Experimental set-up for the validation of phase change models in case of direct and inverse heat transfer problems

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Abstract. A number of models and modelling approaches for phase transitions of phase change materials (PCMs) have been proposed in recent years. However, many of these models have not been thoroughly validated with experimental data. This is in particular the case of the models for thermal hysteresis and partial phase transitions of PCMs, where the design and execution of relevant experiments is difficult. The most widely used experimental techniques for characterization of PCMs - Differential Scanning Calorimetry (DSC) and T-history method – require minimization of the temperature gradients in the test samples and thus the obtained results do not represent very well the behavior of PCMs in thermal energy storage (TES) systems (where large temperature gradients in PCMs are commonplace). An experimental set-up for the acquisition of data suitable for validation of phase change models have been proposed and assembled. The set-up can be used for the model validation in case of both the direct and inverse heat transfer problems. The set-up is based on the monitoring of the phase change front propagation in a rectangular cavity, where the positive or negative heat flux is introduced at one of the cavity walls. Such an arrangement results in (often significant) temperature gradients in a PCM. Unlike in similar experimental set-ups, where a heat transfer fluid (HTF) is used to introduce the heat flux at the wall, the Peltier cells are used in the proposed experimental set-up for this purpose. Also, most experiments reported in the literature only addressed the melting process (heating of a PCM) with the positive heat flux introduced at the wall. The Peltier cells allow for relatively quick switching between the positive and negative heat flux (heating/cooling) and as a result the thermal processes similar to real-life operation of TES systems can be investigated. The cubical cavity with 250 mm long internal edges is made of PMMA. The wall, at which the heat flux is introduced, is made of a 15 mm thick aluminum plate with embedded RTD temperature sensors for wall temperature monitoring. A heat flux sensor is installed on the side of the aluminum plate facing the PCM (the heat flux sensor covers the entire surface of the plate). An extended heat transfer surface in the form of a finned aluminum sink is installed on the Peltier cells to improve the heat transfer between the cells and the ambient environment.

Introduction

Phase change materials (PCMs) and their usage in latent heat thermal energy storage (LHTES) systems have been studied extensively and applied in various engineering areas, notably in the building sector [1], for domestic hot water (DHW) storage [2], temperature stabilisation [3] or in concentrated solar power (CSP) systems [4]. The development of efficient energy storage systems is essential in renewable energy systems, as there is a huge discrepancy between energy supply and energy demand. Although most of the energy will be likely stored in form of electricity using battery systems and hydrogen energy storage in the future, they are limited mainly by their efficiency and environmental impact. Therefore, thermal energy storage (TES) systems should not be overlooked, as they are low maintenance, easy to use, and offer high temperature stability.

The mathematical modelling of such systems is a very useful tool, mainly during the development phase of the LHTES systems itself. However, the accuracy of the modelling approach is limited by the quality of input data, which usually comprise specific heat capacity, thermal conductivity, latent heat of fusion, or material density. Experimental investigation of the above-mentioned properties is quite challenging, time-consuming, highly sensitive to the measurement accuracy, and further complicated by phenomena such as phase change hysteresis (PCH) or supercooling. Also, most commonly used methods, such as the differential scanning calorimetry (DSC) method or the temperature history (T-history) method, are applicable only for the investigation of a small sample, therefore resulting in thermal behaviour which does not represent the amount of PCMs in real-life TES systems.

The PCH phenomena is rarely addressed in the mathematical models of heat transfer in PCMs. The most common definition of PCH is as a shift between the melting and solidification temperatures - in other words, the material has to be cooled down below its melting temperature in order for the solidification to be initiated. Therefore, neglecting PCH could generally lead to high dis-

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crepancies between the simulation and experimental results. In connection with the interruption of the melting/solidification process, the PCH could be further separated into the complete phase change (CPC) or the partial phase change (PPC). The mathematical modelling of CPC is usually quite straightforward, as it is based on direct switching between the heating and cooling curves [5]. However, this approach is not applicable in cases where there is a heating/cooling switch (and vice versa) during the phase transition, resulting in PPC. In such cases, a more advanced model has to be utilised, taking into account the transition period that takes place right after the interruption.

