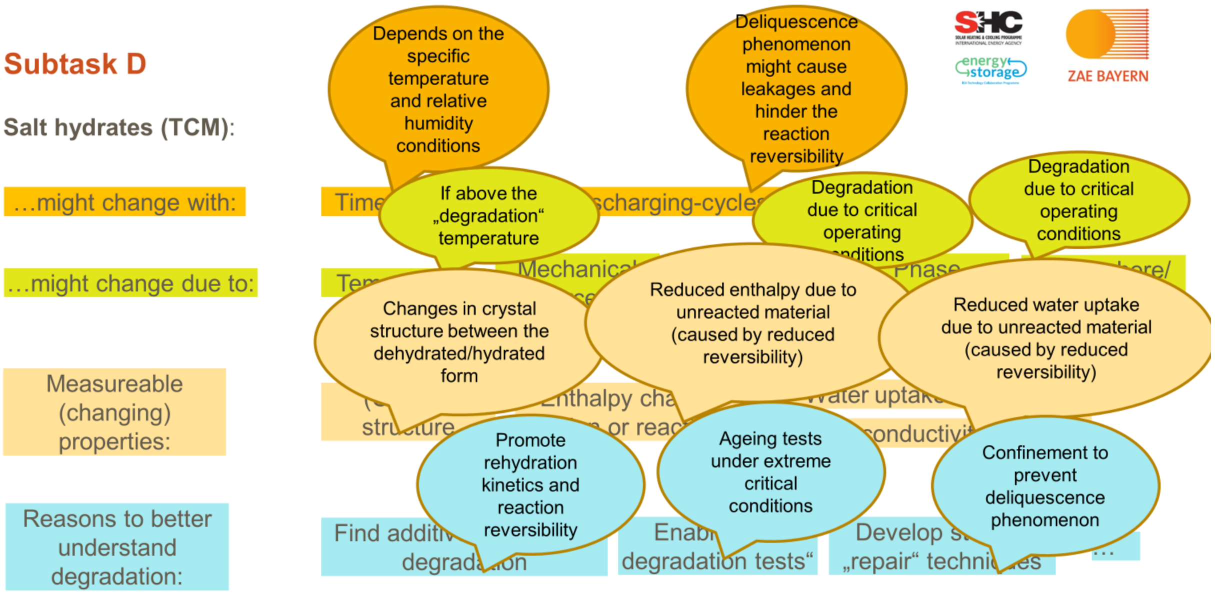
7

Figure 8-6: First approach to structure CTES material stability filled in for TCM composites (source: Univ. Savoy Mont Blanc).



Subtask D

Salt hydrates (TCM):

…might change with: Time … scharging-cycles

…might change due to: Te… Mechanical … Phase … …here/

Measureable (changing) properties: (C… structure … nthalpy cha… … or reac… … ater uptak… … onductivi…

Reasons to better understand degradation: Find additiv… degradation … Enab… degradation tests“ … Develop s… „repair“ techni…es … …

Depends on the specific temperature and relative humidity conditions

Deliquescence phenomenon might cause leakages and hinder the reaction reversibility

If above the „degradation“ temperature

Degradation due to critical operating conditions

Degradation due to critical operating conditions

Changes in crystal structure between the dehydrated/hydrated form

Reduced enthalpy due to unreacted material (caused by reduced reversibility)

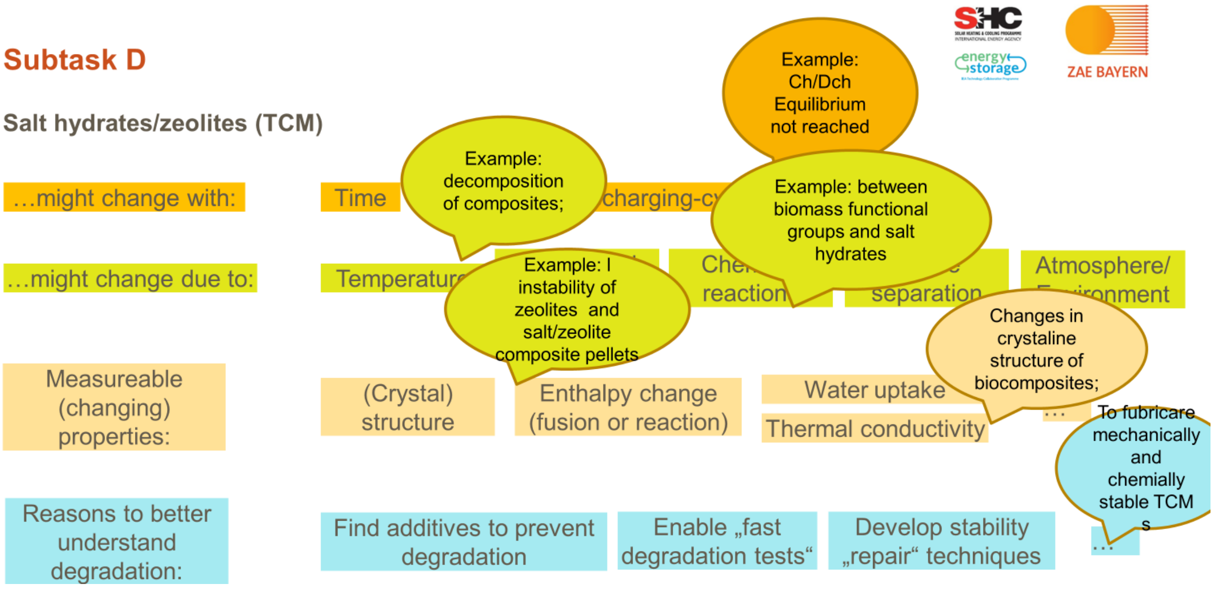
Reduced water uptake due to unreacted material (caused by reduced reversibility)

Promote rehydration kinetics and reaction reversibility

Ageing tests under extreme critical conditions

Confinement to prevent deliquescence phenomenon

Figure 8-7: First approach to structure CTES material stability filled in for salt hydrates as TCM (source: Univ. Messina).



Subtask D

Salt hydrates/zeolites (TCM)

…might change with: Time … charging-cy…

…might change due to: Temperatur… Che… reaction … separation … Atmosphere/ E…ironment

Measureable (changing) properties: (Crystal) structure … Enthalpy change (fusion or reaction) … Water uptake … Thermal conductivity … …

Reasons to better understand degradation: Find additives to prevent degradation … Enable „fast degradation tests“ … Develop stability „repair“ techniques … …

Example: Ch/Dch Equilibrium not reached

Example: decomposition of composites;

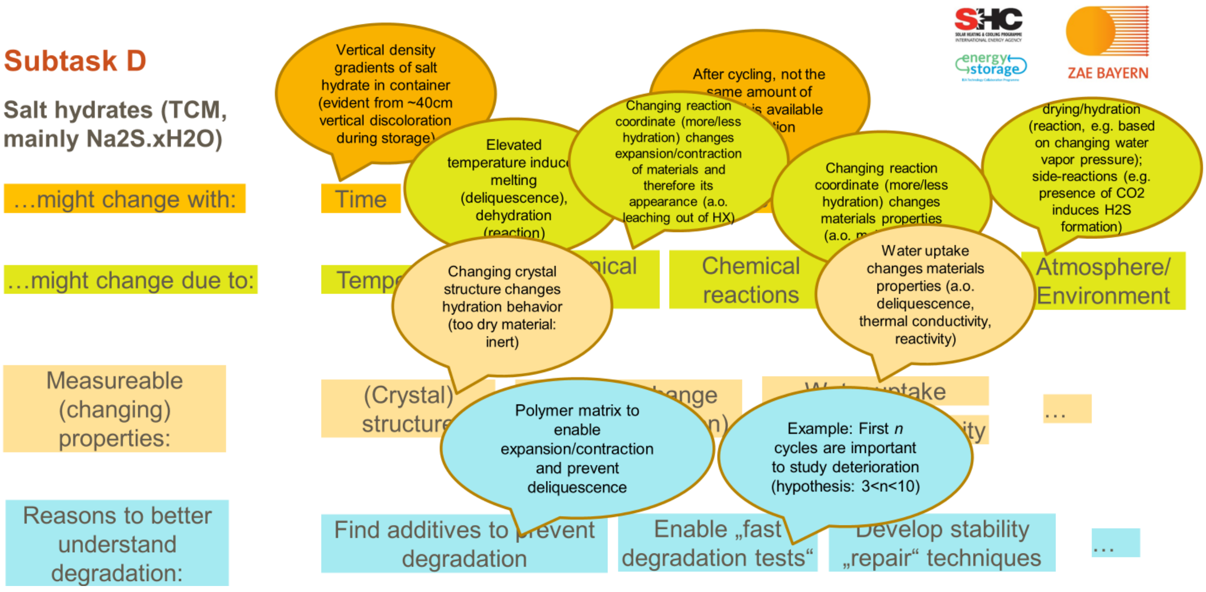
Example: between biomass functional groups and salt hydrates

Example: I instability of zeolites and salt/zeolite composite pellets

Changes in crystaline structure of biocomposites;

To fubricare mechanically and chemially stable TCM s

Figure 8-8: First approach to structure CTES material stability filled in for salt hydrates/zeolites as TCM (source: NRCan).



Subtask D

Salt hydrates (TCM, mainly Na2S.xH2O)

…might change with:

…might change due to:

Measureable (changing) properties:

Reasons to better understand degradation:

Time

Vertical density gradients of salt hydrate in container (evident from ~40cm vertical discoloration during storage)

Elevated temperature induc melting (deliquescence), dehydration (reaction)

After cycling, not the same amount of is available tion

Changing reaction coordinate (more/less hydration) changes expansion/contraction of materials and therefore its appearance (a.o. leaching out of HX)

Changing reaction coordinate (more/less hydration) changes materials properties (a.o. m

drying/hydration (reaction, e.g. based on changing water vapor pressure); side-reactions (e.g. presence of CO2 induces H2S formation)

Temp

nical

Chemical reactions

Atmosphere/ Environment

Changing crystal structure changes hydration behavior (too dry material: inert)

Water uptake changes materials properties (a.o. deliquescence, thermal conductivity, reactivity)

(Crystal) structure

hange n)

uptake ity

…

Polymer matrix to enable expansion/contraction and prevent deliquescence

Example: First *n* cycles are important to study deterioration (hypothesis: 3<n<10)

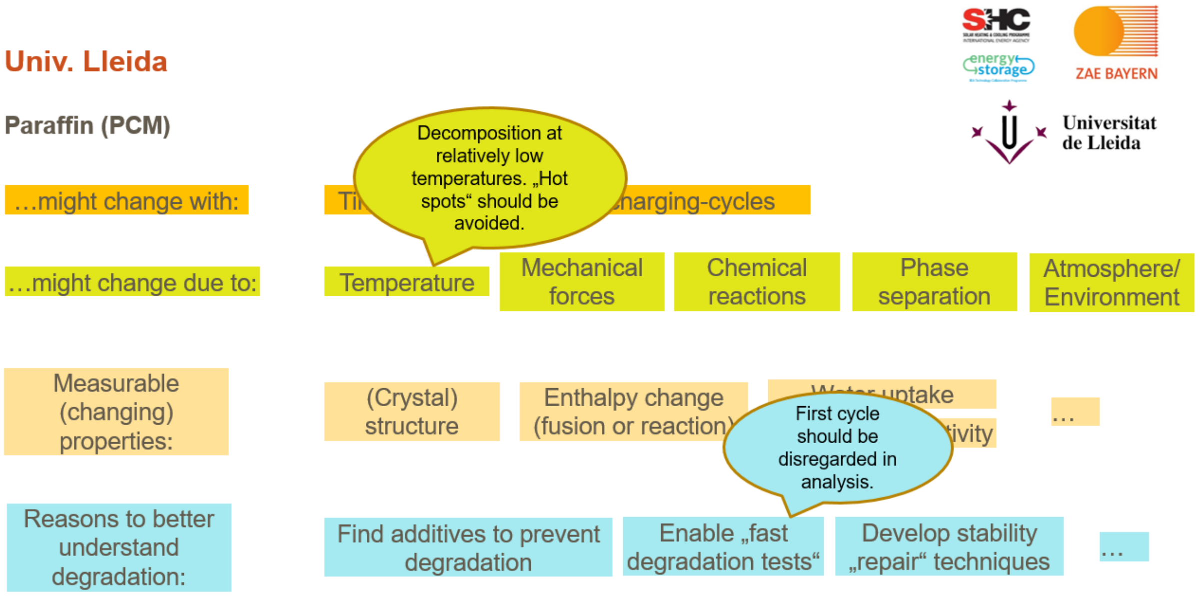
Find additives to prevent degradation

Enable „fast degradation tests“

Develop stability „repair“ techniques

…

Figure 8-9: First approach to structure CTES material stability filled in for salt hydrates as TCM (source: TNO).



