Estimation of the thermal properties of PCMs through inverse modelling

Available online at www.sciencedirect.com

ScienceDirect

Energy Procedia 78 (2015) 1714 – 1719

Energy Procedia

6th International Building Physics Conference, IBPC 2015

Estimation of the thermal properties of PCMs through inverse modelling

Ylenia Cascone[a], Marco Perino[a,]*

[a]Department of Energy, TEBE Research Group, Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129 Torino, Italy

Abstract

Even though the use of Phase Change Materials (PCMs) is promising to improve the energy efficiency of buildings, their application in the building sector is still very limited. One of the obstacles to the diffusion of PCMs is the lack of information regarding their thermo-physical properties. A method for estimating the specific heat-temperature curve of a PCM through inverse modelling is herewith presented. This method combined experimental data with a numerical tool able to simulate multilayer walls with the inclusion of PCM materials. Results were validated against tests on different samples and discussed in comparison with a low-speed DSC measurement.

Peer-review under responsibility of the CENTRO CONGRESSI INTERNAZIONALE SRL

Keywords: Phase Change Materials (PCM); thermo-physical properties; inverse problem

1. Introduction

In recent years, the application of Phase Change Materials (PCMs) has been investigated in many fields. Due to the promising role that these materials could have to improve the energy efficiency of buildings, many researches have focused on their application in the building envelope. However, although the great interest that PCMs have gained, their practical application in the building sector is nowadays still very limited. One of the obstacles to the diffusion of PCMs is the lack of information regarding their thermo-physical properties.

* Corresponding author. Tel.: +39-011-090-4423; fax: +39-011-090-4499.
E-mail address: marco.perino@polito.it

Peer-review under responsibility of the CENTRO CONGRESSI INTERNAZIONALE SRL
doi:10.1016/j.egypro.2015.11.275

Nomenclature

a	amplitude coefficient of the solidification/melting peak (-)
c	specific heat (J/(kg K))
T	temperature (°C)

Subscripts

l	liquid
max	maximum
peak	solidification/melting peak
s	solid

Many manufacturers do not provide data on the enthalpy-temperature curve of their products or these data are not suitable for application in a building energy simulation tool. In addition, the capabilities of building simulation tools may not be totally appropriate to simulate every kind of material. For example, EnergyPlus allows for a single enthalpy-temperature curve as input for each PCM and cannot take the hysteresis phenomenon (different behaviour of the material during solidification and melting) into account. In this case, the evaluation of a single curve which can still simulate the material behaviour in an acceptable way would prove useful.

Among the experiments that can be conducted for measuring the dependency of the specific heat capacity on temperature are the Differential Scanning Calorimetry (DSC) and the T-history method.

The DSC is the most used laboratory measurement to obtain melting temperature and heat of fusion of PCM samples. However, limitations of the DSC approach are the very small sample size and the strong influence of the test procedure on the results [1]. Especially for dynamic measurements with constant heating and cooling rate, a slow rate is needed for PCMs unlikely the typical standards used in DSC analysis for other materials [2, 3]. Following the German RAL standard [4] and further improvements which include proper calibration and baseline measurement, reliable measurements were achieved with dynamic DSC in heating [5].

The T-history method [6] is widely adopted as an alternative to DSC to investigate the thermal behaviour of large PCM samples. Several contributions were proposed to improve its mathematical model [7, 8], its measuring process [9, 10] or both [11]. A horizontal setup was also found to reduce the discrepancies between freezing and melting enthalpy-temperature curves [1]. The T-history method can also be used to evaluate the thermal conductivity of PCMs whose phase change occurs with a clear interface between the two phases. However, thermal conductivity and specific heat cannot be simultaneously determined.