Thermal behaviour of PCMs during the PPC have been studied thoroughly in recent years, however there is still a lot of uncertainty surrounding the PPC transitions and further validation is needed. An efficient method for inverse identification of thermophysical properties of PCMs was presented by Zalewski et al. [6]. As a case study, a cement mortar filled with a microencapsulated PCM was subjected to repeated temperature ramps. Omaraa [7] proposed the inverse identification procedure based on experimental data obtained using the conventional T-history method. A detailed study on the inverse identification of thermal behaviour of PEG6000 PCM was presented by Thonon et al. [8]. An experimental apparatus consisting of a PCM sample was contained between two fluxmeters and it was exposed to heating and cooling cycles imposed by two heat exchangers, which were controlled using thermoregulated baths.

1 Experimental set-up

A novel experimental set-up has been designed, containing the plexiglass container filled with a studied PCM, which was subject to the heating/cooling cycles. The experiment was controlled using Peltier cells, which allow for both heating and cooling cycles. In total, nine Peltier cells were inserted into a 3 by 3 grid and placed between the aluminium plate on the inner side and the passive cooler on the outer side, as shown in Figure 1 and 2. Seven Pt100 sensors were placed inside the aluminium plate to investigate the homogeneity of the heat flux produced by the Peltier cells. ALMEMO FQA019C (250mm × 250mm) heat flux meter was installed on the inner surface of the aluminium plate, measuring the heat flux entering the PCM bulk. Moreover, there are plans to incorporate two more Pt100 sensors to assess the temperature within the PCM layer. The first sensor will be positioned at the center of the cavity, while the second one will be situated 40 mm away from the heated surface. All measurement data were collected using a digital data acquisition (DAQ) system. The material properties of the investigated PCM Rubitherm RT 35 HC are summarised in Table 1. The entire experimental set-up was thermally insulated along its outer surfaces to avoid heat losses to the surroundings.

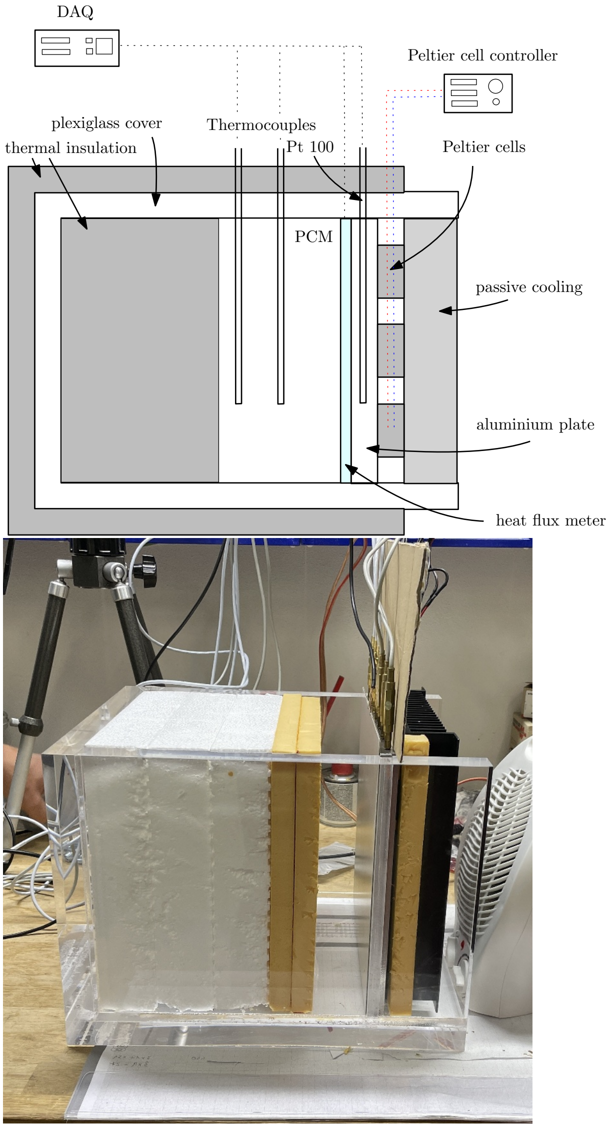

Fig. 1. Experimental set-up.