Univ. Lleida

Paraffin (PCM)

…might change with:

…might change due to:

Measurable (changing) properties:

Reasons to better understand degradation:

Ti

Decomposition at relatively low temperatures. „Hot spots“ should be avoided.

harging-cycles

Temperature

Mechanical forces

Chemical reactions

Phase separation

Atmosphere/ Environment

(Crystal) structure

Enthalpy change (fusion or reaction)

Water uptake

tivity

First cycle should be disregarded in analysis.

…

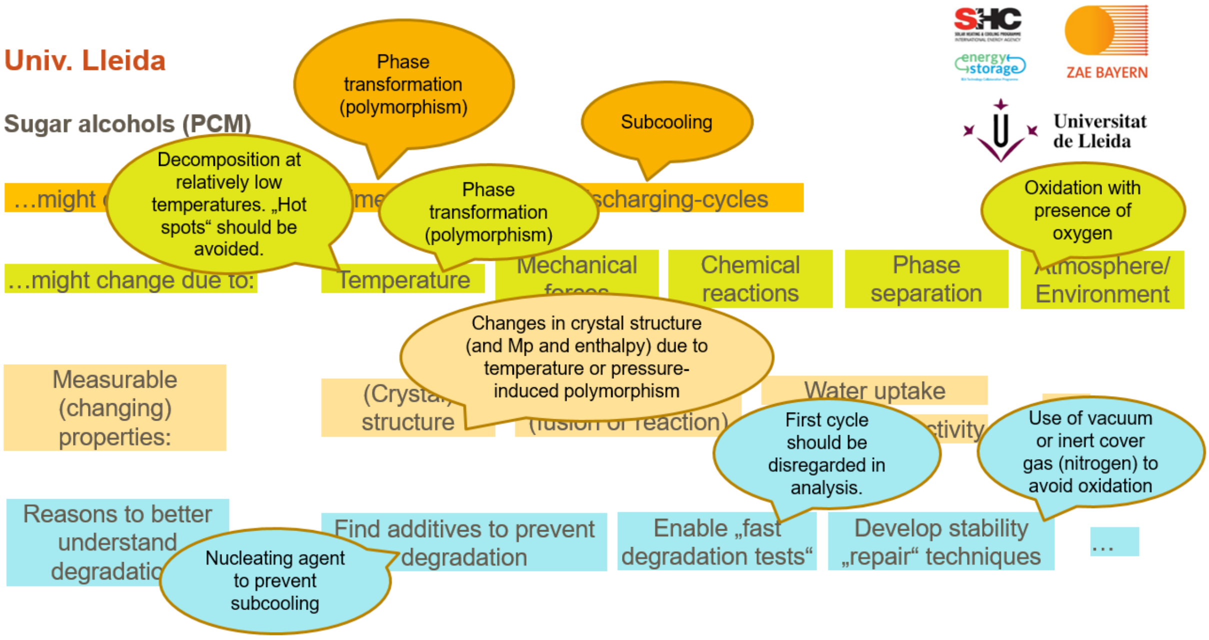
Find additives to prevent degradation

Enable „fast degradation tests“

Develop stability „repair“ techniques

…

Figure 8-10: First approach to structure CTES material stability filled in for paraffin as PCM (source: Univ. Lleida).



Univ. Lleida

Sugar alcohols (PCM)

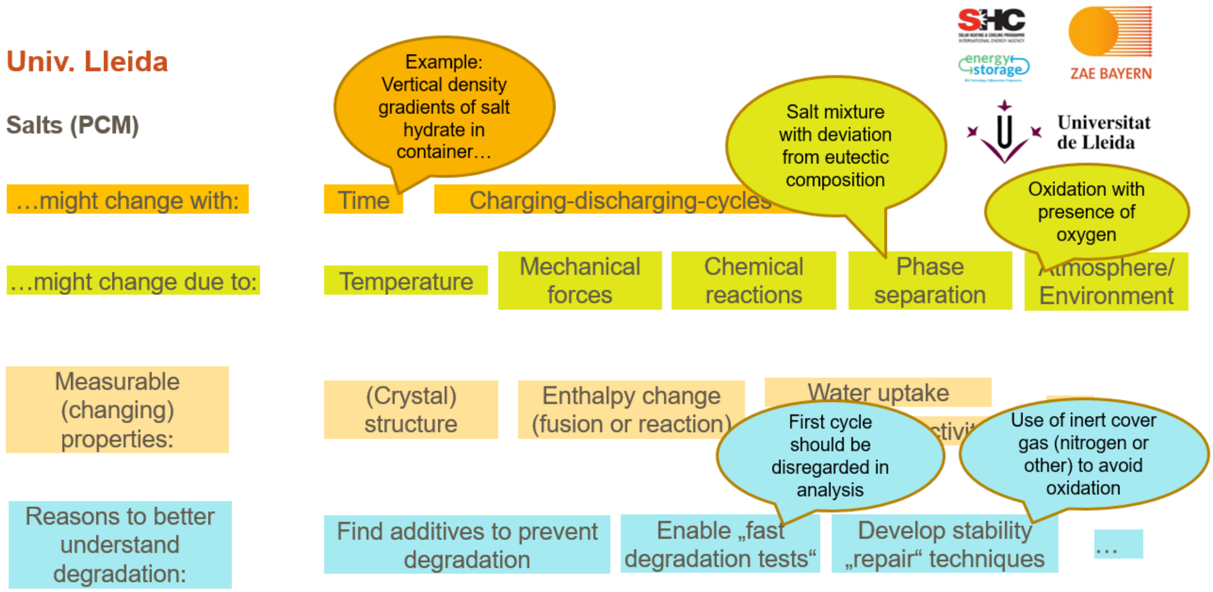
…might c | me | scharging-cycles

…might change due to: | Temperature | Mechanical forces | Chemical reactions | Phase separation | Atmosphere/ Environment

Measurable (changing) properties: | (Crystal) structure | (fusion or reaction) | Water uptake | ctivity

Reasons to better understand degradation: | Find additives to prevent degradation | Enable „fast degradation tests“ | Develop stability „repair“ techniques | …

Figure 8-11: First approach to structure CTES material stability filled in for sugar alcohols as PCM (source: Univ. Lleida).



Univ. Lleida

Salts (PCM)

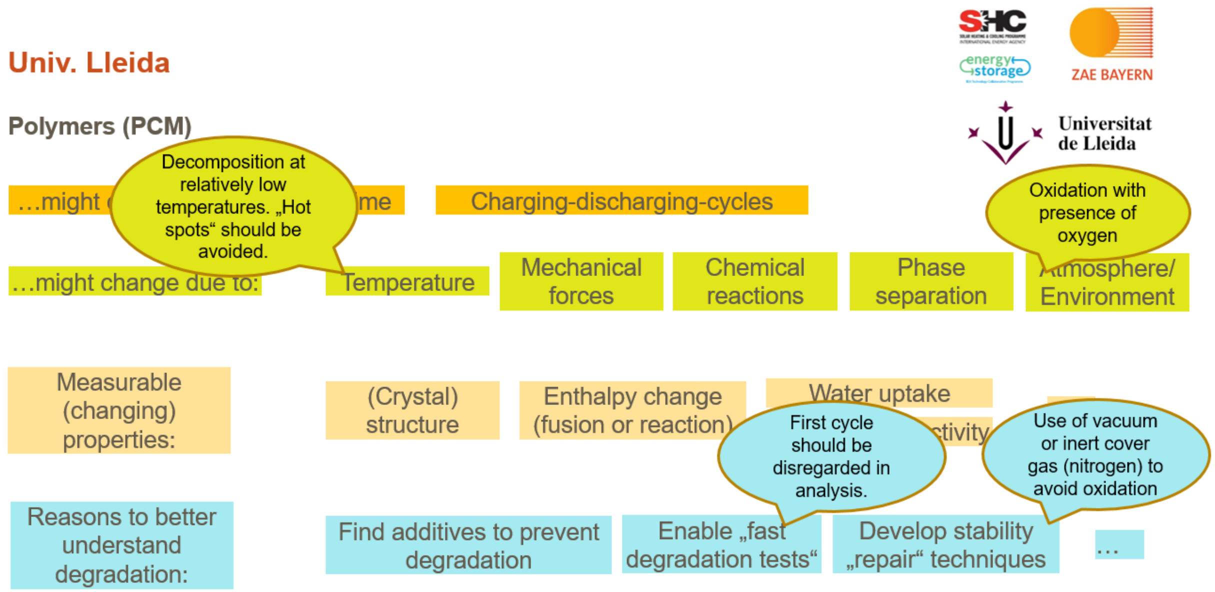
…might change with: | Time | Charging-discharging-cycles

…might change due to: | Temperature | Mechanical forces | Chemical reactions | Phase separation | Atmosphere/ Environment

Measurable (changing) properties: | (Crystal) structure | Enthalpy change (fusion or reaction) | Water uptake | ctivi

Reasons to better understand degradation: | Find additives to prevent degradation | Enable „fast degradation tests“ | Develop stability „repair“ techniques | …

Figure 8-12: First approach to structure CTES material stability filled in for salts as PCM (source: Univ. Lleida).



Univ. Lleida

Polymers (PCM)

Universitat de Lleida

…might | me | Charging-discharging-cycles

Decomposition at relatively low temperatures. „Hot spots“ should be avoided.