Another approach for estimating the thermo-physical properties of materials is through the application of inverse methods. Such problems could be dealt with by means of exhaustive search method or can be formulated as optimisation problems. In this case, the objective is to minimise the discrepancy between measured values (e.g. of temperature or heat flux) and calculated values based on the estimated properties. However, inverse problems are ill-posed; under small changes of the input data existence, uniqueness and stability of the solution are not satisfied. [12]. In recent years, an estimation of thermal conductivity and heat capacity on materials with constant properties was carried out by Derbal et al. [13], who proposed a procedure that can be potentially applied to in-situ measurements. The material to be characterised is placed between two layers of materials with known thermo-physical properties. Thermocouple probes are placed at the different interfaces and record the variations in temperature when the whole multilayer is subjected to stimulation. In addition to thermal conductivity and heat capacity, Chaffar et al. [14] estimated also the surface film coefficient of a homogeneous panel by applying a heat flux and studying the response in terms of the temperature recorded by infrared thermography on the opposite surface. With regards to PCMs, Lachheb et al. [15] proposed a method for estimating thermal conductivity, specific heat and thermal diffusivity of paraffin/graphite PCM composites from laboratory tests under controlled boundary conditions, but material properties were evaluated at room temperature and their dependency on temperature was hence not investigated. Thermal conductivity and specific heat as a function of temperature of PCM-concrete bricks subjected to controlled boundary conditions were estimated by Cheng et al. [16]. The temperature dependency was evaluated through the temperature segment method, which has the advantage of not requiring any a-priori knowledge on the specific heat function. However, the number of segments directly determines the number of variables in the optimisation problem. Temperature-dependent thermal conductivity, heat capacity and thermal diffusivity were simultaneously estimated by Cui et al. [17], who proposed an approach based on the measurement of the temperature distribution within the material and subjected either to Dirichlet or Neumann boundary conditions. Prior information on the functional form of the thermal properties is not necessary.

In the present work, a method for estimating the enthalpy-temperature curve of a PCM through inverse modelling is presented. This method combines experimental data with a numerical tool that is capable of simulating multilayer walls with the inclusion of PCM materials. The experimental setup consisted in a sample of PCM which was subjected to controlled temperature variations on its surfaces. Given the measured surface temperatures of the sample as boundary conditions and the known thermo-physical properties of the material (thermal conductivity and density) to the model, the enthalpy-temperature curve which minimised the difference between measured and simulated heat fluxes was found through an optimisation algorithm. Results were validated against tests on different samples and discussed in comparison with a low-speed DSC measurement.

Even though laboratory tests were used to validate the procedure, in-situ measurements could be also used. However, the accuracy of the estimation would be greatly affected by the uncertainty of the input data.

2. Methodology

A method for estimating the enthalpy-temperature curve of a PCM through inverse modelling is presented. This method combines experimental data with a numerical tool that is capable of simulating multilayer walls with the inclusion of PCM materials.

The experimental setup consisted in three samples which were subjected to controlled temperature variations on their surfaces. One sample was used to retrieve the thermo-physical properties of the PCM under investigation (Sample A), whereas the others were used for validation (Samples B1 and B2). Each sample was placed in a LASERCOMP FOX 600 guarded hot plate and heat flow meter apparatus, which was modified by the manufacturer to allow for sinusoidal temperature variations on its plates with a period of 24 hours and a pre-settable amplitude.

Sample A was composed, from top to bottom, by 15 mm of a shape-stabilised PCM (nominal melting temperature of 21,7 °C) and 120 mm of XPS. To cover the material phase-change range, during testing the upper plate was subjected to a sinusoidal temperature variation with average temperature of 23 °C and amplitude of 5 °C while the lower plate was kept at a constant temperature of 23 °C. Sample B1 was composed by 2 layers of gypsum plasterboard 12.5 mm thick, 50 mm of mineral wool, 5 mm of PCM and 12.5 mm of gypsum plasterboard. During testing the upper plate was kept at a constant temperature of 23 °C while the lower plate was subjected to a sinusoidal temperature variation with average temperature of 23 °C and amplitude of 8 °C. Sample B1 differed from Sample A in the thickness of the PCM layer (10 mm). The test duration was 48 hours.

Material properties other than the specific heat of the PCM where either measured (thermal conductivity), retrieved by the manufacter datasheets (density) or found in literature (specific heat).

Given the measured surface temperatures of Sample A as boundary conditions and the known thermo-physical properties of the materials to the model, the specific heat vs temperature curve of the PCM which minimised the difference between measured and simulated heat fluxes on both faces of the sample was found through an optimisation algorithm. The objective function was formulated as maximisation of the coefficient of determination R^2. Only the last 24 hours were considered to evaluate the fitness accuracy not to account for the effects deriving from the initial conditions.