2 Methods

The inverse identification methodology is built around the inverse problem, mathematical model, and optimisation methods. As the most essential part, the mathematical model is used in both direct and inverse problems. Direct problems use a specific set of input parameters (material properties, boundary conditions, design parameters) and generate, according to the mathematical model, the information about behaviour. However, in the case of inverse problems, some of the input parameters are unknown and subject to inverse identification. Contrary to direct problems, specific information about the behaviour is known - usually from an experiment.

A 1-D heat conduction model was adopted, defined by the heat equation as

$$\rho c_{\mathrm{eff}}(T)\frac{\partial T}{\partial \tau} = \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right), \tag{1}$$

where τ is time, T describes temperature, k is thermal conductivity, ρ is density and x is the spatial coordinate. In

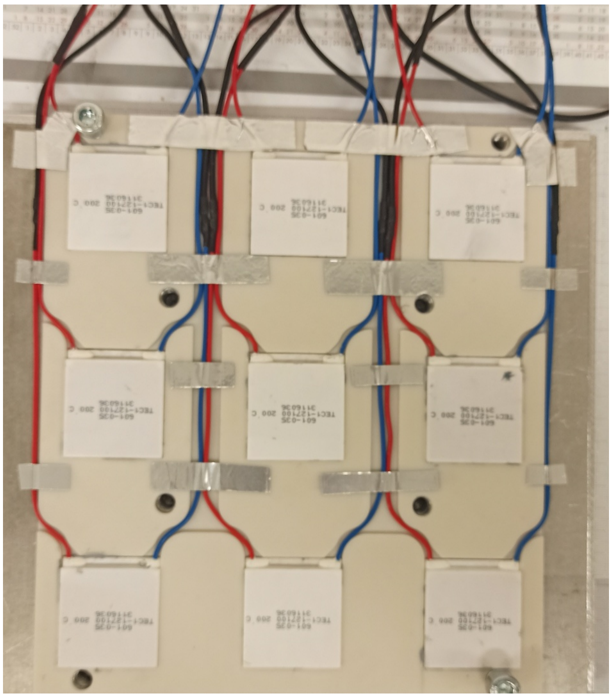

Fig. 2. Peltier cell grid.

Table 1. Material properties of Rubitherm RT 35 HC [9].

Material property	**Value**	**Unit**
Phase change temperature	35	[°C]
Heat storage capacity*	240	[$\text{kJ}\,\text{kg}^{-1}$]
Specific heat capacity	2000	[$\text{J}\,\text{kg}^{-1}\,\text{K}^{-1}$]
Density	800	[$\text{kg}\,\text{m}^{-3}$]
Thermal conductivity	0.2	[$\text{W}\,\text{m}^{-1}\,\text{K}^{-1}$]

*(latent and sensible heat between 27 - 42°C)

terms of phase change modelling, the effective heat capacity method was used. The effective heat capacity function (shown in Figure 4) was defined, similarly as suggested by [8], in the form of an asymmetric Gaussian function as

$$c_{\text{eff}}(T) = \begin{cases} c_{\text{s}} + (c_{\text{M}} - c_{\text{s}}) \exp\left\{\frac{(T - T_{\text{ppc}})^2}{\sigma_{\text{s}}}\right\} & \text{for } T \le T_{\text{ppc}}, \\ c_{\ell} + (c_{\text{M}} - c_{\ell}) \exp\left\{\frac{(T - T_{\text{ppc}})^2}{\sigma_{\ell}}\right\} & \text{for } T > T_{\text{ppc}}, \end{cases} \tag{2}$$

where c_{s} and c_{ℓ} are specific heat capacities in the solid and liquid phase, c_{M} is the height in mode value of the c_{eff} function, T_{ppc} represents the peak phase change temperature, and σ_{s} and σ_{ℓ} define the sharpness of the Gaussian function. Parameters of the c_{eff} function serve as the optimisation variables $\mathbf{p} = (c_{\text{s}}, c_{\ell}, c_{\text{M}}, T_{\text{ppc}}, \sigma_{\text{s}}, \sigma_{\ell})$.