…might change due to: | Temperature | Mechanical forces | Chemical reactions | Phase separation | tmosphere/ Environment

Oxidation with presence of oxygen

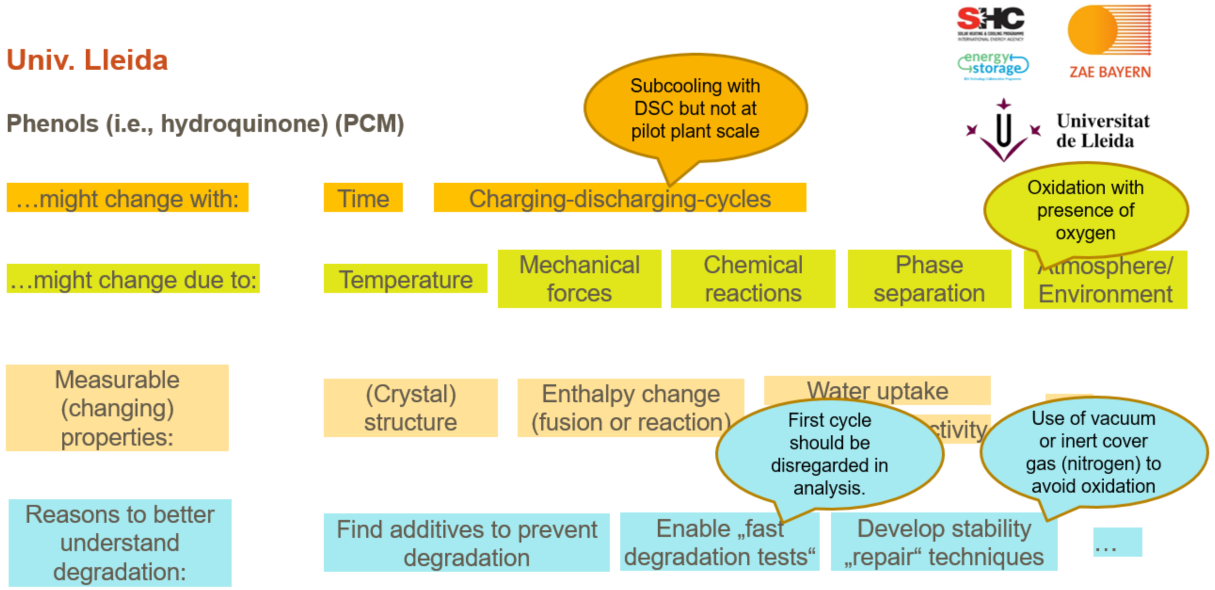
Measurable (changing) properties: | (Crystal) structure | Enthalpy change (fusion or reaction) | Water uptake | ctivity

First cycle should be disregarded in analysis.

Use of vacuum or inert cover gas (nitrogen) to avoid oxidation

Reasons to better understand degradation: | Find additives to prevent degradation | Enable „fast degradation tests“ | Develop stability „repair“ techniques | …

Figure 8-13: First approach to structure CTES material stability filled in for polymers as PCM (source: Univ. Lleida).



Univ. Lleida

Phenols (i.e., hydroquinone) (PCM)

Universitat de Lleida

…might change with: | Time | Charging-discharging-cycles

Subcooling with DSC but not at pilot plant scale

…might change due to: | Temperature | Mechanical forces | Chemical reactions | Phase separation | tmosphere/ Environment

Oxidation with presence of oxygen

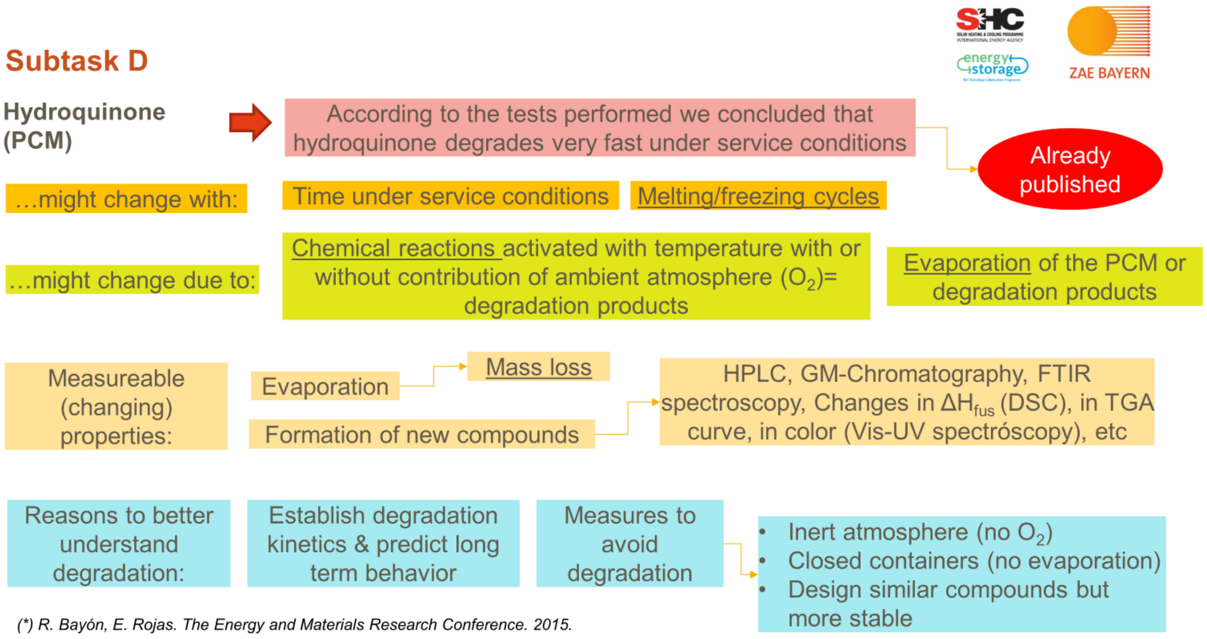
Measurable (changing) properties: | (Crystal) structure | Enthalpy change (fusion or reaction) | Water uptake | ctivity

First cycle should be disregarded in analysis.

Use of vacuum or inert cover gas (nitrogen) to avoid oxidation

Reasons to better understand degradation: | Find additives to prevent degradation | Enable „fast degradation tests“ | Develop stability „repair“ techniques | …

Figure 8-14: First approach to structure CTES material stability filled in for phenols as PCM (source: Univ. Lleida).



Subtask D

SHC energy storage ZAE BAYERN

Hydroquinone (PCM)

According to the tests performed we concluded that hydroquinone degrades very fast under service conditions

Already published

…might change with: Time under service conditions | Melting/freezing cycles

…might change due to: Chemical reactions activated with temperature with or without contribution of ambient atmosphere (O_2)= degradation products | Evaporation of the PCM or degradation products

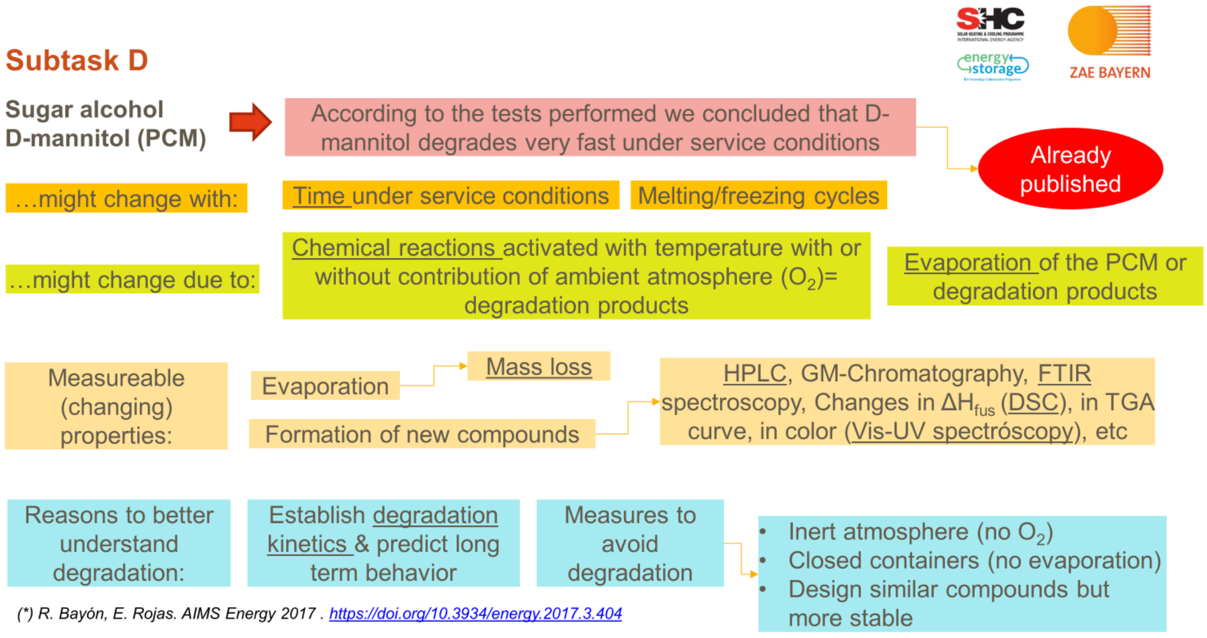
Measureable (changing) properties: Evaporation → Mass loss; Formation of new compounds → HPLC, GM-Chromatography, FTIR spectroscopy, Changes in ΔH_{fus} (DSC), in TGA curve, in color (Vis-UV spectróscopy), etc

Reasons to better understand degradation: Establish degradation kinetics & predict long term behavior | Measures to avoid degradation

- Inert atmosphere (no O_2)
- Closed containers (no evaporation)
- Design similar compounds but more stable

(*) R. Bayón, E. Rojas. The Energy and Materials Research Conference. 2015.

Figure 8-15: Second approach to structure CTES material stability filled in for hydroquinone as PCM (source: CIEMAT).



Subtask D

SHC energy storage ZAE BAYERN

Sugar alcohol D-mannitol (PCM)

According to the tests performed we concluded that D-mannitol degrades very fast under service conditions

Already published

…might change with: Time under service conditions | Melting/freezing cycles

…might change due to: Chemical reactions activated with temperature with or without contribution of ambient atmosphere (O_2)= degradation products | Evaporation of the PCM or degradation products

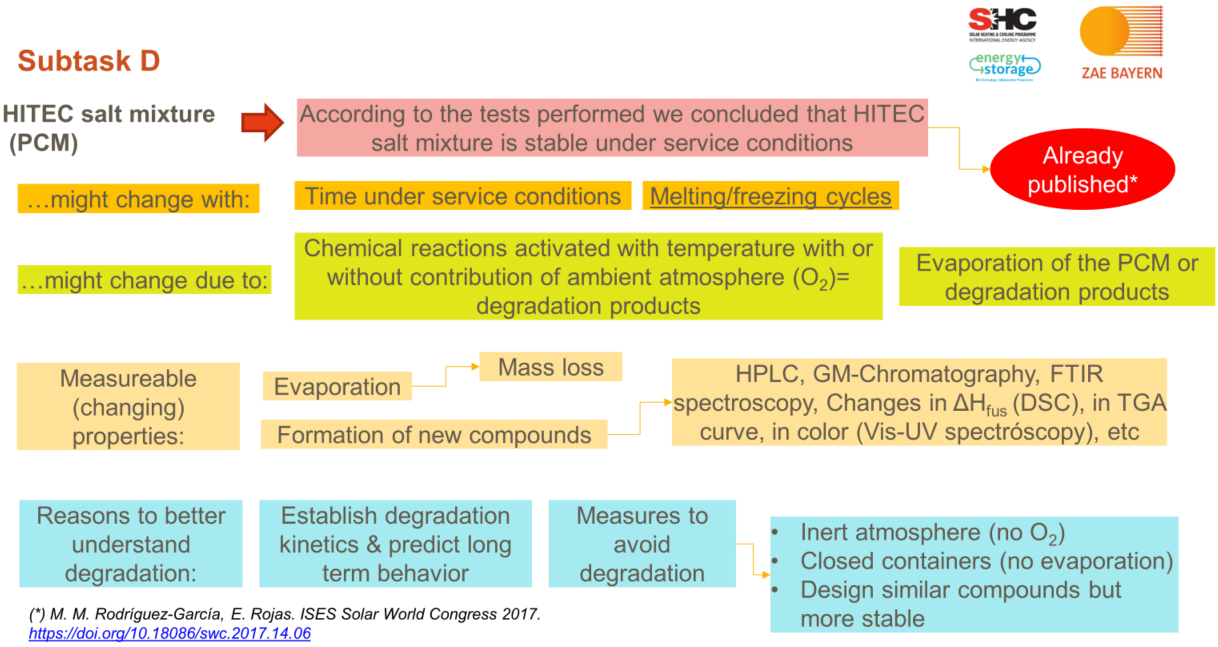
Measureable (changing) properties: Evaporation → Mass loss; Formation of new compounds → HPLC, GM-Chromatography, FTIR spectroscopy, Changes in ΔH_{fus} (DSC), in TGA curve, in color (Vis-UV spectróscopy), etc

Reasons to better understand degradation: Establish degradation kinetics & predict long term behavior | Measures to avoid degradation

- Inert atmosphere (no O_2)
- Closed containers (no evaporation)
- Design similar compounds but more stable

(*) R. Bayón, E. Rojas. AIMS Energy 2017 . https://doi.org/10.3934/energy.2017.3.404

Figure 8-16: Second approach to structure CTES material stability filled in for D-mannitol as PCM (source: CIEMAT).



