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Title

Uncertainty propagation and sensitivity analysis of thermo-physical properties of phase change materials (PCM) in the energy demand calculations of a test cell with passive latent thermal storage

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Abstract

In this work uncertainty propagation and sensitivity analyses have been applied to a case study of an application where PCM is integrated into the envelope of a test cell. The aim of the study is to quantify the influence of the uncertainties associated with the measurements of the thermo-physical properties of PCM on the results of the annual energy consumption. For this purpose, EnergyPlus has been used for the building energy simulation and a Monte Carlo based method has been chosen for the uncertainty and sensitivity analysis. Considering realistic uncertainty ranges for PCM thermo-physical properties, a significant uncertainty of savings on cooling energy demand has been calculated (approximately 10%). Phase change temperature and thermal conductivity have been identified as the most influential input parameters whereas phase change enthalpy is of secondary importance. A method has been proposed in order to calculate a combination of admissible uncertainties for the input variables that reduces output uncertainty to a required value. The method can be used if input variables and the behaviour of the model comply with certain conditions. For the case study, a maximum tolerance for the error

of measurements of phase change temperature and thermal conductivity of ±0.3°C and ±8% respectively is necessary to reduce the uncertainty of savings on cooling energy demand to 5%.

Nomenclature

A_i	Surface of the test cell wall i [m^2]
c_p	Specific heat [J/(kg·K)]
h_m	Specific phase change enthalpy [kJ/kg]
$h(T)$	Enthalpy temperature curve [kJ/kg]
$\hat{h}(T)$	Approximated enthalpy temperature curve [kJ/kg]
k	Number of uncertain input variables
N	Number of simulations
R^2	Coefficient of determination
T	Temperature [°C]
T_i	Temperature interpolation points [°C]
T_m	Phase change temperature [°C]
$\bar{T}_{PCM}$	Average temperature of PCM layer [°C]
W	Saphiro-Wilk test statistic
x	Input variable, spatial coordinate
y	Ouput variable

Greek symbols:

α	Distribution coefficient
β_i	Coefficients of regression

Δ	Increment
ΔT_m	Phase change temperature range [°C]
δ	Uncertainty
λ	Thermal conductivity [W/(m·K)]
ρ	Density [kg/m^3]
σ	Standard deviation

Abbreviations:

ACH	Air Changes per Hour [h^{-1}]
DSC	Differential Scanning Calorimetry
LFA	Laser Flash Apparatus
LHS	Latin Hypercube Sampling
NRMSD	Normalized Root Mean Square Deviation
PCM	Phase Change Materials
SRC	Standardized Regression Coefficient
TES	Thermal Energy Storage
TMA	Thermo-Mechanical Analyser

1. Introduction

Nowadays the building sector is a key area for improving energy efficiency [1]. It is responsible for approximately 40% of the primary energy consumption in developed countries and contributes almost the same percentage to world greenhouse gas emissions. Furthermore, this primary energy consumption has doubled from 1971 to 2010 due to the increase in population and economic growth [2]. Therefore, current policies are focused on enhancing building energy performance and promoting the use of renewable energy sources.

The use of thermal energy storage (TES) is especially suitable in applications in which the availability of energy sources is time-intermittent, as is the case with renewable energies. Among TES materials, Phase Change Materials (PCM) have the advantage of storing and releasing a significant amount of thermal energy within the narrow temperature interval in which their phase change, generally solid-liquid, takes place. Furthermore, not only have these materials been used in thermal storage devices for heating and air cooling setups, but they can also be integrated into the building envelope in order to increase its thermal mass and thus reduce indoor temperature fluctuations. This passive latent TES has both a beneficial effect on reducing energy consumption for heating and cooling and on improving the thermal comfort of occupants. Comprehensive information about the passive applications of PCM in building systems can be found in recent reviews [3-5], whereas PCM and the different techniques for their integration into building elements are extensively reviewed in [6-9].

During the design stage and the calculation process of the performance of PCM applications, the accuracy of the determination of their thermo-physical properties is an important issue. Several authors have highlighted the importance of the accuracy of the measurements of the enthalpy-temperature curves for these materials [10-12]. Although there are widely accepted experimental methodologies for the determination of enthalpy-temperature curves –principally differential scanning calorimetry (DSC) and the T-history method- discrepancies can be found in experimental data obtained by different methods or measurement conditions [12]. PCM frequently exhibit particular phenomena in their thermal behaviour, such as sub-cooling, the presence of thermal gradients in the sample used in calorimetry, hysteresis, crystallization problems due to the sample size or wide melting temperature range, all of which make it difficult to accurately determine their thermal properties [12]. Considering the present limitations of the accuracy of PCM thermal property measurements, Günther et al. [10] defined a tolerable accuracy for the phase change enthalpy ($\delta\Delta h / \Delta h < 10\%$) and temperature ($\delta T < 1$ °C) of PCMs in order to ensure a tolerance of ±10% for power calculations in a general thermal storage application.

It is therefore advisable to take into account the uncertainties of PCM thermal properties when numerically evaluating their behaviour in energy systems. Although there is a significant quantity of numerical studies dealing with the evaluation of the performance of PCM in different systems, few of these analyse the effect of the uncertainty of the PCM thermo-physical properties. Arkar et al. [13] studied the influence of the different apparent thermal capacity-temperature curves of PCM, which had been obtained using several heating and cooling rates by the DSC methodology, on the numerical results of an experimental set up of a PCM-air heat exchanger. They concluded that curves corresponding to the lower temperature change rates of DSC methodology had to be used in order to obtain greater accuracy in the results, and they argued that the similarity between the temperature change rate of the DSC measurements and the experimental set up was the reason for these better results. Dolado et al. [14] carried out an uncertainty propagation and sensitivity analysis for a theoretical model for the simulation of a PCM-air heat exchanger in which PCM was integrated in slabs. The uncertainty propagation of the model input values was used for its empirical validation and, according to the sensitivity analysis results, the most influential input parameters were identified. Furthermore, some recommendations were made for the accuracy of the input parameters. For instance, an accuracy of 0.25 °C for the enthalpy temperature curve was suggested. Zsembinszki et al. [15] applied a sensitivity analysis to a model of a PCM-to-water heat exchanger. The input variables were varied within their estimated uncertainty range. The deviation from the solution of the reference base case problem caused by the alteration of each input variable value was analysed. The PCM properties had a relevant influence on the solution, the melting temperature causing the largest variations in the results. Tabares-Velasco [16] studied the influence of the precision of the definition of the enthalpy temperature curve on the energy consumption calculation of building simulation programs. Hourly temperature evolution and monthly and yearly energy demands were analysed. He established a level of error for the approximation of the linearly defined h-T curve.

Uncertainty propagation and sensitivity analyses have attracted a growing interest for building simulation during the last few years. They have been used for different purposes: in the building design phase [17-19], in the sizing of air heating and cooling systems [20] and in experimental validation [21, 22]. However, the use of these methodologies is not frequent among the numerical studies on the thermal behaviour of PCM in building elements that have been published. To the authors' knowledge, only Guichard et al. [23] have conducted a global sensitivity analysis to a simulation model of a test cell where a PCM layer was integrated into the roof. It was carried out in the context of the empirical validation of the model, aiming to identify the most influent parameters on the deviation observed between the numerical and experimental results. Thermal properties of PCM had a relevant effect on the temperature fluctuation of the roof components. However, the uncertainty range of the numerical results was not calculated and the accuracy of the measurements of PCM thermo-physical properties was considered sufficient for the purpose of the work.

The present study analyses the influence of uncertainties of PCM thermo-physical properties – associated to the current measurement methodologies- on the energy consumption of an experimental cubicle. In this case, PCM is integrated into exterior walls composed of a conventional brick constructive solution. The potential of PCM for smoothing indoor temperature fluctuation and indoor air temperature peaks in these applications has been demonstrated in previous experimental studies such as in those of Castell et al. [24] analysing the thermal behaviour experimental cubicles and those of Vicente et al. [25] testing different brick wall specimens with PCM in an experimental dynamic wall simulator. Castell et al. [24] also demonstrated the ability of PCM for reducing in 15% cooling energy consumption whereas Izquierdo-Barrientos et al. [26], who numerically analysed the influence of phase change temperature on the reduction of heat transfer through a standard Spanish brick wall, highlighted that some undesired dynamic phenomena can be observed if PCM is integrated into a wall with high thermal inertia.

As part of the work in the context of our research projects, the case study chosen for this paper has been taken from the previous work presented by Castell et al. [24]: an experimental cubicle with conventional brick walls containing macro-encapsulated PCM. This experimental methodology, utilizing cubicles or test cells as an approach to large scale testing, has been used recently for the thermal analysis of different envelope configurations (e.g. integrating PCM into the natural stone of a trans-ventilated façade [27], brick construction envelopes [28] and a roof slab with macro encapsulated PCM [29]). The results of this case study, thus, can be compared to –or can complement- those from previous works where similar examples had been chosen for different analysis (e.g. life cycle analysis [30] or optimization of insulation thickness [31]). Furthermore, one of the objectives for future work is the comparison of the simulation model with experimental measurements taking into account uncertainty propagation in both results.

The main objectives of the present study are:

- To evaluate the uncertainty in the estimation of energy savings on heating and cooling which are obtained by the inclusion of a PCM layer inside the cubicle envelope.

- To study the influence of the uncertainty of each thermo-physical property on the overall uncertainty of the results.

- To obtain, for the case study under consideration, the required accuracy for the measurement of PCM thermal properties in order to reduce the uncertainty of energy consumption calculations to a previously specified level.

2. Methodology: Monte Carlo Analysis

A Monte Carlo method has been used for the evaluation of the uncertainty in the results calculated by the numerical model. According to the classification established by MacDonald [32], this is an external method since it analyses the behaviour of the model in terms of the variation of output variables when modifying the input set of parameters. It has been selected for this case study since the determination of the mathematical relation between PCM properties and the results of overall annual energy consumption is not straightforward. Furthermore, the implementation of the method does not require additional modification to the original model and the obtained sample of output variables can be used for sensitivity analysis.

Each input parameter under analysis is considered as an uncertain variable with an associated probability density function. Therefore, the results obtained with the model are necessarily uncertain. The use of a Monte Carlo method allows the estimation of the probability density function of outcomes and their statistical analysis.