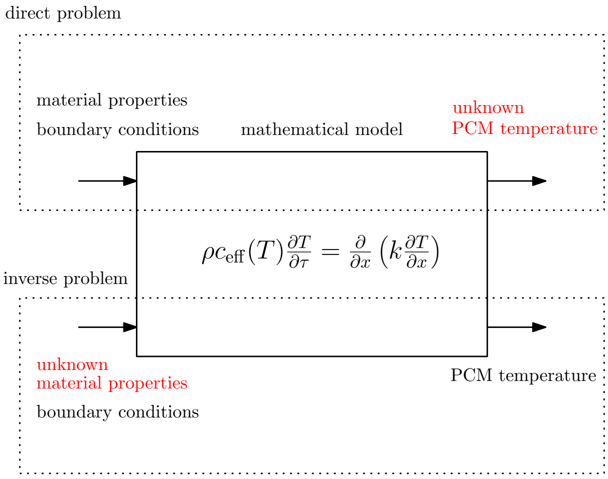

Fig. 3. Direct and inverse problem.

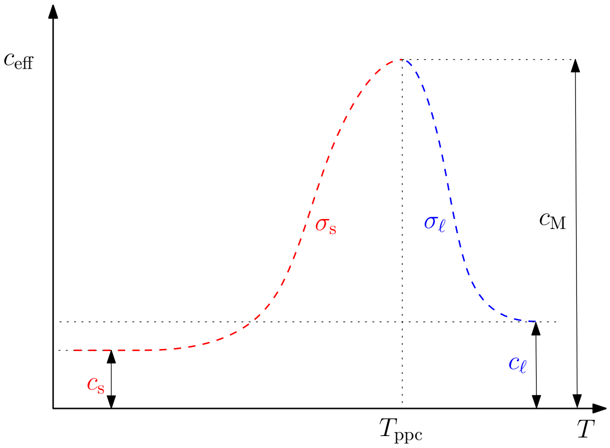

Fig. 4. Parametrization of the effective heat capacity function.

In connection with the experimental measurement, the inverse problem was defined as minimising the sum of square differences between the calculated and measured temperatures in PCM, as is shown in Equation 3

$$\mathtt{OF}(\mathbf{p}) = \sum_{i=0}^{\frac{t_{\max}}{\Delta t}} \left(T^{\text{PCM}}_{\text{sim}} - T^{\text{PCM}}_{\text{exp}}\right)^2 , \tag{3}$$

where i is iteration number, $t_{\max}$ represents the duration of the simulation/experiment, Δt is time step, $T^{\text{PCM}}_{\text{sim}}$ is calculated PCM temperature and $T^{\text{PCM}}_{\text{exp}}$ is the measured PCM temperature.

As a next step, a suitable optimisation method has to be utilised, searching for the set of parameters **p** that would minimise the value of objective function for a given search space. For this purpose, the planned approach involves utilizing the particle swarm optimization (PSO) method. The PSO method is founded on the concept of simulating the behavior of a swarm of particles, where each particle represents a potential solution within the optimization problem (a specific value of the vector **p**). By iterative updating the positions and velocities of these particles based on their own experiences and the collective knowledge of the swarm, PSO aims to converge towards the optimal solution. The iterative nature of this process enables the method to efficiently navigate the search space, increasing the chances of discovering the global optimum. Nevertheless, it is crucial to acknowledge that this method does not provide a guarantee of achieving the global optima. The optimization procedure employed the PSO method from the Global Optimization Toolbox, implemented using MATLAB software.