Subtask D

HITEC salt mixture (PCM)

According to the tests performed we concluded that HITEC salt mixture is stable under service conditions

Already published*

…might change with:

Time under service conditions

Melting/freezing cycles

…might change due to:

Chemical reactions activated with temperature with or without contribution of ambient atmosphere (O_2)= degradation products

Evaporation of the PCM or degradation products

Measureable (changing) properties:

Evaporation

Mass loss

Formation of new compounds

HPLC, GM-Chromatography, FTIR spectroscopy, Changes in ΔH_{fus} (DSC), in TGA curve, in color (Vis-UV spectróscopy), etc

Reasons to better understand degradation:

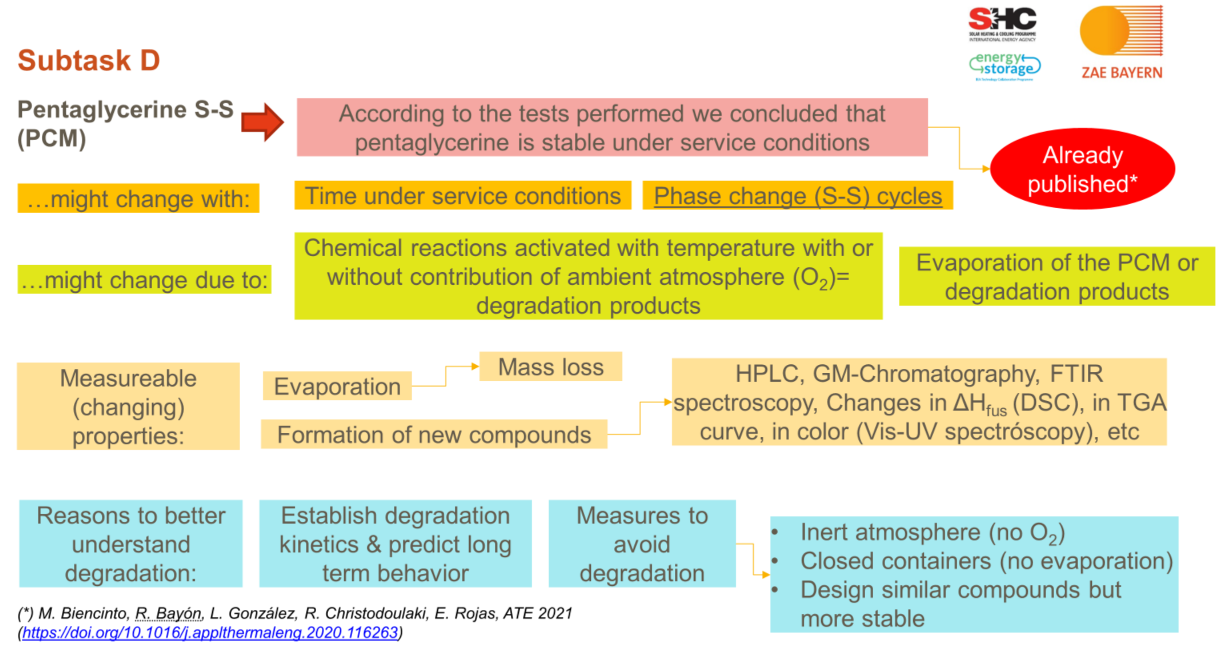
Establish degradation kinetics & predict long term behavior

Measures to avoid degradation

- Inert atmosphere (no O_2)
- Closed containers (no evaporation)
- Design similar compounds but more stable

(*) M. M. Rodríguez-García, E. Rojas. ISES Solar World Congress 2017. https://doi.org/10.18086/swc.2017.14.06

Figure 8-17: Second approach to structure CTES material stability filled in for HITEC salt as PCM (source: CIEMAT).



Subtask D

Pentaglycerine S-S (PCM)

According to the tests performed we concluded that pentaglycerine is stable under service conditions

Already published*

…might change with:

Time under service conditions

Phase change (S-S) cycles

…might change due to:

Chemical reactions activated with temperature with or without contribution of ambient atmosphere (O_2)= degradation products

Evaporation of the PCM or degradation products

Measureable (changing) properties:

Evaporation

Mass loss

Formation of new compounds

HPLC, GM-Chromatography, FTIR spectroscopy, Changes in ΔH_{fus} (DSC), in TGA curve, in color (Vis-UV spectróscopy), etc

Reasons to better understand degradation:

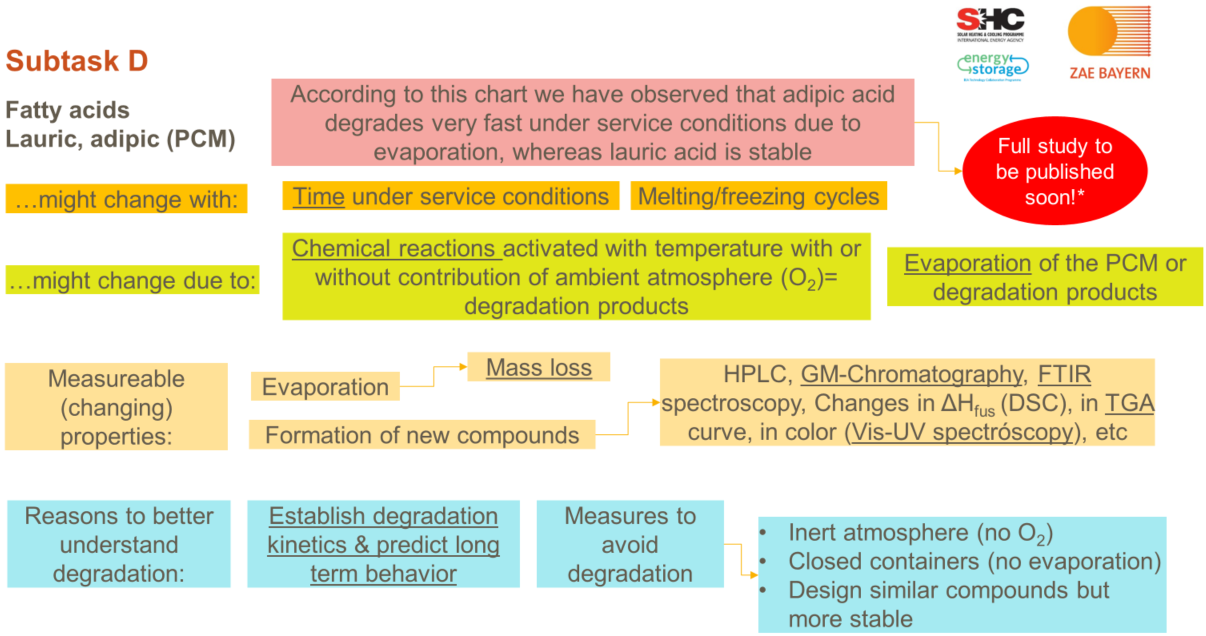
Establish degradation kinetics & predict long term behavior

Measures to avoid degradation

- Inert atmosphere (no O_2)
- Closed containers (no evaporation)
- Design similar compounds but more stable

(*) M. Biencinto, R. Bayón, L. González, R. Christodoulaki, E. Rojas, ATE 2021 (https://doi.org/10.1016/j.applthermaleng.2020.116263)

Figure 8-18: Second approach to structure CTES material stability filled in for pentaglycerine as PCM (source: CIEMAT).



Subtask D

Fatty acids
Lauric, adipic (PCM)

According to this chart we have observed that adipic acid degrades very fast under service conditions due to evaporation, whereas lauric acid is stable

Full study to be published soon!*

…might change with:
Time under service conditions
Melting/freezing cycles

…might change due to:
Chemical reactions activated with temperature with or without contribution of ambient atmosphere (O_2)= degradation products
Evaporation of the PCM or degradation products

Measureable (changing) properties:
Evaporation
Mass loss
Formation of new compounds
HPLC, GM-Chromatography, FTIR spectroscopy, Changes in ΔH_{fus} (DSC), in TGA curve, in color (Vis-UV spectróscopy), etc

Reasons to better understand degradation:
Establish degradation kinetics & predict long term behavior

Measures to avoid degradation
- Inert atmosphere (no O_2)
- Closed containers (no evaporation)
- Design similar compounds but more stable

Figure 8-19: Second approach to structure CTES material stability filled in for fatty acids as PCM (source: CIEMAT).

8.3 Appendix: Dissemination list

8.3.1 Reports, published books

Author(s) / Editor	Title	Report No., Publication Date	Target Audience	Web or Print
Benjamin Fumey, Mirko Kleingries, Gerhard Karger und Heribert Offermanns	Wärmespeicher Was steckt in der Lauge?	Nachrichten aus der Chemie| 70 April 2022, p 41-44	Engineers and Scientists	
Alenka Ristić / Andreas Hauer	Sorption material developments for TES applications / Advances in energy storage: latest developments from R&D to the market (book)	April, 2022, Hoboken; Chichester: J. Wiley & Sons	all	print
Alvaro Rojo Caballero / supervisor Alenka Ristić	Synthesis and characterization of porous carbonaceous matrices	Diploma thesis, 2022, Ljubljana	all	print
Manca Ocvirk / supervisor Alenka Ristić	Synthesis of mesoporous γ-alumina	Master thesis, 2022, Ljubljana	all	print
Suzana Mal / supervisor Alenka Ristić	Synthesis of Hierarchical Aluminophosphate Adsorbents for Thermochemical Solar Energy Storage	Master thesis, 2024, Ljubljana	all	print
Gang Wang	PhD thesis “Flexible heat storage based on stable supercooling of sodium acetate trihydrate”	2022 – publication at DTU is pending	Researcher	Will be available via DTU homepage
van Helden, W., Fumey, B., Englmair, G., Kerscher, F., Cuypers, R., Groulx, D., Lager, D., Doppiu, S., & Rathgeber, C.	Technology Position Paper: Compact Thermal Energy Storage	International Energy Agency, SHC TCP.		