The search was performed through the ($\lambda + \mu$) Evolution Strategy (ES) technique [18, 19], whose implementation was validated against the Rosenbrock function. Evolutionary algorithms are stochastic optimisation algorithms where the optimum seeking process is based on the principles of organic evolution. [20]. These algorithms are based on the competition among individuals in a population. Each individual is a vector of input data whose value in the objective function represents its fitness to survive. Only μ individuals with the best fitness (lowest or highest values according to the type of optimization problem, i.e. minimisation or maximisation) among the population are allowed to reproduce and generate new offspring through crossover and mutation algorithms. In the ($\lambda + \mu$) ES, individuals can survive for more than one generation; both parents and offspring are considered for ranking and crossover. The fitness of the new born individuals is evaluated and the rate of success – i.e. the rate of fitness improvement compared to the previous generation – is used to influence the subsequent mutations. The process continues until a stop criterion is met. The individual with the best fitness represents the final result of the optimisation process.

The numerical simulation of the heat transfer process was carried out by solving the one-dimensional transient heat conduction equation. The solution was retrieved through the application of the finite difference methods with Crank-Nicolson scheme and Gauss-Seidel overrelaxation [21, 22]. A uniform time step and a uniform mesh size were assumed.

The dependency of the specific heat on temperature was modelled according to equation (1) [23]:

$$\begin{cases} c = c_s + (c_{\max} - c_s) \cdot e^{-\left[\left(T_{peak}-T\right)/a_s\right]^2} & \text{if } T \le T_{peak} \\ c = c_l + (c_{\max} - c_l) \cdot e^{-\left[\left(T_{peak}-T\right)/a_l\right]^2} & \text{if } T > T_{peak} \end{cases} \quad (1)$$

Even though a-priori knowledge of the functional form of the specific heat was not strictly necessary, this approach was chosen to reduce the number of search variables and hence reduce the calculation run time. In this way, only six variables were needed to describe the specific heat. Thermal conductivity could also be evaluated, but the focus of the present work was especially on specific heat estimation.

3. Results and discussion

The comparisons between measured fluxes both at the dynamic and static plates and the simulated values after solution of the inverse problem are reported in Fig. 1 (a) for Sample A. To evaluate the accuracy of the estimation, the root mean square error (RMSE) was calculated, for estimation and validation samples, according to equation (2):

$$RMSE = \sqrt{\frac{\sum (\hat{y} - y)^2}{N}} \quad (2)$$

where $\hat{y}$ are the simulated values, y are the measured values and N is the number of measurements. The resulting values of RMSE are summarised in Table 1. A very good agreement between measured and simulated data was found. The highest RMSE of the heat fluxes exchanged with the dynamic plate was found for the evaluation sample (3,486 W/m^2), whereas the highest RMSE of the heat fluxes exchanged with the static plate was found for Sample B2 (0,889 W/m^2).

Heating and cooling curves from a dynamic DSC measurement with a rate of 0,05°C/min are shown in Fig. 2 in comparison with the specific heat vs temperature curve resulting from the inverse problem. The output values of the estimation (specific heat in solid and liquid phase, peak temperature, maximum specific heat and amplitude coefficients of the solidification/melting peak) are reported in Table 2.

Table 1. RMSE of the heat fluxes measured by the guarded hot plate.

Sample	RMSE dynamic plate (W/m^2)	RMSE static plate (W/m^2)
Sample A (estimation)	3,486	0,231
Sample B1 (validation)	2,533	0,774
Sample B2 (validation)	1,994	0,889

Table 2. Estimated values of the unknowns of the inverse problem.

c_s (J/(kg K))	a_s (-)	T_{peak} (°C)	c_{max} (J/(kg K))	c_l (J/(kg K))	a_l (-)
3224	11,11	17,40	14437	2461	3,42