Latin Hypercube Sampling (LHS) [33] has been used for selecting the set of input variables for the simulation. This is frequently used in Monte Carlo analysis since it produces an efficient coverage of the parameter space. McKay et al. [33] demonstrated that if the output function is monotonic within the range of variation of the input variables, LHS produces a better estimation of the mean and population distribution function than random sampling, and stratified for the same dimension of the sample. The LHS algorithm used to generate the sampling for simulation is described below:

-A probability (D_1, D_2,…, D_k) density function is assigned to each uncertain input variable (x_1, x_2,…,x_k). In this study, since no knowledge about the density function describing the uncertainty of PCM thermo-physical properties is available, a normal distribution is considered.

-Each probability density function is divided into N non-overlapping intervals, each having the same marginal probability (1/N). A random sample of each variable is taken from each interval, therefore the set of samples for each variable forms the vector X_{ij} (i=1..N;j=1..k).

-The components of each vector corresponding to the different input variables are randomly matched, thus obtaining the set of input values used in each of the N simulations.

The selection of the sample size (N) is an important issue when using a Monte Carlo method for uncertainty analysis. There is no direct mathematical expression to obtain the minimum number of simulations which ensures the required accuracy for the results, since the variability of the statistical estimators depends on the output function which is, in principle, unknown. However, theoretical results used in previous works [34, 35] can be utilised in this case in order to estimate the errors due to the dimension and method used for sampling. Assuming a normal distribution of the results and a random sampling of the solution, it can be demonstrated that a slight reduction in the confidence intervals for the estimation of the mean and standard deviation is reached if the number of simulations is increased over 100 runs. Furthermore, according to the results of Mckay et al. [33], LHS estimators for the mean, the variance and the population distribution are expected to have a lower variance if the output function is monotonic. Therefore, a sample of 100 simulations has been selected for the uncertainty propagation analysis.

3. Case study

3.1 Description

3.1.1 Experimental cubicle [24]

The house-shaped cubicles being modelled are based on the experimental installation of the GREA research group, situated in Puigverd, (Lleida, Spain) (Fig. 1). They represent a typical Mediterranean construction. The cubicles consist of four walls of 2.4x2.4x0.15 m. The walls consist of 5 material layers (enumerated from outside to inside): a cement mortar finish, a hollow brick structure, an air chamber of 5 cm, perforated bricks and a plaster layer. The PCM, which is macro-encapsulated into CSM panels supplied by Rubitherm [36], is located between the air chamber and the perforated bricks. The roof was constructed using concrete precast beams and a 5 cm concrete slab. The internal finish is plaster. The external finish consists of a layer of cement mortar and a double asphalt membrane. More details can be found in [24, 37].

The following specifications are used for the cubicle simulation. They represent the operation conditions of the experimental cubicles [24] and have already been used in Carreras et al. [31]:

- An internal set point temperature of 24°C is fixed for the whole year.
- Heating and cooling loads are calculated for the annual period.
- A fixed infiltration rate of 0.12 ACH (air changes per hour) is assumed [38]. No mechanical or natural ventilation is considered.
- There is no internal mass and no human occupancy.
- Thermal properties of the construction materials employed are given in [37].

3.1.2 Thermo-physical properties of PCM

The PCM selected as a reference material for this case study is RT-27 supplied by Rubitherm [36]. The enthalpy-temperature curves, measured using the T-history method [39, 40] are plotted in figure 2. These experimental data have already been presented in previous works from the University of Zaragoza [11]. Thermal conductivity (table 1) measurements have been accomplished by the Netzsch Company [41] utilizing laser flash methodology (LFA) (457 MicroFlashTM model). The density of the material has been determined by weighing (microbalance) and measuring the volume of the samples.

3.2 Uncertainty on thermo-physical properties of PCM

The values of the uncertainty associated to each property have been selected according to the results of previous works on determining thermo-physical properties of PCM. Regarding the enthalpy-temperature curve, a parameterized analytical function has been used rather than the experimentally determined one in order to simplify the analysis. The aim of this approach is to separate the contribution of the main factors which are involved in this temperature dependent magnitude. This analytical function representing the h-T curve was used in [14]. The sigmoidal function (Eq. 1) which has been approximated to the experimental data is shown in figure 2.

$$h(T) = h_0 + c_p \cdot (T - T_0) + \frac{h_m}{1+e^{-\frac{T-T_m}{\Delta T_m}}} \quad \text{Eq. 1}$$

Each parameter of the curve is directly related to a thermal property or measurable magnitude (c_p: heat capacity of the PCM, h_m: phase change enthalpy, T_m: phase change temperature, ΔT_m: related to the phase change temperature range). These parameters are graphically identified in figure 3.

Table 1 shows the values of the adjusted parameters for the analytic h-T function. The uncertainty associated to each parameter has been assigned taking into account the results of previous works on the determination of the enthalpy-temperature curves of PCM with the most commonly used methodology: differential scanning calorimetry (DSC) [10, 42] and T-history [10, 11]. The measurement of thermal conductivity of a PCM by the LFA technique has the major difficulty of determining this magnitude at the liquid state, since this methodology was originally developed for measurements in solids. In this work an accuracy of 10% has been considered, in accordance with the experimental results of Delgado et al. [43] and Coquard et al. [44]. Since this error is higher than the variation of this magnitude from solid to liquid phase, the same constant value for the thermal conductivity of both phases is used in this work. The selected uncertainty for density measurements is 2%, in accordance with the results of Peñalosa et al. [45] where the density of several PCM where measured utilizing a densimeter and a thermo-mechanical analyser (TMA). Since the one dimensional model of EnergyPlus is not able to cope with the temperature variations of density, a constant value is selected corresponding to the lower density within the operating temperature range as recommended by Mehling et al. [46] and the RAL-PCM Quality Association [47].

3.3 Simulation of PCM in the test cell envelopes with EnergyPlus [48]

EnergyPlus [48, 49] is the building energy simulation software used in this work for the calculations of the energy performance of the test cells. The program is able to simulate conduction heat transfer in building elements using a finite difference numerical algorithm [50]. Tabares-Velasco et al. [51] verified and experimentally validated the model for calculating heat transfer through PCM layers integrated into building elements. EnergyPlus is widely used for the study of the behaviour of PCM when incorporated into construction elements. Some examples of its use can be found in the work of Pedersen [50] on the simulation of PCM incorporated into building envelopes, and the works of Soares et al. [52], Evola et al. [53] and Alam et al. [54] on the simulation of PCM wallboards.

In EnergyPlus, a one dimensional finite different scheme can be utilized for calculation of conduction heat transfer through building envelopes. This model enables the simulation of materials which have temperature dependent thermo-physical properties -specific heat and thermal conductivity- such as PCM. A fully implicit or a Crank-Nicholson scheme can be selected for time discretization. Enthalpy-temperature variation is taken into account in each time step using an equivalent heat capacity obtained from equation 2 [50]. The program is not able to simulate either sub-cooling or hysteresis [55]. However, for this case study, where no relevant effects of these phenomena have been observed, this capability is not necessary.

Enthalpy-temperature curve is entered into the software in the form of a tabulated enthalpy-temperature set of data. EnergyPlus linearly interpolates these data to calculate the enthalpy corresponding to each node and time step [50].

$$c_{p,i}{}^{j+1} = \frac{h_i{}^{j+1} - h_i{}^{j+1}}{T_i{}^{j+1} - T_i{}^{j+1}} \quad \text{Eq. 2}$$

According to the recommendation made by Tabares-Velasco et al. [56], a previous quantification of the errors due to the time discretization method and to the temporal and spatial resolution has been made. For this purpose, the base case with a PCM layer integrated into the cubicle envelope has been simulated utilizing meshes with different spatial and time resolutions and time discretization methods: first order -fully implicit- and second order -Crank Nicholson-.

Some of the simulation data are summarized in table 2. It has been observed that if the selected values for these numerical parameters are close to those proposed by Tabares-Velasco et al. [51], the obtained errors in the whole year energy demand calculations are insignificant. Therefore, a Crank-Nicholson scheme with a time step of 3 minutes and a spatial width of 5mm has been chosen since this represents a low simulation time and the error is acceptable for the analysis.

3.3.1 Input data for enthalpy-temperature curve

Since the enthalpy-temperature has to be input by means of a table of values, a set of 12 temperature interpolation points (T_i, i=1..12) has been defined in order to minimize the normalized root-mean-square deviation (NRMSD) between the approximation to the analytic enthalpy-temperature curve and the real one (Eq. 3). The objective is to reduce the errors between different simulations caused by the approximated curve that uses EnergyPlus.

$$NRMSD = \frac{1}{h_m}\sqrt{\frac{\int_{T_1}^{T_{12}}\left(h(T)-\hat{h}(T,T_i)\right)^2 \cdot dT}{(T_{12}-T_1)}} \quad \text{Eq. 3}$$

If this optimized set of temperature interpolation points is made dimensionless and applied to the enthalpy-temperature curve corresponding to each case, it can be proved that all the simulations have the same minimum normalized deviation (NRMSD). In this study a NRMSD of 0.004 has been reached, which is one order of magnitude lower than the maximum level proposed by Tabares-Velasco [16]. The analytical enthalpy-temperature curve and the approximation function entered into EnergyPlus, in which the interpolation points have been highlighted, are plotted in figure 4.

4. Results

4.1 Calculation of energy consumption

This section presents the results of the energy consumption calculation for the case studies. The monthly energy consumption of two cases –one without PCM and the other with a 2 cm layer of PCM- is compared in figure 5. Table 3 presents the data of energy consumptions and savings of two cases with different thicknesses of the PCM layer (1cm and 2 cm). Comparing them with a reference test cell without PCM, it can be seen that although the PCM reduces the energy consumption during the whole year, it has a more relevant relative influence on cooling energy demand. The reduction in energy consumption is due to two effects: the reduction of the thermal transmittance of the test cell envelope, owing to the addition of the thermal resistance of the PCM layer, and the effect of the phase change.

In order to identify each contribution, a second comparison can be made taking two new reference cases. In these cases, the walls have the same thermal transmittance as the cubicles with a PCM layer. These secondly defined reference cases have a material layer located at the same relative position as the PCM capsules in the test cell envelope. The material layer has the same thickness as the PCM and equivalent thermal properties (thermal capacity and conductivity) but it does not undergo the phase change process.