Author(s) / Editor	Title	Report No., Publication Date	Target Audience	Web or Print
HUBMAN, Anže, VOLAVŠEK, Janez, URBIČ, Tomaž, ZABUKOVEC LOGAR, Nataša, MERZEL, Franci	Water–aluminum interaction as driving force of Linde Type A aluminophosphate hydration	https://dirros.openscience.si/IzpisGradiva.php?id=16888, DOI: 10.3390/nano13172387.		
Englmair, G.	Case 1: DTU optimerer faseskiftende materialers høje energitæthed til kompakt og decentral energilagring. In Status Styrker Synergier: DaCES Rapport om Energilagring i Danmark 2023 (pp. 15).	DaCES – Dansk Center for Energilagring (website)		

8.3.2 Journal articles, conference papers, etc.

Author(s)	Title	Publication / Conference	Bibliographic Reference
Serrano, A., Duran, M., Dauvergne, J. L., Doppiu, S., & Del Barrio, E. P.	Tailored transition temperature plastic crystals with enhanced thermal energy storage capacity.	Solar Energy Materials and Solar Cells, 220, 110848. (2021).	10.1016/j.solmat.2020.110848
Dauvergne, J. L., Serrano, Á., & Del Barrio, E. P.	Fast estimation of the enthalpy–temperature function of Phase Change Materials.	Experimental Thermal and Fluid Science, 122, 110317. (2021).	10.1016/j.expthermflusci.2020.110317
Serrano, A., Borreguero, A. M., Iglesias, I., Acosta, A., Rodríguez, J. F., & Carmona, M.	Diffusion of Shape Stabilized PEG-SiO2 as a Driver for Producing Thermoregulating Facing Bricks	Materials, 14(6), 1395. (2021).	10.3390/ma14061395
Mahroug, I., Doppiu, S., Dauvergne, J. L., Serrano, A., & Palomo del Barrio, E.	Li4 (OH) 3Br-Based Shape Stabilized Composites for High-Temperature TES Applications: Selection of the Most Convenient Supporting Material.	Nanomaterials, 11(5), 1279. (2021).	10.3390/nano11051279
Borreguero, A. M., Izarra, I., Garrido, I., Trzebiatowska, P. J., Datta, J., Serrano, Á., … & Carmona, M.	Thermal and Mechanical Behavior of Elastomers Incorporated with Thermoregulating Microcapsules.	Applied Sciences, 11(12), 5370. (2021).	10.3390/app11125370
Mahroug, I., Doppiu, S., Dauvergne, J. L., Echeverria, M., Toutain, J., & del Barrio, E. P.	Study of peritectic compound Li4 (OH) 3Br for high temperature thermal energy storage in solar power applications.	Solar Energy Materials and Solar Cells, 230, 111259. (2021).	10.1016/j.solmat.2021.111259
Perez-Arce, J., Serrano, A., Dauvergne, J. L., Centeno-Pedrazo, A., Prieto-Fernandez, S., Palomo Del Barrio, E., & Garcia-Suarez, E. J	Sustainable lignin-based polyols as promising thermal energy storage materials.	Journal of Applied Polymer Science, 138(46), 51356. (2021).	10.1002/app.51356
Mailhé, C., Duquesne, M., Palomo del Barrio, E., & Godin, A. (2021).	On the Use of Infrared Thermography for the Estimation of Melting Enthalpy.	Applied Sciences, 11(13), 5915.	10.3390/app11135915

Author(s)	Title	Publication / Conference	Bibliographic Reference
Mint Brahim, M., Godin, A., Azaïez, M., & Palomo Del Barrio, E.	Thermal characterization of complex shape composite materials using Karhunen–Loève decomposition techniques.	Inverse Problems in Science and Engineering, 29(13), 2676-2695. (2021).	10.1080/17415977.2021.1945050
Duquesne, M., Mailhé, C., Doppiu, S., Dauvergne, J. L., Santos-Moreno, S., Godin, A., … & Palomo del Barrio, E.	Characterization of Fatty Acids as Biobased Organic Materials for Latent Heat Storage.	Materials, 14(16), 4707. (2021).	10.3390/ma14164707
Dauvergne, J. L., Nikulin, A., Doppiu, S., & Palomo del Barrio, E.	Experimental Investigations on Electric-Field-Induced Crystallization in Erythritol.	Materials, 14(17), 5110. (2021).	10.3390/ma14175110
De La Pinta Alonso, N., Santos Moreno, S., Doppiu, S., Igartua Aldamiz, J. M., Palomo del Barrio, E., & López, G. A.	NPG–TRIS Thermal Storage System. Quantification of the Limiting Processes: Sublimation and Water's Adsorption.	Crystals, 11(10), 1200. (2021).	10.3390/cryst11101200
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Author(s)	Title	Publication / Conference	Bibliographic Reference
		Thermodynamics	
Lourdes Bouzas; Ana Garcia-Romero; Pello Larrinaga; Gonzalo Diarce.	Experimental Assessment of a Plate-Based LHTES: Comparison Between Compressed Expanded Graphite Plates Infiltrated with a PCM, and Bulk PCM Plates Macroencapsulated n Aluminum	CNIT 13 - 13th National and 4th International Conference in Engineering Thermodynamics	
Eukene Garcia; Gonzalo Diarce.	On the use of TGA for the study of degradation of thermal energy storage materials:analysis of the influence of evaporation	CNIT 13 - 13th National and 4th International Conference in Engineering Thermodynamics	
Eukene Garcia; Gonzalo Diarce.	On the use of TGA for the study of degradation of thermal energy storage materials: analysis of the influence of evaporation and mass sample	Medicta 2023, Oporto	
A. Crespo, A. Frazzica, C. Fernández, A. de Gracia	Optimizing the discharge process of a seasonal sorption storage system by means of design and control approach	Journal Publication	Journal of Energy Storage, Volume 60, April 2023, 106652. DOI: 10.1016/j.est.2023.106652
G. Airò Farulla, V. Palomba, D. Aloisio, G. Brunaccini, M. Ferraro, A. Frazzica, F. Sergi	Optimal design of lithium ion battery thermal management systems based on phase change material at high current and high environmental temperature	Journal Publication	Thermal Science and Engineering Progress, Volume 42, 1 July 2023, 101862. DOI: 10.1016/j.tsep.2023.101862
G. Airò Farulla, V. Brancato, V. Palomba, Y. Zhang, G.E. Dino, A. Frazzica	Experiments and Modeling of Solid–Solid Phase Change Material-Loaded Plaster to Enhance Building Energy Efficiency	Journal Publication	Energies, Volume 16, March 2023 2384. DOI: 10.3390/en16052384

Author(s)	Title	Publication / Conference	Bibliographic Reference
A. Frazzica, V. Palomba, A. Freni	Development and Experimental Characterization of an Innovative Tank-in-Tank Hybrid Sensible–Latent Thermal Energy Storage System	Journal Publication	Energies, Volume 16, February 2023 1875. DOI: 10.3390/en16041875
Talebi, Elija; Morgenstern, Leander; Würth, Manuel; Kerscher, Florian; Spliethoff, Hartmut	Effect of particle size distribution on heat transfer in bubbling fluidized beds applied in thermochemical energy storage	Journal Publication	Fuel 344, 2023
Morgenstern, L.; Talebi, E.; Kerscher, F.; Spliethoff, H.	Experimental investigation of CaO/Ca(OH)2 for thermochemical energy storage – commissioning of a 0.5 kWh experimental setup	Journal Publication	Fuel 345, 2023
Morgenstern, L.; Ohmstedt, S.; Kerscher, F.; Spliethoff, H.	Particle Properties of CaO/Ca(OH)2 Throughout Cyclisation in a Fluidized Bed for Thermochemical Energy Storage – Consequences for Fluidization	Conference Proceedings	Heat Powered Cycles Conference 2023, 2023, p. 520 - 528
Benjamin Fumeya Robert Weber Luca Baldini	Heat transfer constraints and performance mapping of a closed liquid sorption heat storage process	Publication	Applied Energy 335 (2023) 120755
Zhu, Y., Englmair, G., Huang, H., Dragsted, J., Yuan, Y., Fan, J., & Furbo, S.	Numerical investigations of a latent thermal energy storage for data center cooling.	Applied Thermal Engineering	Applied Thermal Engineering, 236 Part B, Article 121598. https://doi.org/10.1016/j.applthermaleng.2023.121598
Filonenko, K., Dominkovic, D. F., Jensen, A. U., & Englmair, G.	Investigation of cold storage integration in a Danish data center.	Building Simulation Conference Proceedings	In Building Simulation Conference Proceedings (Vol. 18, pp. 2875 - 2878). International Building Performance Simulation

Author(s)	Title	Publication / Conference	Bibliographic Reference
			Association. https://doi.org/10.26868/25222708.2023.1560
König-Haagen, A., Höhlein, S., Lázaro, A., Delgado, M., Diarce, G., Groulx, D., Herbinger, F., Patil, A., Englmair, G., Wang, G., Abdi, A., Chiu, J. N. W., Xu, T., Rathgeber, C., Pöllinger, S., Gschwander, S., & Gamisch, S.	Analysis of the discharging process of latent heat thermal energy storage units by means of normalized power parameters.	Journal of Energy Storage,	Journal of Energy Storage, 72, Article 108428. https://doi.org/10.1016/j.est.2023.108428
Dannemand, M., Englmair, G., Kong, W., & Furbo, S	Experimental investigations of multiple heat storage units utilizing supercooling of sodium acetate trihydrate: Stability in application size units.	Journal of Energy Storage,	Journal of Energy Storage, 86, Article 111194. https://doi.org/10.1016/j.est.2024.111194
Simonsen, Galina; Ravotti, Rebecca; O'Neill, Poppy; Stamatiou, Anastasia	Biobased phase change materials in energy storage and thermal management technologies	Renewable and sustainable energy reviews, 184, 2023, 113546	
Martinez Garcia, Jorge; Gwerder, Damian; Guarda, Dario; Fenk, Benjamin; Stamatiou, Anastasia; Worlitschek, Jörg; Schütz, Philipp	Study of the solidification behaviour of calcium chloride hexahydrate by in-situ X-ray computed tomography	Research and Review Journal of Nondestructive testing, 1(1), 2023, 1-6	
Martinez Garcia, Jorge; Gwerder, Damian; Wahli, Fabian; Guarda, Dario; Fenk, Benjamin; Stamatiou, Anastasia; Worlitschek, Jörg; Schütz, Philipp	Volumetric quantification of melting and solidification of phase change materials by in-situ X-ray computed tomography	Journal of energy storage, 61, 2023, 106726	
Anastasia Stamatiou, Jorge Martinez-Garcia, Rebecca Ravotti, Poppy O'Neill, Benjamin Fenk, Dario Guarda, Simone Mancin, Damian Gwerder, Ludger J. Fischer, Jörg Worlitschek, Philipp Schuetz	Using in-situ X-ray computed tomography to study the crystallization of salt hydrates	Proceedings of the Eurotherm Seminar "Innovative solutions for thermal energy storage deployment", 2023	
Sebastian Gamisch, Moritz Kick, Franziska Klünder, Julius Weiss, Eric Laurenz, Thomas Haussmann	Thermal Storage: From Low-to-High-Temperature Systems	Energy Technology published	https://doi.org/10.1002/ente.202300544.