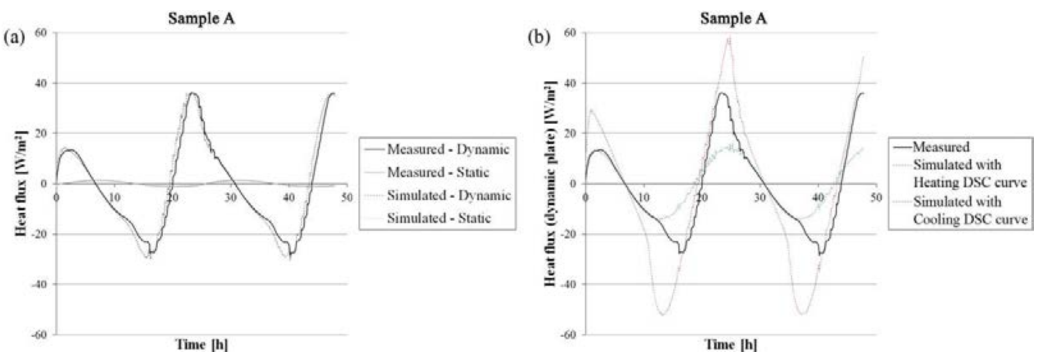

Fig. 1. Measured vs simulated heat fluxes for Sample A with: (a) data from inverse problem estimation; (b) data from DSC measurements.

Although the low speed of the DSC measurement, a significant hysteresis can be observed. A comparison between measured fluxes at the dynamic plate and simulated values with specific heat data from the DSC is reported in Fig. 1 (b). Only some portions of the curves are in agreement with the measured data; with a RMSE respectively of 15,76 W/m^2 and 10,52 W/m^2 for simulations with heating and cooling DSC curves, the errors are very high.

The estimations of the specific heat in liquid phase and of the maximum value of the specific heat were in agreement with the DSC melting curve (Fig. 2). The estimated peak temperature was instead in agreement with the DSC solidification curve. The estimated peak temperature (17,4 °C) was lower than the nominal melting temperature (21,7 °C), falling even outside the strict validity range of the estimation (18 °C – 28 °C, which can be extended to 16 °C – 30,5 °C after validation with Samples B1 and B2). Due to peak temperature shift, no accurate information on the specific heat in solid phase could be retrieved. Further experimental tests should be performed at lower temperatures for a more comprehensive characterisation of the PCM.

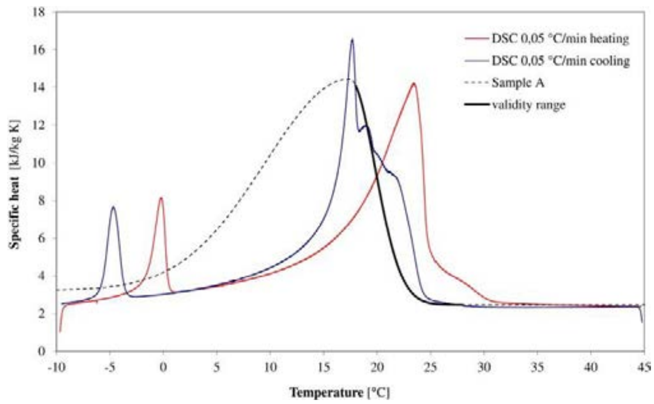

Fig. 2. Specific heat as a function of temperature: estimation vs DSC measurements.

4. Conclusions

A method for estimating the specific heat as a function of temperature of a PCM through inverse modelling was presented. This method combined experimental data with a numerical tool that was capable of simulating multilayer walls with the inclusion of PCM materials. The experimental setup consisted in a sample of PCM which was subjected to controlled temperature variations on its surfaces. Given the measured surface temperatures of the sample as boundary conditions and the known thermo-physical properties of the material to the model, the specific heat-temperature curve which minimised the difference between measured and simulated heat fluxes was found through an optimisation algorithm. The resulting curve was compared with a low-speed DSC measurement. The estimations of the specific heat in liquid phase and of the maximum value of the specific heat were in agreement with the DSC melting curve. The estimated peak temperature was instead in agreement with the DSC solidification curve. The estimated peak temperature was lower than the nominal melting temperature, falling even outside the strict validity range of the estimation. Due to this peak temperature shift, no accurate information on the specific heat in solid phase was retrieved. Future work will deal with further experimental tests, which will be performed at lower temperatures for a more comprehensive characterisation of the PCM. The accuracy of a single enthalpy-temperature curve retrieved by inverse methods for application in building energy simulation software will also be investigated.

Acknowledgements

Authors are grateful to Dr. Stefano Fantucci for his help in performing some of the experimental tests.