The results of this additional analysis are also presented in table 3 (1cm and 2cm without latent heat). The monthly savings on energy consumption owing to the latent heat storage are plotted in figure 6. Additionally, an average temperature of PCM ($\bar{T}_{PCM}$), which has been calculated using the implicitly defined equation 4, is overlapped onto this representation. In this graphic, the period of time where the phase change takes place can be clearly identified and related to energy savings. The results confirm what was initially expected: latent heat does not have a representative relative influence on heating energy consumption -during the winter period the temperature of PCM remains far from the phase transition- and its contribution is restricted to the summer months with a reduction of nearly 8% of cooling energy consumption. As can be observed, the ratio between the cooling energy savings owing to the latent heat storage and to the reduction of the thermal transmittance of the test cell envelope varies in this case study from 1:1 –with a 1cm PCM layer- to 1:2 –with a 2cm PCM layer-. Since this second contribution is of higher importance, a more effective reduction of energy consumption can be expected if an additional thermal insulation layer is integrated into the envelope.

$$h(\bar{T}_{PCM}) = \frac{\sum_{i=1}^{n_{PCM\ layers}} \int_{x=0}^{x=e_{PCM}} A_i \cdot h(T) \cdot dx}{\sum_{i=1}^{n_{PCM\ layers}} \int_{x=0}^{x=e_{PCM}} A_i \cdot dx} \quad \text{Eq. 4}$$

4.2 Evaluation of uncertainty on energy consumption

The results of the 100 simulations have been used to quantify the uncertainty. An approximation for the probability density function has been obtained and the value of the mean and standard deviation has been estimated. As an example, in figure 7 the relative frequency histogram for cooling energy demand is shown. Table 4 gathers the results of the statistical analysis which has been made for the results obtained in different cases. A test of normality, an expansion of the Shapiro-Wilk test [57], has been done for the sample of the calculated results. In all cases the sample data fit properly with a normal distribution. Accepting a normal distribution behaviour for the results, an uncertainty interval (±δ) for a confidence level of 97.5% has been calculated. Although the relative uncertainty of the energy consumption calculations is low, less than 2%, it cannot be ignored if this uncertainty is compared to the energy savings deriving from the inclusion of the PCM layer.

4.3 Sensitivity analysis: influence of input parameters uncertainty

The Standardized Regression Coefficient method [58] has been used for the sensitivity analysis evaluation. The main goal of this study is to quantify the contribution of the errors in the estimation of input variable values to the uncertainty of the results. The method is based on a least square fitting of the sample data obtained by the Monte-Carlo method to a linear function such as equation 5.

$$y = \beta_0 + \sum_{i=1}^{6} \beta_i \cdot x_i \quad \text{Eq. 5}$$

Standard Regression Coefficients (SRC) are obtained by normalizing each linear coefficient (β_i) following equation 6.

$$SRC_i = \frac{\beta_i \cdot \sigma_i}{\sigma_y} \quad \text{Eq. 6}$$

where σ_i and σ_y are, respectively, the standard deviation of the corresponding sample of input variable (i) and the result variable which is being analysed. This coefficient gives an idea of the relative influence of the error associated to the estimation of each input variable on the overall uncertainty of the results. Positive values of this coefficient indicate that an increase in the input variable implies a rise in the result variable.

This methodology has the advantage that it uses data obtained by the Monte Carlo method. However, its applicability is restricted to cases which have an acceptable fit to a linear function. Saltelli [58] gives a limit for the R_y^2 (Eq. 7) of the regression model of 0.7.

$$R_y{}^2 = \frac{\sum_{i=1}^{N}(\hat{y}_i - \bar{y})^2}{\sum_{i=1}^{N}(y_i - \bar{y})^2} \text{ Eq. 7}$$

In figure 8 the SRC of each input variable is represented for each case study (1cm and 2cm PCM layer). In all cases the linear regression fits properly (R_y^2>0.9). For each case study the coefficients associated to different output variables are shown separately. For cooling energy consumption, where the phase change process has a more relevant relative influence, the uncertainty of the phase change temperature has the most important effect. Thermal conductivity is the most influential factor in periods of time when PCM does not undergo a phase change. In the simulations of the test cell with a 1cm PCM layer, variables related to phase change are more influential on the results since the thermal resistance of the PCM has a lower relative importance in the overall envelope heat transmittance.

The analysis of SRC provides information about the tendency of the results with the variation of input variables. In this simplified case study, energy consumption is expected to be a decreasing function with respect to properties related to PCM thermal energy storage density – density, specific heat and enthalpy- and an increasing function with respect to its thermal conductivity. However, there is a minimum level of energy consumption for a certain value of phase change temperature. In both cases which have been studied, positive values of the associated SRC have been obtained, which means that the phase change temperature is above its optimum value.

A second order polynomial regression has been fitted to the calculations (Eq. 8). The aim of using this regression is to detect the second order effects and to identify the main interactions between the input variables.

$$y = \beta_0 + \sum \beta_i \cdot x_i + \sum \beta_{ij} \cdot x_i \cdot x_j \text{ Eq. 8}$$

In order to compare the influence of the different coefficients, a standard regression coefficient can be defined for the second order terms (Eq. 9).

$$SRC_{ij} = \frac{\beta_{ij} \cdot \sigma_i \cdot \sigma_j}{\sigma_y} \text{ Eq. 9}$$

The following figure (fig. 9) shows the values of the SRC for the proposed second order polynomial regression to the cooling energy calculation. The representation of SRCs lower than 0.01 has been omitted. As can be seen, there are significant second order effects related to phase change temperature.

4.4 Study of uncertainty propagation and sensitivity analysis of a case with a phase change temperature optimized PCM

This section analyses the uncertainty propagation and sensitivity analysis of an idealized case: the melting temperature of the PCM has been selected in order to minimize the cooling energy consumption. The objective is to demonstrate how the design conditions can modify the conclusions of the sensitivity analysis by comparing its results with those obtained in the previous sections.

The evolution of the cooling energy consumption with the variation of the melting temperature and phase change temperature range is shown in figure 10. It can be seen that the lower values for the minimum energy consumption are reached with PCM with the narrowest temperature phase change range; in this case, a pure PCM –with no sub-cooling or hysteresis effect- would be the optimal one. In addition, the optimum phase change temperature does not significantly depend on the temperature range. These results match those obtained by Neeper [59].The optimum enthalpy-temperature curve used for this analysis maintains the previous phase temperature range, 0.9°C, and has a phase change temperature of T_m=24.8°C.

Table 5 summarizes the main features of the statistical analysis made regarding the sample of cooling energy calculations. The SRCs corresponding to a second order polynomial regression are shown in figure 11. Since the uncertainty propagation has, in this case, been made around an optimum, the SRC associated to the linear variation of energy consumption with the phase change temperature (SRC_{Tm}) is close to zero. Compared to the previously analysed case, the uncertainty of the results is reduced because of the lower contribution of the phase change temperature to the variation of the energy consumption. This fact has to be verified if a SRC sensitivity analysis is conducted on a model where a relevant non-linear behaviour of the solution is expected.

5. Reduction of the uncertainty of saving on energy consumption

In the previous sections the uncertainty of energy consumption calculations owing to errors in measurements of the PCM thermo-physical properties has been quantified. These uncertainties are relevant if they are compared to the savings in energy consumption resulting from the inclusion of a PCM layer. Therefore, in this section the reduction of this uncertainty by improving the accuracy of the measurements of the PCM thermo-physical properties is analysed.

In table 6 the cooling energy consumption of the different cases is shown. Energy savings with their associated uncertainties are included. The savings have been calculated using the reference case without a PCM layer. The uncertainty of cooling energy savings is in some cases important (e.g. about 10% for the 1cm PCM layer calculation). This error can cause a significant deviation in the estimation of the profitability of the investment.

In the cases analysed in this work, where the probability density function of the output variable can be approximated by a normal distribution, the output variable has a good fit with a linear function and randomly independent input variables are considered, the previously obtained regression can be used in order to estimate the uncertainty of the output variable if the original errors of the input variables - $\delta x_{i,0}$- are modified to δx_i (Eq. 10).

$$\delta y = \delta y_0 \cdot \sqrt{\sum_{i=1}^{k} SRC_i^{\,2} \cdot \left(\frac{\delta x_i}{\delta x_{i,0}}\right)^2} \quad \text{Eq. 10}$$

where δy_0 is the originally estimated uncertainty for the output variable.

Equation 10 can be utilized with the purpose of determining a combination of uncertainties for the input variables that reduces the error of the output to a required level (δy_{req}). In this work a method to assign a reduction of the uncertainty to each input variable is proposed. The required uncertainties of input variables are calculated making a distribution inversely proportional to the corresponding SRC (Eq. 11).

$$\delta x_i = \frac{\alpha}{SRC_i} \cdot \delta x_{i,0} \text{ Eq. 11}$$

where $\delta x_{i,0}$ is the original error of input variables, δx_i is the uncertainty required to achieve an acceptable error for the result and α is a distribution coefficient. It has to be taken into account that for variables with low SRC the evaluation of α/SRC_i can be higher than 1, which means that the uncertainty of these variables could even be raised. However, since this is not practical for common applications, in the proposed method these variables are maintained at the original level of uncertainty. An iterative algorithm (fig. 12) has been used to calculate the required accuracy for the input variables.

In each iteration (j) the uncertainty for each variable (i) is calculated according to equation 12.

$$\delta x_i^j = min\left(\frac{\alpha^j}{SRC_i} \cdot \delta x_{i,0}, \delta x_{i,0}\right) \text{ Eq. 12}$$

where the factor α_j is calculated following equation 13.

$$\alpha^j = \sqrt{\frac{\left(\frac{\delta y}{\delta y_0}\right)^2 - \sum_{SRC_i | \alpha_i^{j-1} \geq 1} SRC_i^{\,2}}{n^{j-1}}} \text{ Eq.13}$$

where n^{j-1} is the number of parameters whose uncertainty has to be reduced according to the following condition (Eq. 14):

$$\frac{\alpha^{j-1}}{SRC_i} < 1 \text{ Eq. 14}$$

This method has been used to calculate the required uncertainty of input variables that reduce the error in cooling energy savings to 5%. In table 7 the results of these calculations are summarized and in figure 12 a graphical example of the application of the method is shown. For the cases that have been studied, improvements in the uncertainty of the experimental measurements of phase change temperature and thermal conductivity should be made in order to reach the required uncertainty of the output variable. Additionally, the expected uncertainty of calculations considering the tolerance for the measurements of PCM thermo-physical properties defined in previous works [10, 46, 60] and by the RAL-PCM quality association [47] is shown. As can be seen in table 7, if the tolerance levels defined in these previous works are assumed, the obtained errors in the numerical results are higher than the objective value used in this work of 5%. For the particular cases analysed in this paper, the required accuracy for phase change temperature is more restrictive, whereas a higher uncertainty range can be accepted for the thermal conductivity measurement.