Author(s)	Title	Publication / Conference	Bibliographic Reference
Sebastian Gamisch, Stefan Gschwander, Stefan J. Rupitsch	Numerical and Experimental Investigation of Wire Cloth Heat Exchanger for Latent Heat Storages	Energies 2021	https://doi.org/10.3390/ en14227542
Christoph Rathgeber, Stefan Hiebler. Rocío Bayón, Luisa F. Cabeza, Gabriel Zsembinszki , Gerald Englmair, Mark Dannemand, Gonzalo Diarce, Oliver Fellmann, Rebecca Ravotti, Dominic Groulx, Ali C. Kheirabadi, Stefan Gschwander, Stephan Höhlein, Andreas König-Haagen, Noé Beaupere, Laurent Zalewski	Experimental Devices to Investigate the Long-Term Stability of Phase Change Materials under Application Conditions	Applied Sciences 2020	https://www.mdpi.com/2076-3417/10/22/7968
Andreas König-Haagen , Stephan Höhlein, Ana L´azaro, M´onica Delgado, Gonzalo Diarce, Dominic Groulx, Florent Herbinger, Ajinkya Patil, Gerald Englmair, Gang Wang, Amir Abdi, Justin N.W. Chiu, Tianhao Xu, Christoph Rathgeber, Simon Pöllinger, Stefan Gschwander, Sebastian Gamisch	Analysis of the discharging process of latent heat thermal energy storage units by means of normalized power parameters	Journal of Energy Storage 2023	https://doi.org/10.1016/j.est.2023.108428
Wenye Lin, Stefan Gschwander, , Wenji Song, Ziping Feng, Mohammed M. Farid	Preparation, characterisation and property modification of a calcium chloride hexahydrate phase change material slurry with additives for thermal energy transportation	International Journal of Refrigeration	https://doi.org/10.1016/j.ijrefrig.2024.02.010
L. Kouchachvili, D. Bardy, R. Djebbar and L.E.W Hogg,	Screening of natural zeolites as potential host matrices for the development of low-cost, high performance thermal energy storage materials,	Material Science and Engineering (MSE) Congress, Darmstadt, Germany, 2020	MSE 2020 Conference proceedings

Author(s)	Title	Publication / Conference	Bibliographic Reference
Lia Kouchachvili, Dylan Bardy,Reda Djebbar, and LuVerne E.W. Hogg	Canadian natural zeolites as stable host matrices for low-cost, high-performance composite thermochemical energy storage materials	EnerSTOCK, 2021, Abstract	EnerStock 2021 conference proceedings
Lia Kouchachvili, D.A. Bardy, and Reda Djebbar	Enhancing the thermal energy storage density of natural zeolites	7th International Conference on Multifunctional, Hybrid and Nanomaterials, 2022	Conference proceedings
Lia Kouchachvili · D. A. Bardy · Reda Djebbar · LuVerne E. W. Hogg	Natural zeolites as host matrices for the development of low-cost and stable thermochemical energy storage materials	Journal of Porous Materials, 2022	https://doi.org/10.1007/s10934-022-01277-3
Lia Kouchachvili · Guillaume Gagnon-Caya · Reda Djebbar	Wood-derived biochar as a matrix for cost-effective and high-performing composite thermal energy storage materials	Journal of Porous Materials, 2024.	https://doi.org/10.1007/s10934-024-01638-0
Anh Kiet Nguyen, Pheobe Chalmers, Stephen Harrison, Reda Djebbar	Performance model for phase-change thermal energy storages	Eurosun 2024, Cyprus 2024 conference, Pending publication with ISES	Eurosun 2024 conference proceedings
Stephen Harrison, Roy Indranil, Anh Kiet Nguyen	Experimental Evaluation of a Phase-change Thermal Storage	EnerStock 2024, Lyon France conference	EnerStock 2024 conference proceedings
Schmit, H., Pöllinger, S., Rathgeber, C., Tafelmeier, S., Hoock, P., Hiebler, S., Müller-Baum, K. & Hörl, C.	Development of a phase change material for vaccine transport without dry ice.	Energy Storage 6.1 (2024): e557.	10.1002/est2.557
Schmit, H., Schubert, T., Ristic, A., Velte-Schäfer, A., Hügenell, P., Füldner, G., Lävemann, E. & Hiebler, S.	Experimental determination of characteristic curves of two commercial zeolites and the composite of γ-Al2O3 and CaCl2 for sorption heat storage.	Journal of Energy Storage 97 (2024): 113011.	10.1016/j.est.2024.113011
Rathgeber, C., Schmit, H., Hiebler, S., & Hoock, P.	Development of Phase Change Materials Based on Mixtures of Salt Hydrates	14th International Renewable Energy Storage Conference	10.2991/ahe.k.210202.003

Author(s)	Title	Publication / Conference	Bibliographic Reference
	Through Theoretical Prediction and Experimental Investigation.	2020 (IRES 2020) (pp. 14-18). Atlantis Press.	
Tomás Costa, Yolanda Sanchez-Vicente, Zili Yang, Lee A. Stevens, Fabio de S. Dias and Sol-Carolina Costa Pereira	Thermophysical properties of tetrabutylammonium chloride, paraffin and fatty acids for thermal energy applications†	RSC Adv., 2024, 14, 26246-26258	DOI: 10.1039/D4RA03782K
Elisangela Jesus D'Oliveira, Ulugbek Azimov, Sol-Carolina Costa Pereira, Khalid Lafdi	Effect of particle size on the thermal conductivity of organic phase change materials with expanded graphite	Journal of Energy Storage Volume 92, 1 July 2024, 112090	https://doi.org/10.1016/j.est.2024.112090
Elisangela Jesus D'Oliveira, Sol Carolina Costa Pereira, Dominic Groulx, Ulugbek Azimov	Thermophysical properties of Nano-enhanced phase change materials for domestic heating applications	Journal of Energy Storage Volume 46, February 2022, 103794	https://doi.org/10.1016/j.est.2021.103794
Ryan Callaghan, Elisangela J. D'Oliveira, Dominic Groulx*, S. Carolina Costa Pereira	CHARACTERIZATION OF A SMALL-SCALE PCM-HEAT EXCHANGER: IMPACT OF PCM SELECTION	Proceedings of the 17th International Heat Transfer Conference, IHTC-17 14 – 18 August 2023, Cape Town, South Africa	https://ihtc17.org/
Adeel Arshad, Syed Atif Iqrar, Sol Carolina Costa Pereira, Muhammad Wakil Shahzad, Kashif Nawaz, William Worek	Cooling performance of an active-passive hybrid composite phase change material (HcPCM) finned heat sink: Constant operating mode	International Journal of Heat and Mass Transfer Volume 207, 15 June 2023, 123973	https://doi.org/10.1016/j.ijheatmasstransfer.2023.123973
Laura Quant, Rocío Bayón, Redlich J. García, Gonzalo Diarce, Ana García-Romero, Esther Rojas	Kinetic Analysis Of TGA Measurements When Evaporation Is A Degradation Process In PCM	Proceedings of Eurosun 2022	https://doi.org/10.18086/eurosun.2022.13.16

Author(s)	Title	Publication / Conference	Bibliographic Reference
Rocío Bayón, Redlich J. García, Laura Quant, Esther Rojas	Study of Thermal Degradation of Adipic Acid as PCM Under Stress Conditions: A Kinetic Analysis	Proceedings of Eurosun 2022	https://doi.org/10.18086/eurosun.2022.13.02
Rocío Bayón, Redlich García-Rojas, Margarita Rodríguez-García, Esther Rojas	Assessment of isoconversional methods and peak functions for the kinetic analysis of thermogravimetric data and its application to degradation processes of organic phase change materials	Journal of Thermal Analysis and Calorimetry	Accepted un July 2024
BELINSON, M., GROULX, D.*	Numerical Study of a Latent Heat Storage System's Performance as a function of the Phase Change Material's Thermal Conductivity	Applied Science – Special Issue: Advanced in Materials for Thermal Energy Storage, 2024, v. 14, 3318	
CALLAGHAN, R.L.*, GROULX, D.	Experimental Characterization of a PCM-Heat Exchanger: Impact of PCM Properties on Comparison Metrics	(2023) Eurotherm Seminar: Innovative Solutions for Thermal Energy Storage Deployment, Lleida (Spain), 4 p.	
CALLAGHAN, R.L., D'OLIVEIRA, E.J., GROULX, D.*, COSTA PEREIRA, S.C.	Characterization of a Small-Scale PCM-Heat Exchanger: Impact of PCM Selection,	17th International Heat Transfer Conference, Cape Town (2023) (South Africa), 10 p.	
BELINSON, M., GROULX, D.*	Numerical Assessment of the Impact of a PCM Thermal Conductivity on a Storage System's Performance	14th IIR Conference on Phase-Change Materials and Slurries for Refrigeration and Air Conditioning- PCM 2024, Paris (France), 8 p.	
CALLAGHAN, R.L., BELINSON, M., GROULX, D.*	Impact of Using Different Phase Change Materials on a PCM-HX's Performance	Enerstock 2024 - The 16th IAE EST CP International	

Author(s)	Title	Publication / Conference	Bibliographic Reference
		Conference on Energy Storage, Lyon (France), 4 p.	
MARTHELEUR, D., GROULX, D.	Thermal Management of High-Powered Short-Duration Electronics aided by a Phase Change Material Thermal Energy Storage System,	Eurotherm 2024 – 9th European Thermal Sciences Conference, Lake Bled (Slovenia), 6 p.	
Schmit Henri, Schubert Tobias, Ristić Alenka, Velte-Schäfer Andreas, Hügenell Philipp, Füldner Gerrit, Lävemann Eberhard, Hiebler Stefan	Experimental determination of characteristic curves of two commercial zeolites and the composite of γ−Al2O3-CaCl2 for sorption heat storage	Journal of energy storage	vol. 97, Par tB, 2024, Page: 113011 DOI: 10.1016/j.est.2024.113011
Marčec Jan, Ristić Alenka, Zabukovec Logar Nataša	New Insights into ZIF-90 Synthesis	*Molecules*	2024, vol. 29, iss. 16, [article no.] 3731, p 1-13 DOI: 10.3390/molecules29163731
Ristić Alenka; Mal Suzana; Zabukovec Logar Nataša; Bérut Elise; Bois Laurence; Outin Jonathan; Ondarts Michel; Le Pierrès Nolwenn; Serrano Angel; Duran Mikel; Santos Sergio; Palomo Del Barrio Elena ; Doppiu Stefania	Improving materials for compact thermal energy storage: Two case studies on tailor-made polyalcohols mixtures (PCMs) and composites of chlorides confined in gamma-alumina or silica-PEG (TCMs)	*ACS Applied Energy Materials*	accepted
Mlakar Urška, Koželj Rok, Ristić Alenka, Stritih Uroš	Experimental testing system for adsorption space heating	*Strojniški vestnik*	2024, vol. 70, no. 3/4, p. 107-115 DOI: 10.5545/sv-jme.2023.788
Marčec Jan, Ristić Alenka	Zeolitic imidazolate framework materials for potential adsorption thermal battery applications	*10th Slovenian-Serbian-Croatian Symposium on Zeolites* *May 23-25, 2024, Ljubljana, Slovenia*	