References

[1] Gschwander S, Lazaro A, Cabeza LF, Günther E, Fois M, Chui J. Development of a Test-Standard for PCM and TCM Characterization – Part 1: Characterization of Phase Change Materials. IEA Report A2.1 part 1. Task 42/Annex 24; 2011.
[2] Castellón C, Günther E, Mehling H, Hiebler S, Cabeza LF. Determination of the enthalpy of PCM as a function of temperature using a heat-flux DSC-A study of different measurement procedures and their accuracy. Int J Energy Res 2008;32:1258-65.
[3] Günther E, Hiebler S, Mehling H, Redlich R. Enthalpy of phase change materials as a function of temperature: required accuracy and suitable measurement methods. Int J Thermophys 2009;30:1257-69.
[4] German Institute for Quality Assurance and Certification E.V. RAL-GZ 896 – Phase Change Material. Sankt Augustin: RAL, 2009.
[5] Lazaro A, Peñalosa C, Solé A, Diarce G, Haussmann T, Fois M, Zalba B, Gshwander S, Cabeza, LF. Intercomparative tests on phase change materials characterisation with differential scanning calorimeter. Appl Energ 2013;109:415-420.
[6] Zhang YP, Jiang Y, Jiang Y. A simple method, the T-history method, of determining the heat of fusion, specific heat and thermal conductivity of phase-change materials. Measur Sci Technol 1999;10:201-5.
[7] Marín JM, Zalba B, Cabeza LF, Mehling H. Determination of enthalpy-temperature curves of phase change materials with the temperature-history method: improvement to temperature dependent properties. Measur Sci Technol 2003;14:184-189.
[8] Sandnes B, Rekstad J. Supercooling salt hydrates: stored enthalpy as a function of temperature. Sol Energy 2006;80:616-625.
[9] Kravvaritis ED, Antonopoulos KA, Tzivanidis C. Improvements to the measurement of the thermal properties of phase change materials. Measur Sci Technol 2010;21:5103-5112.
[10] Kravvaritis ED, Antonopoulos KA, Tzivanidis C. Experimental determination of the effective thermal capacity function and other thermal properties for various phase change materials using the thermal delay method. Appl Energ 2011;88:4459-4469.
[11] Stanković SB, Kyriacou PA. Improved measurement technique for the characterization of organic and inorganic phase change materials using the T-history method. Appl Energ 2013;109:433-440.
[12] Gosselin L, Tye-Gingras M, Mathieu-Potvin F. Review of utilization of genetic algorithms in heat transfer problems. Int J Heat Mass Tran 2009;52:2169-2188.
[13] Derbal R, Defer D, Chauchois A, Antczak E. A simple method for building materials thermophysical properties estimation. Constr Build Mater 2014;63:197-205.
[14] Chaffar K, Chauchois A, Defer D, Zalewski L. Thermal characterization of homogeneous walls using inverse method. Energ Buildings 2014;78:248-255.
[15] Lachheb M, Karkri M, Albouchi F, Mzali F, Ben Nasrallah S. Thermophysical properties estimation of paraffingraphite composite phase change material using an inverse method. Energ Convers Manage 2014;82:229-237.
[16] Cheng R, Pomianowski M, Wang X, Heiselberg P, Zhang Y. A new method to determine thermophysical properties of PCM concrete brick. Appl Energ 2013;112:988-998.
[17] Cui M, Gao X, Zhang J. A new approach for the estimation of temperature-dependent thermal properties by solving transient inverse heat conduction problems. Int J Therm Sci 2012;58:113-119.
[18] Rechenberg I. Evolutionsstrategie: Optimierung technischer systeme und prinzipien der biologischen evolution. Stuttgart: Frommann-Holzboog; 1973.
[19] Schwefel HP. Numerical optimization of computer models. Chichester: Wiley; 1981.
[20] Alotto PG, Eranda C, Brandstätter B, Fürntratt G, Magele C, Molinari G, Nervi M, Preis K, Repetto M, Richter KR. Stochastic algorithms in electromagnetic optimization. IEEE T Magn 1998;34:3674-3684.
[21] Öızşık MN. Heat Conduction. 2nd ed. New York: John Wiley & Sons; 1993.
[22] Öızşık MN. Finite Difference Methods in Heat Transfer. Boca Raton: CRC Press; 1994.
[23] Kuznik F, Virgone J, Roux JJ. Energy efficiency of room wall containing PCM wallboard: A full scales experimental investigation. Energ Buildings 2008;40:148-156.