6. Conclusions

An uncertainty propagation and sensitivity analyses have been carried out on an application in which PCM is included in a test cell envelope. The aim of this approach is to study the effect of the error in the measurements of PCM thermo-physical properties on the results of simulations. Although there are a few works on uncertainty propagation in thermal energy storage systems with PCM [14, 15], this methodology has been rarely applied to building elements with PCM in passive applications. The reference case has been taken from an experimental set up located in Lleida and described in Castell et al. [24]. A Monte-Carlo based method has been used for the uncertainty propagation study.

A significant uncertainty for savings in cooling energy demand has been calculated (approximately ±10%). The most influential parameters are phase change temperature (T_m) and thermal conductivity (λ), while the error in estimation of phase change enthalpy (h_m) is of minor importance. The effect of uncertainties of density and specific heat measurements is negligible.

Compared with the results of Dolado et al. [14], the importance for T_m and h_m is similar. In this case, since the heat transfer configuration is different, thermal conductivity has a higher relevance. Furthermore, in this application there is an optimum for the operation of the test cell envelope varying phase change temperature, while for the other variables the energy demand has a monotonic behaviour. The uncertainty propagation has been analysed using a design with an optimized phase change temperature with the aim of studying the effect of this particular situation on the conclusions of the analysis. Comparing the results to the original case study, the uncertainty is reduced due to the lower contribution of the phase change temperature to the global error. Nevertheless, since this result corresponds to a unique situation and the sensitivity of the influence of phase change temperature on the results is high, this conclusion cannot be generalized. This fact has to be analysed if a significant non-linear effect of one of the input variables within its corresponding uncertainty range on the solution is expected.

A method to calculate a combination of admissible uncertainties for the input variables that reduces output uncertainty to a required value has been proposed. The method can be used if the input and output probability density functions can be approximated with a normal distribution and the linear regression of the output variable fits correctly. Applying this method to the case study analysed in this work, uncertainties of phase change temperature and thermal conductivity should be reduced to ±0.3°C and ±8% respectively in order to reduce the uncertainty of calculations to 5%. For this particular case, comparing the results with the limitations for the error levels defined in different previous works [10, 46, 60] and by the RAL-PCM Quality Association [47], the calculated tolerance for phase change temperature is more restrictive. The acceptable error tolerance of each input variable depends on the sensitivity to the corresponding input parameter of the output variable which is being observed in each particular case study. This fact has to be taken into account when estimating the required tolerance for the input variables in order to ensure a certain level of accuracy for the simulation results.

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Figure captions

Figure 1. Section of the constructive solution for the cubicles [24].

Figure 2. Enthalpy-temperature curve of RT-27.

Figure 3. Analytic enthalpy-temperature curve, identification of its parameters.

Figure 4. Approximated enthalpy-temperature curve.

Figure 5. Comparison between monthly energy consumption of a test cell with a 2 cm layer of PCM and another without PCM.

Figure 6. Monthly energy savings owing to latent heat energy storage (2cm layer of PCM).

Figure 7. Relative frequency histogram for the calculation of annual cooling energy demand (case with a 2cm PCM layer).

Figure 8. SRCs for the results data (a: 1cm PCM layer, b: 2cm PCM layer).

Figure 9. Comparison of the linear and quadratic regression (cooling energy consumption, 1cm PCM layer).

Figure 10. Influence of T_m and ΔT_m on cooling energy consumption (2cm PCM layer).

Figure 11. Comparison between the SRCs of the correlations of the two cases with a 2cm layer of PCM for cooling energy consumption (Tm=24.8°C and Tm=25°C).

Figure 12. (a) Algorithm to obtain the requirements for accuracy of PCM thermo-physical properties. (b) Example of the application of the algorithm to the case corresponding to the test cell with a 1cm PCM layer (cooling energy consumption).

Table(s)

Table 1. Thermo-physical properties of PCM and their associated uncertainty.

	Reference value	Temperature range used in the measurements	Measurement methodology	Uncertainty	References
h_m	170 kJ/kg (*)	15-35°C	T-history, DSC	±10%	[10, 12]
T_m	26 °C (*)	15-35°C	T-history, DSC	±1°C	[10, 12]
ΔT_m	0.9 °C (*)	15-35°C	T-history, DSC	±0.2°C	[10, 12]
c_p	3 kJ/(kg·K) (*)	15-35°C	DSC	±5%	[42]
λ	0.16 W/(m·K) (**)	15-35°C	LFA+DSC+Densimeter +TMA	±10%	[43,44]
ρ	752 kg/m^3	35°C	Densimeter+TMA	±2%	[45]

(*) Parameters of the approximated analytical h-T curve.

(**) Average value

Table 2. Influence of the time step and spatial resolution on the numerical results of the model.

Δt [min]	Δx [mm]	Heating energy demand [kW·h]	$e_{heating}$ [%]	Cooling energy demand [kW·h]	$e_{cooling}$ [%]
3	6.67	2489.93	-0.0030%	232.72	-0.0142%
3	5	2489.97	-0.0016%	232.74	-0.0068%
3	3.33	2489.97	-0.0013%	232.75	-0.0008%
2	5	2489.96	-0.0016%	232.74	-0.0079%
2	4	2489.96	-0.0017%	232.74	-0.0074%
2	0.28	2489.98	-0.0011%	232.75	-0.0003%
1	0.14	2490.00	-	232.75	-

Table(s)

Table 3. Energy consumption and savings of the simulated test cells.

Cases	Heating			Cooling		
	Energy consumption [kW·h]	Energy savings [kW·h]	Savings owing to latent heat [kW·h]	Energy consumption [kW·h]	Energy savings [kW·h]	Savings owing to latent heat [kW·h]
Without PCM	2806.1	-	-	294.7	-	-
1cm without latent heat	2648.9	157.2 (5.6%)	-	272.2	22.5 (7.6%)	-
1cm with PCM	2628	178.1 (6.3%)	20.9 (0.7%)	253.1	41.6 (14.1%)	19.1 (6.8%)
2cm without latent heat	2508.6	297.5 (10.6%)	-	252.7	42 (14.3%)	-
2cm with PCM	2489.8	316.3 (11.3%)	18.1 (0.7%)	232.7	62 (21%)	20 (6.5%)

Table(s)

Table 4. Summary of the statistical analysis applied to the sample data of the results.

	1cm PCM layer		**2cm PCM layer**	
	Cooling energy consumption	Heating energy consumption	Cooling energy consumption	Heating energy consumption
Mean [kW·h]	253.10	2628.01	232.70	2489.78
Standard deviation [kW·h]	1.94	6.56	1.81	11.22
W (Shapiro-Wilk test [49])	0.996	0.999	0.994	0.999
Uncertainty [kW·h]	±4.35	±14.71	±4.06	±25.16
Energy savings [kW·h]	41.6 (±10.5%)	178.1 (±8.3%)	62.0 (±6.5%)	316.3 (±5.7%)

Table(s)

Table 5. Comparison between the results of the statistical analysis applied to the sample data for cooling

	T_m=24.8°C	T_m=25°C (section 4.4)
Mean [kW·h]	231.02	232.70
Standard deviation [kW·h]	1.28	1.81
W (Shapiro-Wilk test [25])	0.999	0.994
Cooling energy savings [kW·h]	63.68±2.87	62.0±4.06

Table 6. Uncertainty of annual energy savings due to inclusion of a PCM layer.

	Cooling energy consumption [kW·h]	Cooling energy savings [kW·h]	Uncertainty
Without PCM layer	294.7		
PCM 1cm	253.1	41.6±4.4	±10.5%
PCM 2cm	232.7	62.0±4.1	±6.5%
PCM 2cm (optimized T_m)	231.0	63.7±2.9	±4.5%

Table(s)

Table 7. Required uncertainty for the measurements of PCM thermo-physical properties.

	1cm PCM layer			**2cm PCM layer**	
	Uncertainty on measurements	Tolerance defined in previous works	Required uncertainties	Uncertainty on measurements	Tolerance defined in previous works
λ	±10%	±5% [47]	±8%	±10%	±5% [47]
ρ	±2%	±1% [47]	±2%	±2%	±1% [47]
c_p	±5%	±10%	±5%	±5%	±10%
T_m	±1°C	±1°C [10, 60]	±0.3°C	±1°C	±1°C [10, 60]
ΔT_m	±0.2°C	±0.2°C	±0.2°C	±0.2°C	±0.2°C
h_m	±10%	±10% [10, 46, 60]	±10%	±10%	±10% [10, 46, 60]
Cooling energy savings	±10.5%	±9.4%	±5%	±6.5%	±5.4%