Author(s)	Title	Publication / Conference	Bibliographic Reference
Byrne Ciara et all.	The influence of working fluids on the heat storage performance of ZIF-93	*10th Slovenian-Serbian-Croatian Symposium on Zeolites* *May 23-25, 2024, Ljubljana, Slovenia*	
Ristić Alenka, Mal Suzana, Zabukovec Logar Nataša	Water adsorption on microporous chabazites as thermal energy storage materials	*Eurotherm 2024: 9th European Thermal Sciences Conference, 10/06/2024 - 13/06/2024, Lake Bled, Slovenia*	Journal of physics. Conference series (Online), vol. 2766. DOI: 10.1088/1742-6596/2766/1/012233
Mlakar Urška, Ristić Alenka, Stritih Uroš	Experimental system for testing adsorption heat storage materials	*Eurotherm Seminar #116 : Innovative solutions for thermal energy storage deployment : 24-26 May 2023 : Lleida, Spain*	
Alenka Ristić, Urška Mlakar, Suzana Mal, Franz Hengel, Wim van Helden, Uroš Stritih, Nataša Zabukovec Logar	Extruded Water Adsorbent APO-Tric for Adsorption Thermal Battery Utilizing Solar Energy	*Eurosun2024,* 26.-29. August, 2024, Limassol, Cyper	
Schmit Henri, Schubert Tobias, Ristić Alenka, Velte-Schäfer Andreas, Hügenell Philipp, Füldner Gerrit, Lävemann Eberhard, Hiebler Stefan	Experimental determination of characteristic curves of two commercial zeolites and the composite of γ−Al2O3-CaCl2 for sorption heat storage	*Journal of energy storage*	vol. 97, Par tB, 2024, Page: 113011 DOI: 10.1016/j.est.2024.113011
Marčec Jan, Ristić Alenka, Zabukovec Logar Nataša	New Insights into ZIF-90 Synthesis	*Molecules*	2024, vol. 29, iss. 16, [article no.] 3731, p 1-13 DOI: 10.3390/molecules29163731

Author(s)	Title	Publication / Conference	Bibliographic Reference
Jakob Werner-Hörmann	Synthesis and characterization of novel calcium salt dicarboxylate hydrates as thermochemical energy storage materials	36th Workshop on "Novel Materials and Superconductors 2023, Schladming, Austria	(https://repositum.tuwien.at/handle/20.500.12708/153160)
Jakob Werner-Hörmann	From waste to resource: investigating calcium dicarboxylate hydrates as thermochemical energy storage materials for waste heat storage.	Exner Lectures 2023, Vienna, which was awarded with the poster award "fundamental milestone	
Jakob Werner-Hörmann	Solving energy challenges through chemical bonds: calcium dicarboxylate hydrates as thermochemical energy storage materials	6th EuChemS Inorganic Chemistry Conference, Vienna	(Book of abstracts: ISBN 978-3-9504809-5-5).
Jakob Werner-Hörmann	Calcium dicarboxylate salt hydrates as thermochemical energy storage materials for household applications,	37th Workshop on Chemistry and Physics of Novel Materials, February 2024, Schladming	
Jakob Werner-Hörmann	Thermochemical storage materials on microfluidic chips: heat storage powerhouses?	Exner Lectures 2024, Vienna	
Jakob Werner-Hörmann	Thermochemistry meets microfluidics: going small to go big	TCH Science days, Vienna, 2024	
Smith, Jakob Werner, Andreas Weinberger, Peter	Dehydration performance of a novel solid solution library of mixed Tutton salts as thermochemical heat storage materials	Journal Article	DOI: 10.1016/j.est.2023.110003.
Soares, N., Matias, T., Durães, L., Simões, P.N., Costa, J. J.	Thermophysical characterization of paraffin-based PCMs for low temperature	Energy, 269, 126745. (2023)	10.1016/j.energy.2023.126745

Author(s)	Title	Publication / Conference	Bibliographic Reference
	thermal energy storage applications for buildings.		
Brites, J. G., Garruço, M., Fernandes, M. S., Sá Pinto, D. M., Gaspar, A. R.	Seasonal storage for space heating using solar DHW surplus.	Renewable Energy, 231, 120889. (2024)	10.1016/j.renene.2024.120889
Aliyari, N., Fernandes, M. S., Gaspar, A. R.	Efficiency Analysis of An Integrated Cascade Sorption Energy Storage into A Solar DHW System.	EUROSUN 2024 Proceedings	In revision
Leander Morgenstern, Sören Ohmstedt, Florian Kerscher, Hartmut Spliethoff	Particle Properties of CaO/Ca(OH)2 Throughout Cyclisation in a Fluidized Bed for Thermochemical Energy Storage – Consequences for Fluidization	HPC 23, 2023	10th Heat Powered Cycles Conference Proceedings https://doi.org/10.5281/zenodo.10245219
Elija Talebi, Leander Morgenstern, Manuel Würth, Florian Kerscher, Hartmut Spliethoff	Effect of particle size distribution on heat transfer in bubbling fluidized beds applied in thermochemical energy storage	Fuel 344, 128060 (2023)	https://doi.org/10.1016/j.fuel.2023.128060
Leander Morgenstern, Elija Talebi, Florian Kerscher, Hartmut Spliethoff	Experimental investigation of CaO/Ca(OH)2 for thermochemical energy storage – commissioning of a 0.5 kWh experimental setup	Fuel 345, 128220 (2023)	https://doi.org/10.1016/j.fuel.2023.128220
Leander Morgenstern, Sören Ohmstedt, Elija Talebi, Florian Kerscher, Hartmut Spliethoff	Pilot-scale investigation of high-temperature thermochemical energy storage based on the material system CaO/Ca(OH)2 in a bubbling fluidized bed	Powder Technology 440, 119775 (2024)	https://doi.org/10.1016/j.powtec.2024.119775
Adam Buruzs, Fabrizia Giordano, Manuel Schieder, Christoph Reichl, Maité Goderis, Wim Beyne, Michel De Paepe and Tilman Barz	CFD simulation of solid/liquid phase change in commercial PCMs using the slPCMlib library	Journal of Physics: Conference Series, Volume 2766, 9th European Thermal Sciences Conference (Eurotherm 2024)	10.1088/1742-6596/2766/1/012223

Author(s)	Title	Publication / Conference	Bibliographic Reference
		10/06/2024 - 13/06/2024 Lake Bled, Slovenia	
Daniel Lager, Jovana Kovacevic	Evaluation of thermochemical materials for thermal energy storage	EUROTHERM SEMINAR #116 Innovative solutions for thermal energy storage deployment 24-26 May 2023 University of Lleida Lleida, Spain	10.21001/Eurotherm.seminar.116.2023
Schmit, H., Pöllinger, S., Rathgeber, C., Tafelmeier, S., Hoock, P., Hiebler, S., Müller-Baum, K. & Hörl, C.	Development of a phase change material for vaccine transport without dry ice.	Energy Storage 6.1 (2024): e557.	10.1002/est2.557
Schmit, H., Schubert, T., Ristic, A., Velte-Schäfer, A., Hügenell, P., Füldner, G., Lävemann, E. & Hiebler, S.	Experimental determination of characteristic curves of two commercial zeolites and the composite of γ-Al2O3 and CaCl2 for sorption heat storage.	Journal of Energy Storage 97 (2024): 113011.	10.1016/j.est.2024.113011
Rathgeber, C., Schmit, H., Hiebler, S., & Hoock, P.	Development of Phase Change Materials Based on Mixtures of Salt Hydrates Through Theoretical Prediction and Experimental Investigation.	14th International Renewable Energy Storage Conference 2020 (IRES 2020) (pp. 14-18). Atlantis Press.	10.2991/ahe.k.210202.003
Majó, M., Calderón, A., Svobodova-Sedlackova, A., … Fernández, A.I., Barreneche, C.	New database of sustainable solid particle materials to perform a material-based design for a thermal energy storage in concentrating solar power	Solar Energy Materials and Solar Cells, 2025, 281, 113309	10.1016/j.solmat.2024.113309
Koçak, B., Majó, M., Barreneche, C., Fernández, A.I., Paksoy, H.	Performance analysis of a molten salt packed-bed thermal energy storage system using three different waste materials	Solar Energy Materials and Solar Cells, 2024, 278, 113199	10.1016/j.solmat.2024.113199

Author(s)	Title	Publication / Conference	Bibliographic Reference
Salgado-Pizarro, R., Navarro-Rivero, M.E., Ding, Y., Barreneche, C., Fernández, A.I.	Thermal evaluation of polymorphic transitions in layered hybrid organic-inorganic perovskites for energy storage applications	Journal of Energy Storage, 2024, 100, 113483	10.1016/j.est.2024.113483
Salgado-Pizarro, R., Puigjaner, C., García, J., Fernández, A.I., Barreneche, C.	Copper- and manganese-based layered hybrid organic-inorganic compounds with polymorphic transitions as energy storage materials	Journal of Materials Chemistry A, 2024, 12(29), pp. 18544–18553	10.1039/d4ta01060d
Majó M.; Svobodova-Sedlackova, A.; Fernández, A. I.; Calderón, A.; Barreneche, C.	Evaluation of volcanic ash as a low-cost high-temperature thermal energy storage material for concentrated solar power	Journal of Energy Storage, 2024, 89, 111729	10.1016/j.est.2024.111729
Majó M.; Svobodova-Sedlackova, A.; Fernández, A. I.; Calderón, A.; Barreneche, C.	Thermal cycling test of solar salt in contact with sustainable solid particles for concentrating solar power (CSP) plants	Energies, 2024, 17(10), 2349	10.3390/en17102349
Svobodova-Sedlackova, A., Palacios, A., Jiang, Z., … Navarro, H., Barreneche, C.	Thermal stability and durability of solar salt-based nanofluids in concentrated solar power thermal energy storage: An approach from the effect of diverse metal alloys corrosion	Journal of Energy Storage, 2024, 75, 109715	10.1016/j.est.2023.109715

8.3.3 Conferences, Workshops, Seminars

Conference / Workshop / Seminar Name	Activity & Presenter	Date & Location	# of Attendees
ISEC 2022	Poster, Wim van Helden, AEE INTEC	6-7 April 2022	~ 350
VI IMPRES Symposium	Oral presentation (Mikel Durán, CIC EnergiGune)	Barcelona, Spain, 25th October 2022	
VI IMPRES Symposium	Oral presentation (Sergio Santos)	Barcelona, Spain, 25th October 2022	
E-MRS Fall meeting	Oral presentation (Maria Taeño, CIC EnergiGune)	19-22 September 2022	
Eurosun 2022	Oral presentation (Ángel Serrano, CIC EnergiGune)	Kassel, Germany, 25th September 2022	
Eurosun 2022	Poster presentation (Stefania Doppiu, CIC EnergiGune)	Kassel, Germany, 25th September 2022	
3rdEuropean Symposium on Nanofluids (ESNf2021)	Oral presentation (Luis González, CIC EnergiGune)	9-10 September 2021, Iasi, Romania	
Enerstock2021	Oral presentation (Ángel Serrano, CIC EnergiGune)	June 9 – 11, 2021, Ljubljana, Slovenia	
Enerstock2021	Oral presentation (Sergio Santos, CIC EnergiGune)	June 9 – 11, 2021, Ljubljana, Slovenia	
ISEC 2022	Poster, Bernhard Zettl, FHOÖ	6-7 April 2022	~ 350
CONECT 2022	Presentation, Nayrana Dabora-Prado, FHOÖ	11-13 May 2022	
IRES 2022	Poster, Evgeny Legotin, FHOÖ	20-22 September 2022	
EUROSUN 2022	Poster and presentation, Gayaneh Issayan, FHOÖ	25-29 September 2022	
IRES 2021	Presentation, Gesa Backofen, TUM	16.03. – 18.03.2021, online	
WE Heraeus Seminar	Poster, Gesa Backofen; TUM	22.03.- 24.04.2021, TU Duisburg Essen	
ECOS 2021	Presentation, Gesa Backofen; TUM	28.06. – 02.07.2021, online	