3 Pilot measurements

A series of initial measurements was performed. As a first step, the heat generation section of the developed experimental apparatus consisting of Peltier cell grid, passive cooling, aluminium plate and surface heat flux meter was tested. The homogeneity of the heat flux produced by the Peltier cells was investigated by measuring the temperatures (using 7 Pt100 sensors) inside the aluminium plate and by means of thermal imaging. The heat flux in the direction of PCM bulk was measured using ALMEMO FQA019C heat flux meter placed on the inner surface of the aluminium plate. As can be seen in Figure 5 and 6, the Peltier cells were able to produce a homogeneous temperature field with the average of maximum differences in surface temperatures of 1.04 °C.

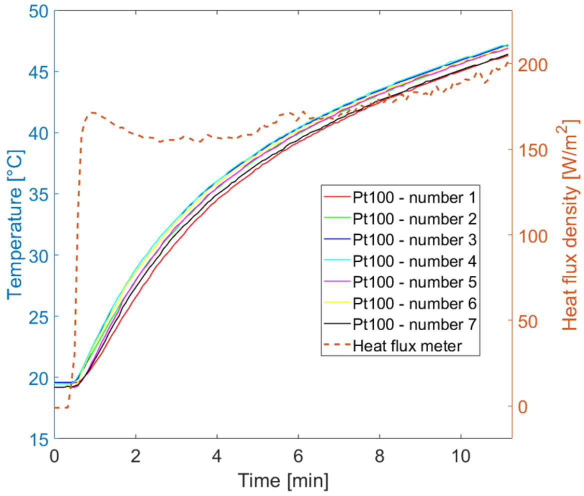

Fig. 5. Temperature evolution during heating cycle.

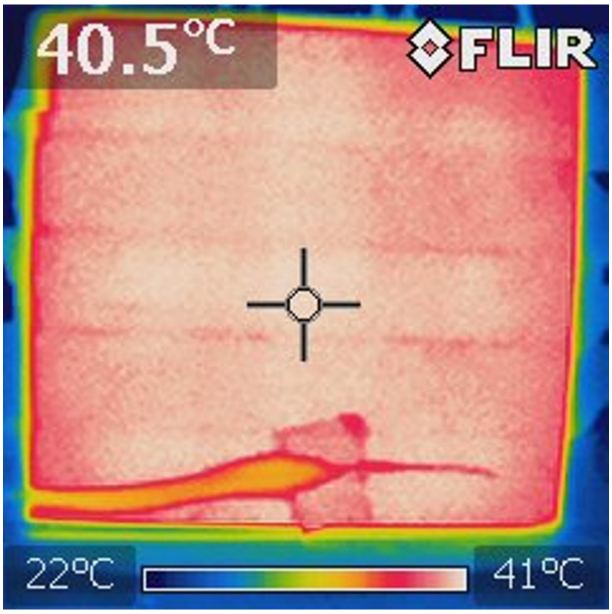

Fig. 6. Thermal image of the aluminium surface temperature.

Conclusion

The main results of the presented study can be summarised as follows

- The experimental set-up was developed in a way that allowed for the cyclic heating and cooling stress to be imposed on the studied PCM.
- The homogeneity of the temperature distribution was investigated using the thermal imaging and temperature measurements by 7 Pt100 sensors inside the heated aluminium plate. The results have shown an evenly distributed surface temperature with the average of maximum surface temperature differences of 1.04 °C during the heating process.
- The testing of the experimental set-up provides the foundation for future research on the inverse identification of material properties of PCMs. In future studies, PCM will be subject to series of interrupted melting and solidification cycles during which the heat flux to (or from) the PCM, as well as the PCM temperatures at different locations will be monitored. The measured data will be used for the study of complex thermal behaviour with the use of the mathematical model and heuristic optimisation methods.
- Close monitoring of natural convection is crucial as it can emerge as a significant driving force in the overall heat transfer process. To mitigate the effects of buoyancy flow in future studies, it is recommended to reduce the height of the investigated cavity and lower the heating/cooling rate.

Acknowledgement

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