Figure(s)
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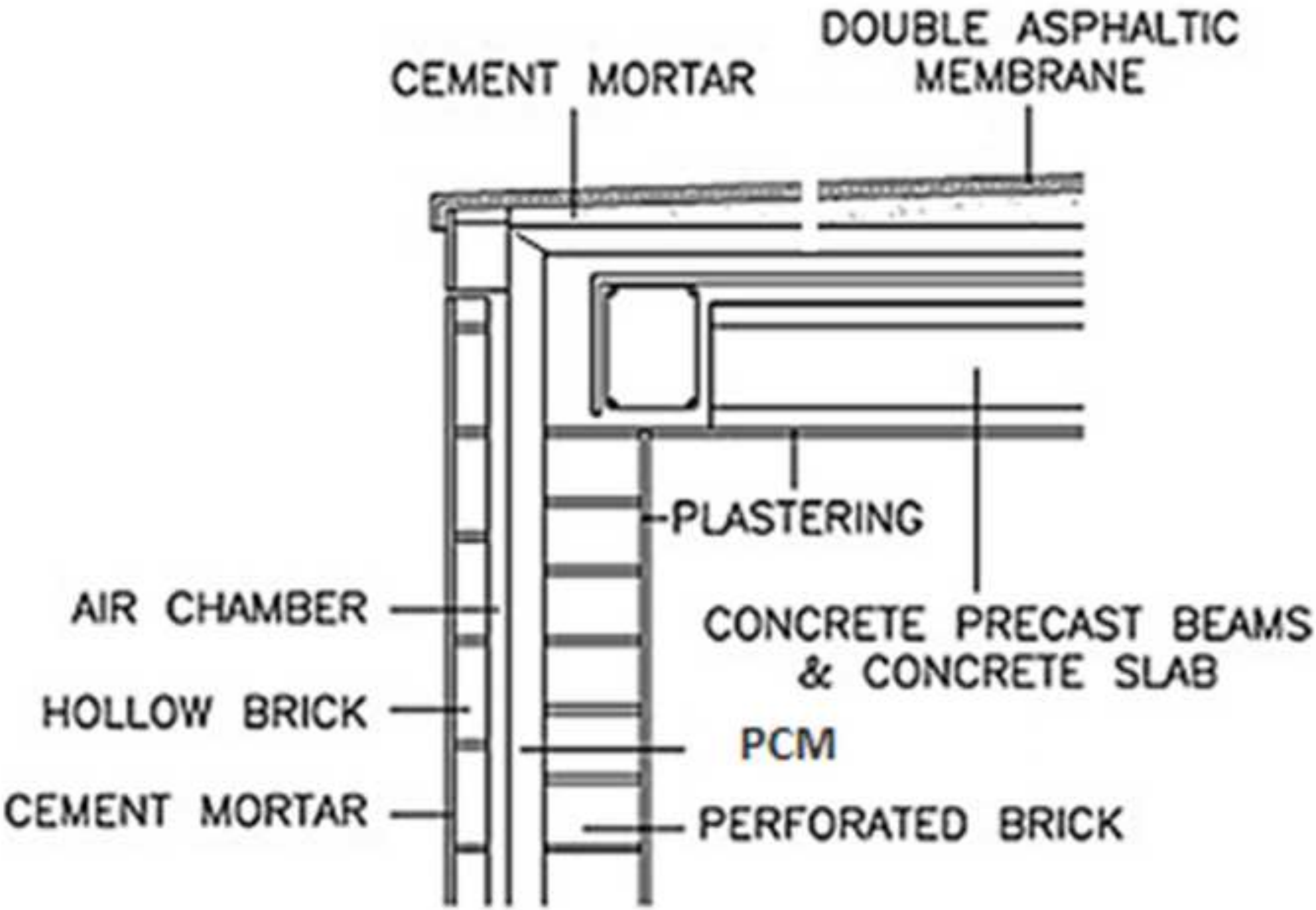

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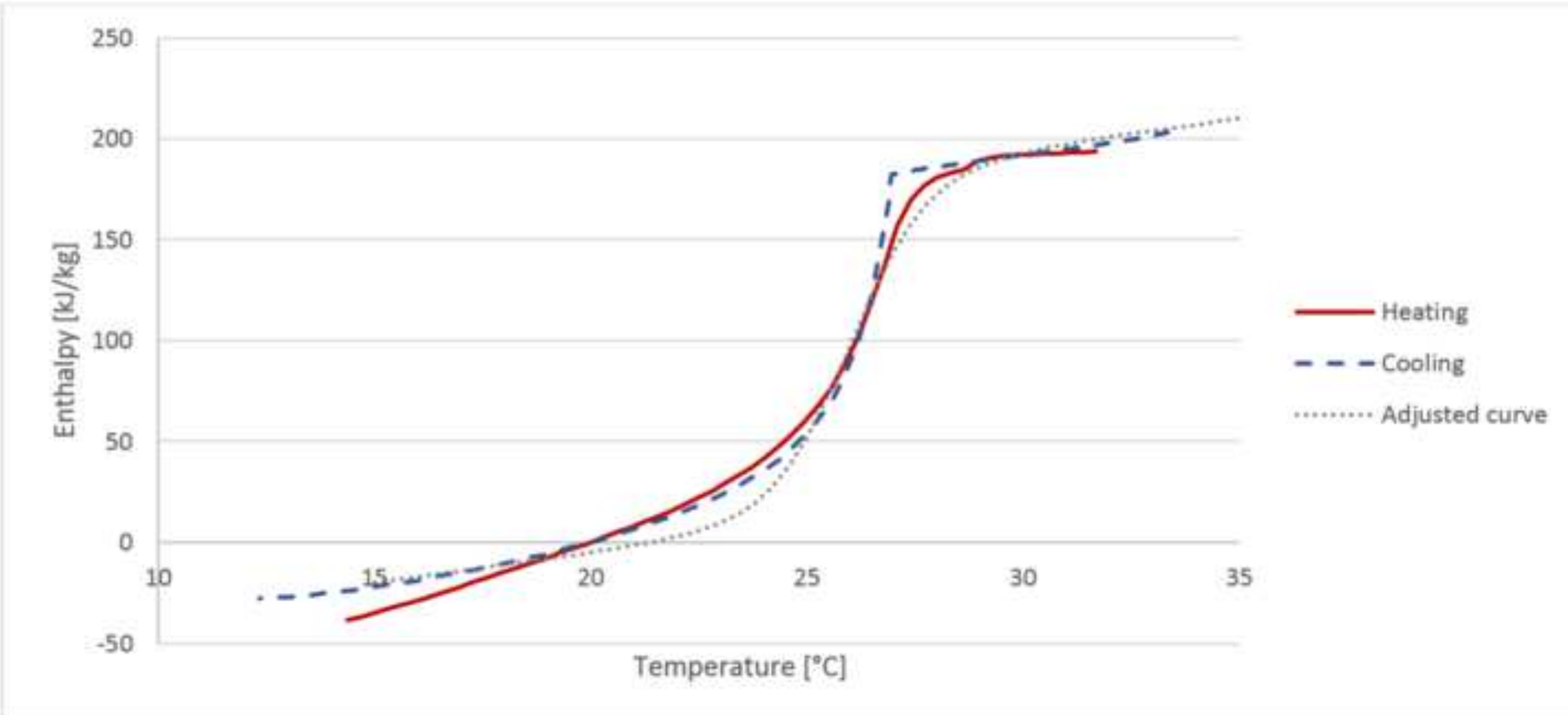