Conference / Workshop / Seminar Name	Activity & Presenter	Date & Location	# of Attendees
TOPCon – Konferenz für Energiesystemanalyse	Presentation, Gesa Backofen; TUM	24.05. – 25.05.2022, Berlin, Germany	
ECOS 2022	Presentation, Gesa Backofen; TUM	03.07. – 07.07.2022, Kopenhagen, Denmark	
Kongress Energieeffizienzforschung für Industrie und Gewerbe	Poster, Florian Kerscher; TUM	17.05-18.05.2022, Jülich, Germany	
CFB 13	Presentation, Elija Talebi; TUM	10.05. – 14.05.2021, online, Vancouver, Canada	
FBC 24	Presentation, Elija Talebi; TUM	08.05.-11.05.2022 Gothenburg Schweden	
FBC 24	Presentation, Leander Morgenstern; TUM	08.05.-11.05.2022, Gothenburg Schweden	
ISEC 2022	Poster, Urška Mlakar; NIC	6-7 April 2022	~ 350
14th International Conference “Fundamentals of Adsorption”	Keynote, Nataša Zabukovec Logar; NIC	May 22- 27, 2022, Denver, USA	
EuroSun 2022 : ISES and IEA SHC International Conference on Solar Energy for Buildings and Industry	Oral presentation, Alenka Ristić; NIC	25 - 29 September 2022, Kassel, Germany	500
International conference on metal-organic frameworks and open frameworks compounds: MOF2022	Poster Byrne, Ciara Susan; NIC	4-7 September 2022, Dresden, Germany	700
20th International Zeolite Conference	Oral presentation Byrne, Ciara Susan; NIC	3-8 July 2022, Valencia, Spain	500
9th meeting of ENMIX -Young Researchers	Oral presentation	October 5th, 2022, Thessaloniki, Greece	100

Conference / Workshop / Seminar Name	Activity & Presenter	Date & Location	# of Attendees
	Byrne, Ciara Susan; NIC		
EuroSun 2022	Poster, Elise Bérut, LOCIE	25-29 Sept 2022, Kassel (Germany)	~ 430
18ème congrès de la Société Française de Génie des Procédés (SFGP 2022)	Poster, Elise Bérut; LOCIE	7-10 Nov 2022, Toulouse (France)	~ 500
Journée scientifique CODEGEPRA - SFGP région Sud-Est (scientific day)	Presentation, Elise Bérut; LOCIE	24 Nov 2022, Chambéry (France)	~ 35
EUROSUN 2022	Presentation, Englmair et al., DTU	26 -29.09.2022, Kassel	~500
EUROSUN 2022	Poster, Fan et al., DTU	26 -29.09.2022, Kassel	~500
Webinar on Thermal Energy Storage for Buildings; Danish	Presentation Gerald Englmair, Presentation Simon Furbo, DTU	03.10.2022	~30
Solar Energy and Thermal Storage Workshop at DTU	Presentation Englmair, DTU	30.11.2022	~50
ISEC 2022	Poster, Rocío Bayón, CIEMAT	6-7 April 2022	~ 350
Eurosun 2022	Poster, Rocío Bayón, CIEMAT	25-29 September 22	~ 350
Eurosun 2022	Poster, Laura Quant, CIEMAT	25-29 September 22	~ 350
15th IIR Gustav Lorentzen 2022	Conference Paper, Jorge Salgado-Beceiro, SINTEF	13-15 June 2022	~ 350
EuroSun 2022	Oral Presentation, Olav Galteland, SINTEF	25-29 Sept 2022	~ 480
Thermal Energy Storage Workshop 2023, Trondheim, Norway	Organized by Jorge Salgado-Beceiro and Ragnhild Sæterli (SINTEF Energy Research)	30/11/2023 – 01/12/2023	100+
Eurotherm Seminar #116	Development of protective coatings for lithium/sodium sulfate salts intended for high-temperature thermal energy storage_	23-May-23 Lleida, Spain	

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	Ángel Serrano (CIC energiGUNE)		
13CNIT	Oral presentation: Bayón R, Rabasco P. Study of different fatty acids as PCM for latent storage: dependence of thermal degradation with molecular structure.	29/11-01/12/2023 Castellón de la Plana (Spain)	
Eurotherm Seminar #116	Oral presentation Mina Shahi	25-5-2023, Lleida	~30
International sustainable energy conference (ISEC) 2024	Poster presentation Mina Shahi	10-4-2024, Graz	n.a.
Enerstock 2024	Oral presentation Mina Shahi	5-6-2024, Lyon	n.a.
ICT 2024 Conference	Oral Presentation Mina Shahi	7-2-2024	~200
Exner Lectures 2023	Presentation. “Crystals and gases unite to save energy” Smith, Jakob	May 22, 2023, Vienna, Austria	100?
Exner Lectures 2023	Poster presentation. “From waste to resource: investigating calcium dicarboxylate hydrates as thermochemical energy torage materials for waste heat storage” Werner, Jakob	Exner Lectures 2023	100?
36th Workshop on Novel Materials and Superconductors	Poster presentation: Novel Materials and Superconductors Smith, Jakob	February 8, 2023 Schladming, Austria	50?
36th Workshop on Novel Materials and Superconductors	Poster presentation: “Synthesis and characterization of novel calcium salt dicarboxylate hydrates as thermochemical energy storage materials” Werner, Jakob	February 8, 2023 Schladming, Austria	50?
6th EuChemS Inorganic Chemistry Conference	Poster presentation: Exploring the Synergies of Gamma Alumina and Tutton Salt Hydrates in Thermochemical Energy Storage	September 3 – 7, 2023 Vienna, Austria	500?

Conference / Workshop / Seminar Name	Activity & Presenter	Date & Location	# of Attendees
6th EuChemS Inorganic Chemistry Conference	Poster presentation: “Solving energy challenges through chemical bonds: calcium dicarboxylate hydrates as thermochemical energy storage materials” Werner, Jakob	September 3 – 7, 2023 Vienna, Austria	500?
Zbornik povzetkov Slovenski kemijski dnevi 2023	Exploring the synergies of gamma alumina and sulfate salt hydrates in thermochemical energy storage	13.-15. september, Portorož, Slovenia	200?
International Renewable Energy Storage Conference IRES 2023	Presentation “Comparison Of Ageing At Elevated Temperature And Cycling Experiments Of HD-PE: A Degradation Study”, Franziska Klünder	Aachen	
ESAT 2024: 33rd European Symposium on Applied Thermodynamics	Oral Presentation, Yolanda Sanchez Vicente, Northumbria	9-12 June 2024	~ 250
Heat Powered Cycles Conference 2023	Oral Presentation, Elisangela Jesus D'Oliveira, Northumbria	3rd-6th September	~ 250
EventISES and IEA SHC International Conference on Solar Energy for Buildings and Industry - Kassel	Oral Presentation, Elisangela Jesus D'Oliveira, Northumbria	25 Sept 2022 → 29 Sept 2022	~ 250
13CNIT2023	Oral Presentation, Rocío Bayón	November 2023	
Eurosun 2024	Oral Presentation, Rocío Bayón	August 2024	
6th EuChemS Inorganic Chemistry Conference	Keynote, Alenka Ristić, NIC	September 3-7, 2023, Vienna/Austria.	400
FEZA 2023 : 9th Conference of the Federation of the European Zeolite Associations,	Poster, Jan Marčec, NIC	Portorž-Portorose Slovenija, 2-6 July 2023	400
10th Slovenian-Serbian-Croatian Symposium on Zeolites	Oral presentations, Jan Marčec, Ciara Byrne, NIC	May 23-25, 2024, Ljubljana, Slovenia	80

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Enerstock2024	Oral presentation, Ciara Byrne, NIC	June, 2024, Lyon, France	250
EIRES Lunch Lecture at Eindhoven Institute for Renewable Energy Systems	Oral presentation, Alenka Ristić and Nataša Zabukovec Logar, NIC	Netherlands, 12th May 2023, on-line	50
34. Deutsche Zeolith-Tagung	Poster, Ciara Byrne, NIC	21.-23. Februar 2023, Universitat Wein, Austria	100
5th European Conference on Metal Organic Frameworks and Porous Polymers : (EuroMOF2023)	Poster, Jan Marčec, NIC	Granada 2023 : [24-27 September 2023	1500
29th Annual Meeting of the Slovenian Chemical Society	Poster, Alenka Ristić, NIC	13.-15. september 2023, Portorož, Portorose, Slovenija	300
29th Annual Meeting of the Slovenian Chemical Society	Poster, Smith Jakob, TU Vienna	13.-15. september 2023, Portorož, Portorose, Slovenija	300
30th Annual Meeting of the Slovenian Chemical Society	Oral presentation, Poster, Jan Marčec, NIC	18.-20. september 2024, Bernardin, Portorož, Slovenia	300
Eurosun2024	Oral Presentation, Alenka Ristić, NIC	26.-29. August, 2024, Limassol, Cyprus	250
37th Workshop on Chemistry and Physics of Novel Materials	Thermochemical energy storage with Tutton salt composites, Jakob Smith	February 4, 2024 Schladming, Austria	
6th EuChemS Inorganic Chemistry Conference	Poster presentation: Exploring the Synergies of Gamma Alumina and Tutton Salt Hydrates in Thermochemical Energy Storage, Jakob Smith	September 3 – 7, 2023 Vienna, Austria	500?
Zbornik povzetkov Slovenski kemijski dnevi 2023	Exploring the synergies of gamma alumina and sulfate salt hydrates in thermochemical energy storage, Jakob Smith	13.-15. September, Portorož, Slovenia	200?

Conference / Workshop / Seminar Name	Activity & Presenter	Date & Location	# of Attendees
2nd StoRIES Summer School	Novel Sulfate Hydrates As Thermochemical Energy Storage Materials: Presentation with the EERA JP Energy Storage Award: Early-stage Researcher Best Poster Presentation Award, Jakob Smith	June 3, 2024, Rome, Italy	
EUROSUN 2024	Oral presentation, Nasrin Aliyari, University of Coimbra	26-30 August 2024, Limassol, Cyprus	
HPC 2023	Presentation, Leander Morgenstern; TUM	03.09. – 06.09.2023, Edinburgh Schottland	
ISEC 2024	Poster, Florian Kerscher; TUM	10.04. – 11.04.2024, Graz, Austria	
Industriewende-Dialog „Thermische Energiespeicher“, Forschungsnetzwerk Industrie und Gewerbe	Presentation, Florian Kerscher; TUM	14.06.2024, online, Germany	
EuroSun 2022	Oral Presentation / A.Inés Fernández	2022/ Kassel, Germany	
EuroSun 2022	Oral Presentation / Rebeca Salgado-Pizarro	2022/ Kassel, Germany	
IMPRES 2022	Oral Presentation / Camila Barreneche	2022 / Barcelona, Spain	
IMPRES 2022	Oral Presentation / A. Inés Fernández	2022 / Barcelona, Spain	
IMPRES 2022	Oral Presentation / Marc Majó	2022 / Barcelona, Spain	
IMPRES 2022	Poster / Marc Neira	2022 / Barcelona, Spain	
IMPRES 2022	Oral Presentation / Rebeca Salgado-Pizarro	2022 / Barcelona, Spain	
Eurotherm Seminar #116 - Innovative solutions for thermal energy storage deployment	Oral Presentation / Rebeca Salgado-Pizarro	2023 / Lleida, Spain	
Eurotherm Seminar #116 - Innovative solutions for thermal energy storage deployment	Oral Presentation / Marc Majó	2023 / Lleida, Spain	
ENERSTOCK 2024	Oral Presentation / Marc Majó	2024 / Lyon, France	

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ENERSTOCK 2024	Oral Presentation / Rebeca Salgado-Pizarro	2024 / Lyon, France	
ENERSTOCK 2024	Oral Presentation / Camila Barreneche	2024 / Lyon, France	
ENERSTOCK 2024	Oral Presentation / A. Inés Fernandez	2024 / Lyon, France	