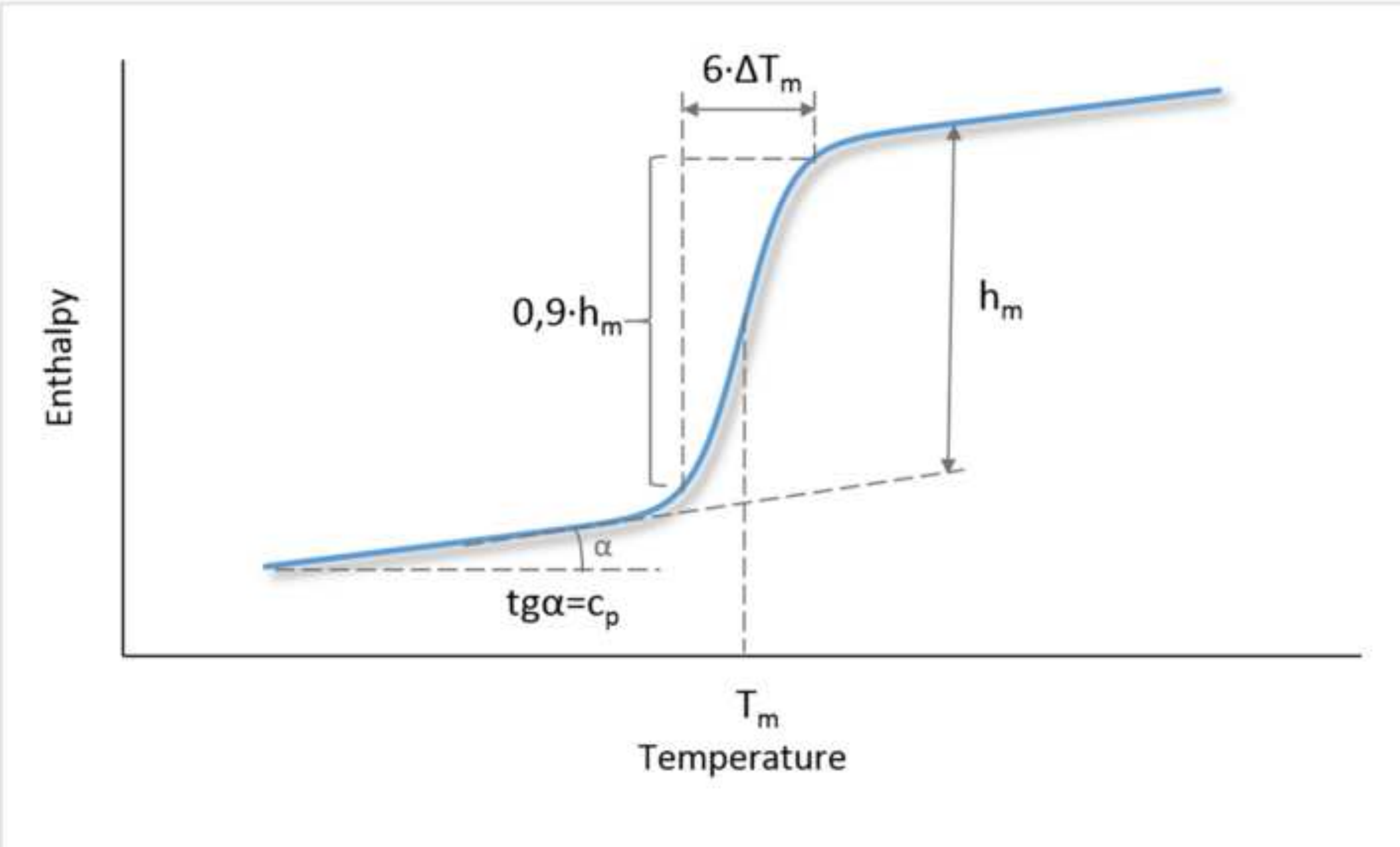
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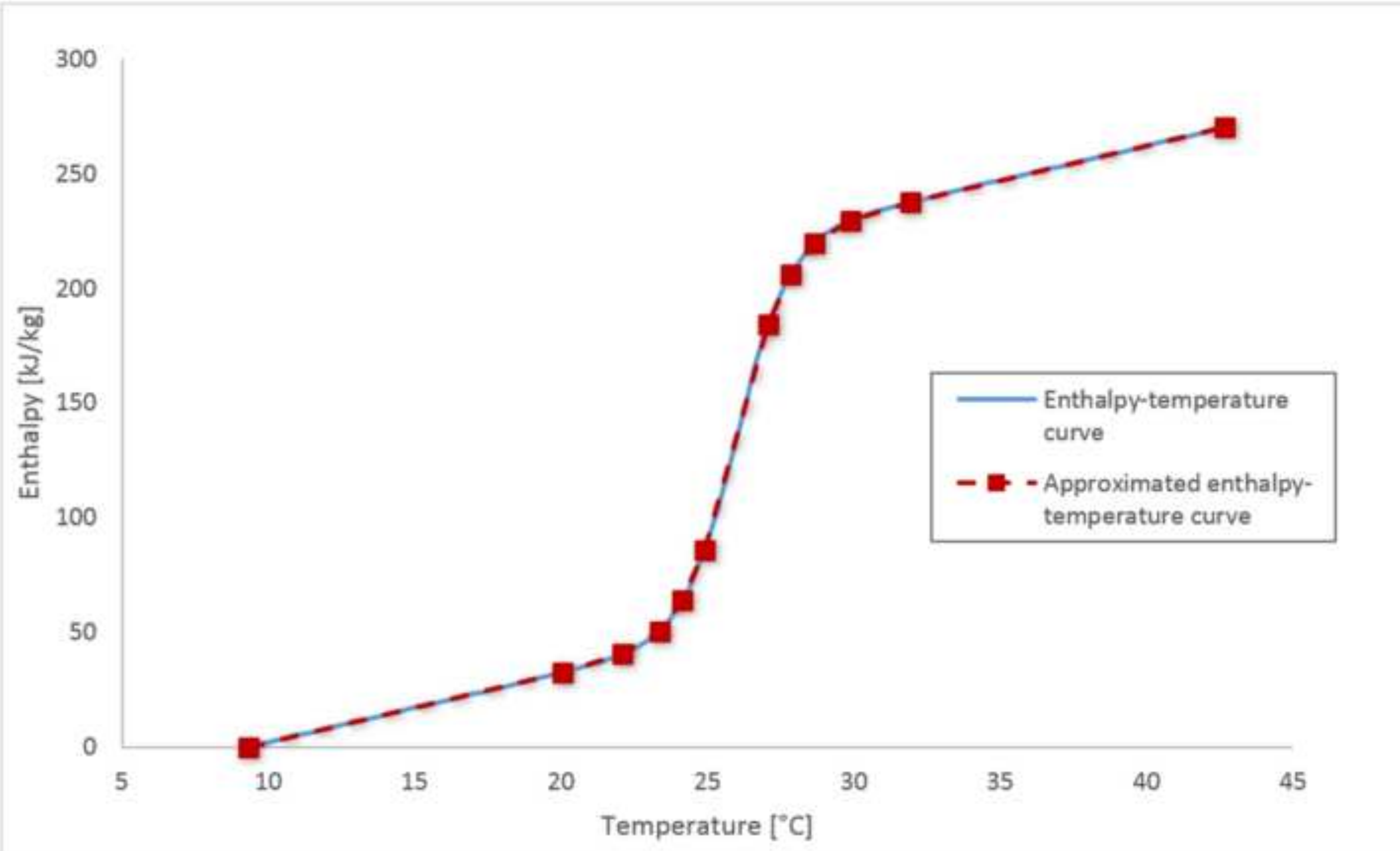
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Approximated enthalpy-temperature curve

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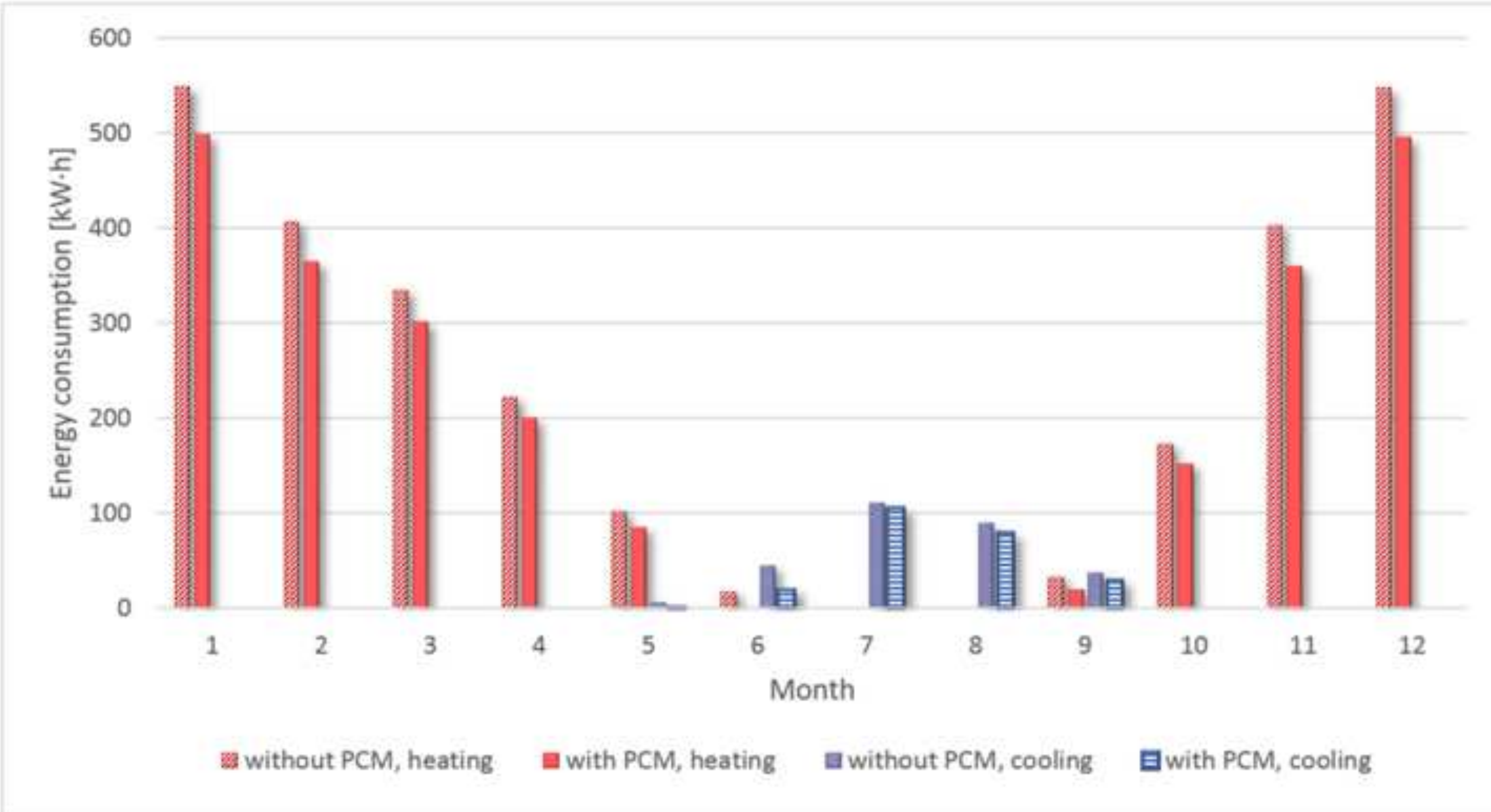

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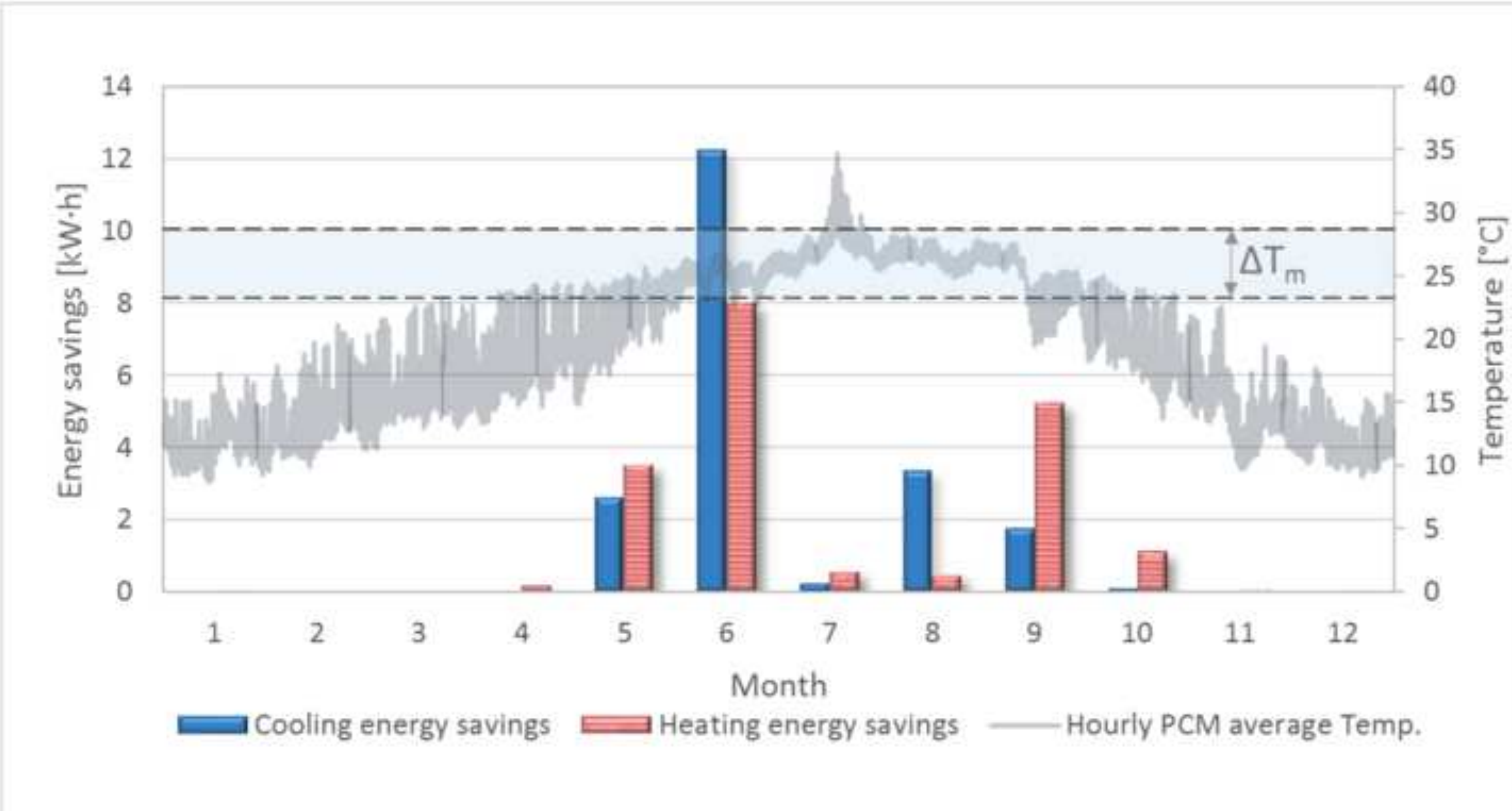

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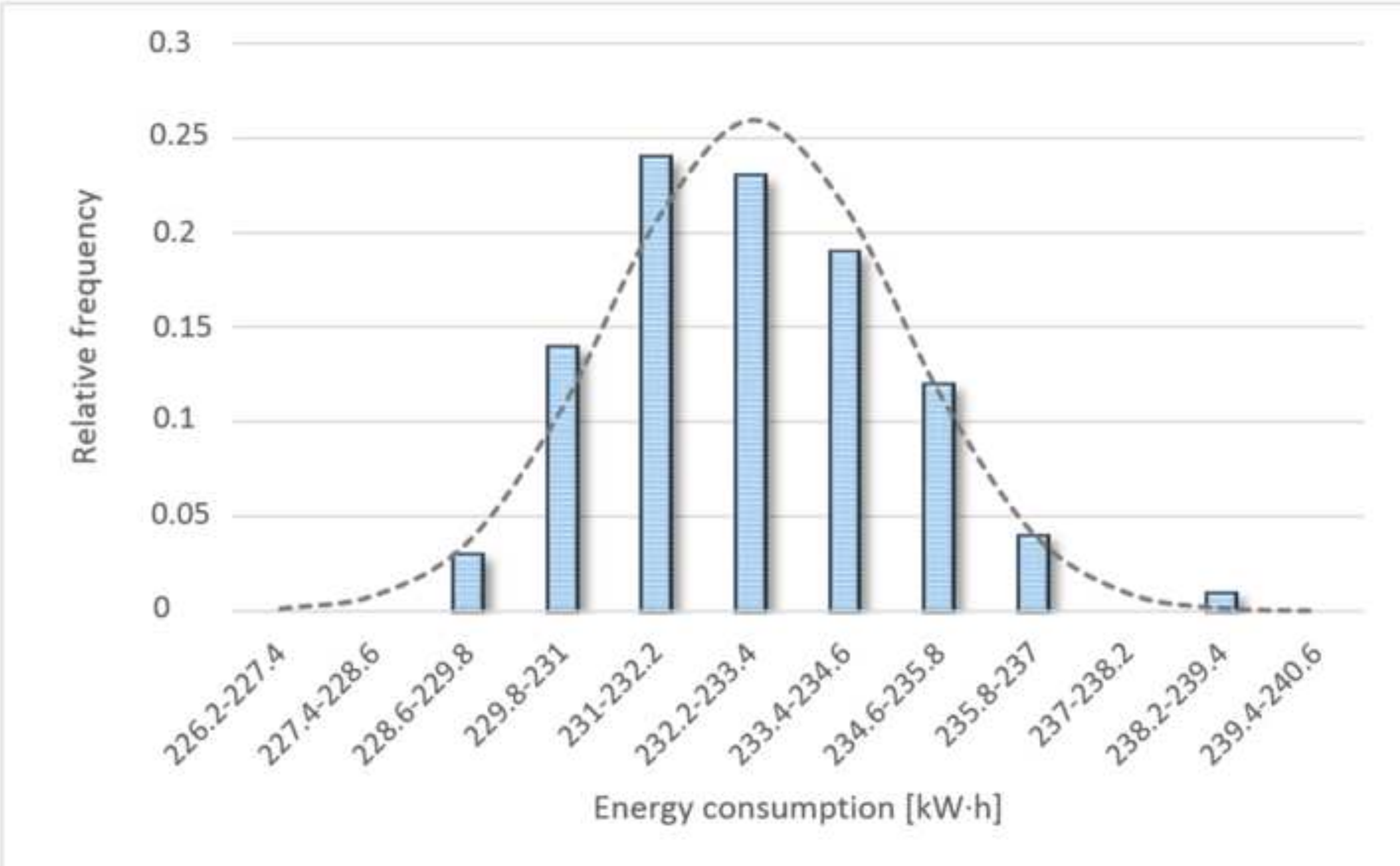

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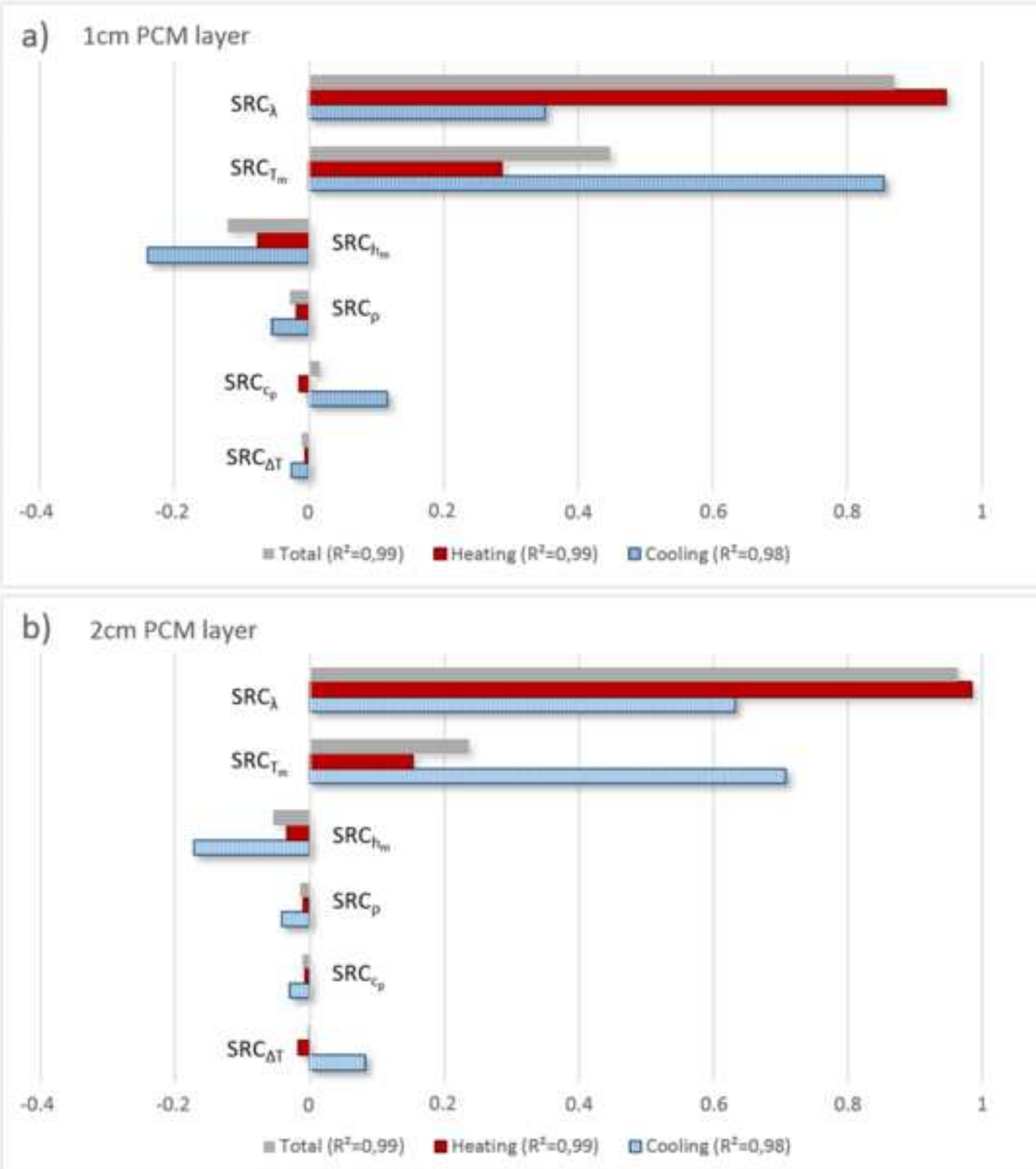

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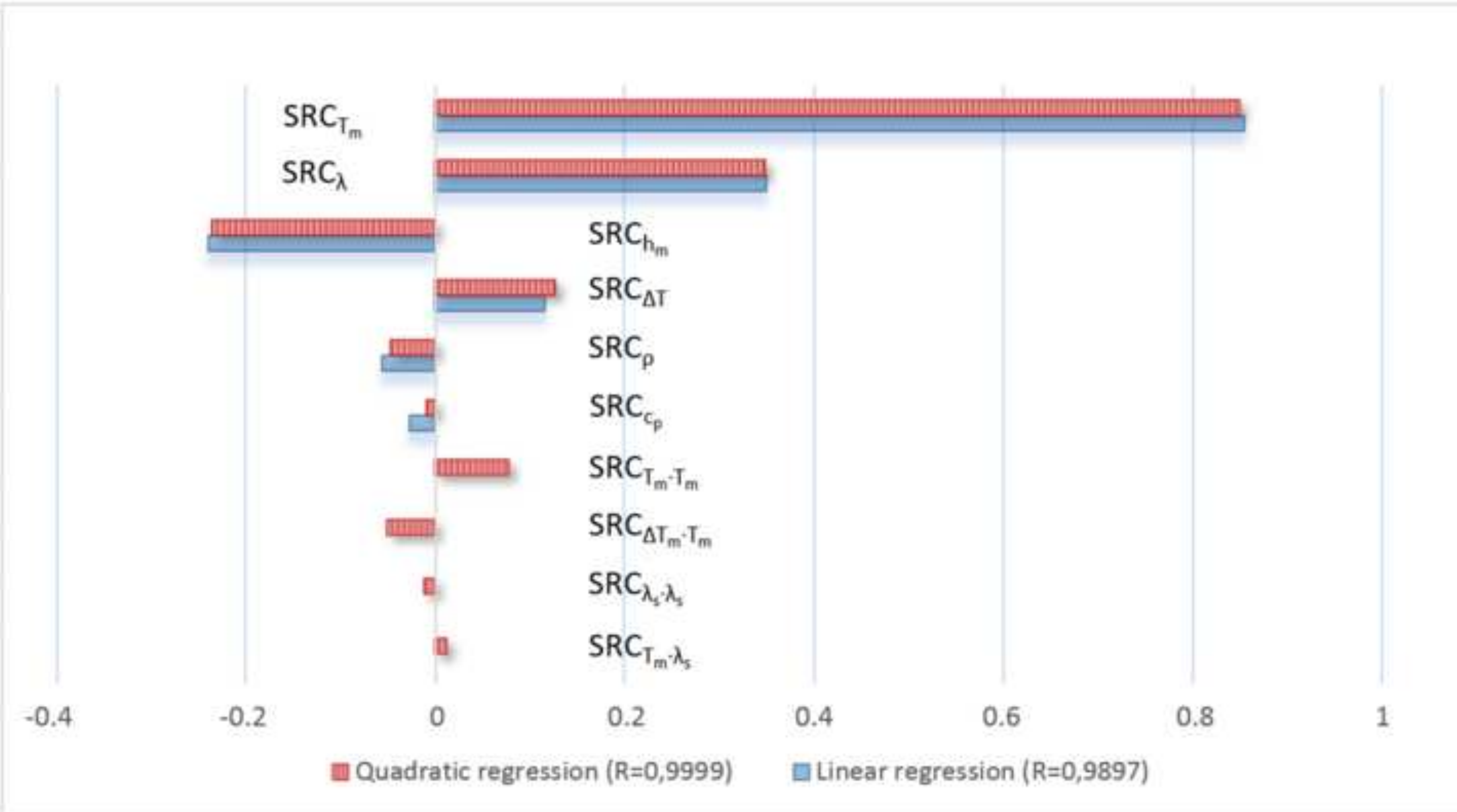

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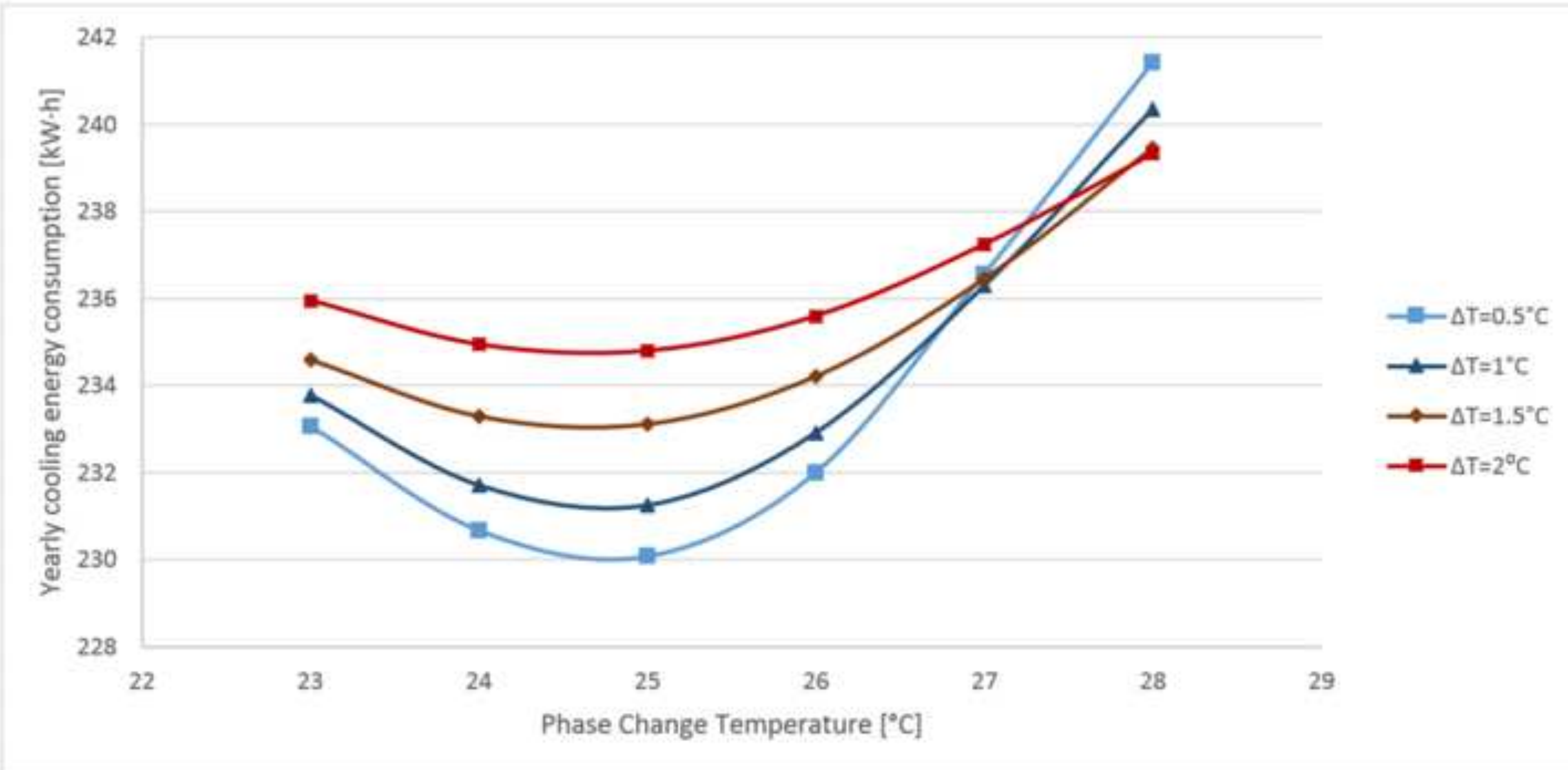

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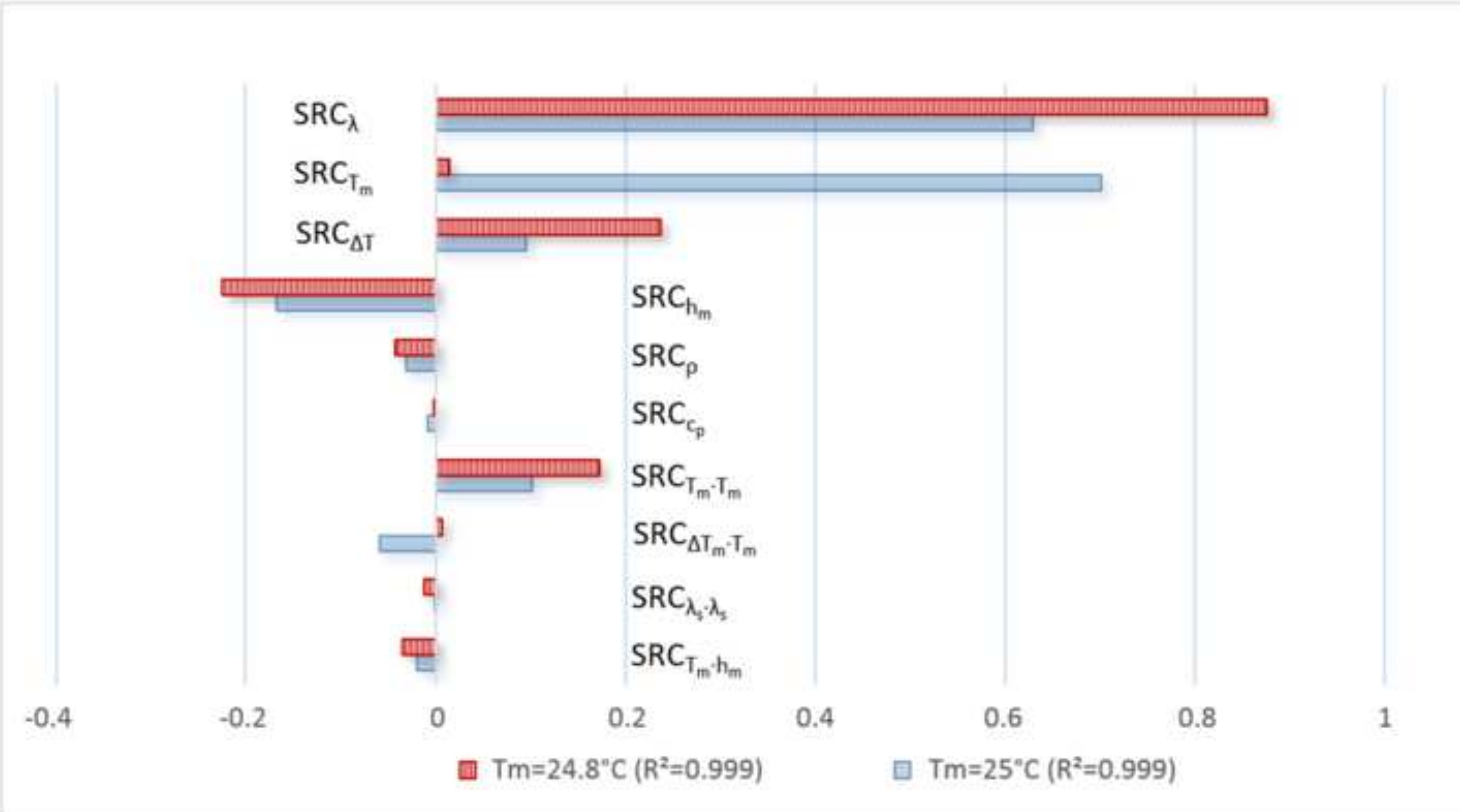

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