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A NEW METHOD TO DETERMINE THERMAL PROPERTIES OF THE MIXTURE OF PCM AND CONCRETE

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ABSTRACT

Integration of phase change materials in building envelopes is a technology that with high potential to decrease the building energy consumption and improve indoor thermal comfort. Accurate measurement of thermal physical properties of PCM-concretes is very important for simulation and evaluation of its energy saving performance. However, there isn't an effective way to measure thermal physical properties of PCM-concretes accurately. The shortcomings of using traditional testing methods to measure thermal physical properties of PCM-concretes were firstly analyzed. Then a new method based on the inverse problem was proposed to deal with the measurements of thermal conductivity and specific heat of PCM-concretes during the phase change process. This method transforms the determination process to an optimization problem, which regarded the difference between the measured and calculated heat flux and temperature as the objective function, and the thermal conductivity and specific heat distribution with temperature will be automatically adjusted through the Sequential Quadratic Programming (SQP) algorithm. The equivalent specific heat of 4 wt% and 6 wt% PCM concretes were determined using the proposed methods. The accuracy (the maximum error is less than 2%) is acceptable for engineering use. The influences of temperature segments and optimization algorithms were analyzed. The results showed that, SQP method is with the highest accuracy and least complexity compared with the Particle Swarm Optimization and Genetic Optimization methods. Finally, some suggestions to apply this method to other similar problems were proposed to extend its application scope.

Keywords: phase change material, thermal physical properties, inverse problem

NONMENCLATURE

Abbreviation	
DSC	Differential Scanning Calorimetry
GA	Genetic Algorithm
PCM	Phase Change Material
PSO	Particle Swarm Optimization
RE	Relative Error
SQP	Sequential Quadric Programming
Symbols	
c_p	Specific heat [J kg^{-1}℃$^{-1}$]
d	Direction
h	Convective heat transfer coefficient [W m^{-2}℃$^{-1}$]
I	Current [A]
k	Thermal conductivity [W m^{-1}℃$^{-1}$]
L	Length [m]
q	Heat flux [W]
R	Radius of the tube [m]
T	Temperature [℃]
t	Time [s]
V	Tension [V]
v	Velosity [m s^{-1}]
x	Position
λ	Step size
ρ	Density [kg m^{-3}]
δ	Half of the thickness of the layer [m]
ω	Relative weights
Subscripts	
cal	Calculated
flux	Heat flux
mea	Measured
temperature	Temperature

1. INTRODUCTION

Since the energy crisis has become a worldwide problem, thermal energy conservation has been considered more and more important during the current years. During the past 20 years, several forms of bulk encapsulated phase change materials were available in the market for active and passive solar applications. Many researchers have investigated the methods of integrating the gypsum wallboard and other architecture materials with phase change materials [1-3]. Thus, it is of great importance to measure the thermal physical properties of the PCMs used in the building envelopes accurately in order to evaluate its thermal performance. If we can know thermal properties of materials in which PCM was integrated, then it would be possible to perform accurate dynamic whole building simulations.

However, it has never been an easy task to measure the thermal physical properties accurately of phase change material in the building envelopes. Because of the phase change process and the inhomogeneity of the bulk materials, it is impossible to use traditional methods to measure the thermal physical properties of the PCMs mixed with concretes. The research presented by Hunger et al. [4] takes into account the challenge of measuring the specific heat capacity of self compacting PCM-concrete, however the proposed calculation methodology simplifies the problem and experimental set-up without considering the influence of the surrounding temperature on the heat transfer within the sample.

Although some new kinds of methods have been proposed to test the thermal physical properties of the PCMs in the past, they are all born with some specific limitations. For example, the Differential Scanning Calorimetry (DSC) methods can only measure the thermal properties of small piece of phase change materials, which may be different from bulk materials. Zhang [5] et al. put forward a new method-the T-history method to test the thermal physical properties of phase change materials, which is much easier and quicker than the DSC method. However, according to present knowledge, there is no methodology to test the PCMs integrated with concretes. For example, the samples tested by the DSC method are usually very small, whose thermal physical properties may be largely different from those of bulk materials. Therefore, to be able to measure bigger sample of PCM and to get an accurate result, it is necessary to apply the T-history method. When applying T-history method the *Biot* number of the tube has to be less than 0.1, which ensures the temperature distribution in the sample can be regarded as uniform. Consequently, the length of the tube would have to be very large if the bulk material, such as combined PCM and concrete was tested. However, set up of such a long sample would not be feasible.

The aims of this paper are to: (1) put forward a novel method based on the inverse problem to determine the thermal properties of the PCM and concrete mixtures; (2) analyze the influences on the optimization accuracy of key parameters; (3) compare the optimization accuracy and time complexity of various optimization algorithms. Finally, possible further improvements of the proposed method are discussed.

2. MEASUREMENT OF THERMAL PHYSICAL PROPERTIES OF PHASE CHANGE MATERIALS

2.1. MEASUREMENT OF SPECIFIC HEAT OF PHASE CHANGE MATERIALS

2.1.1. Differential Scanning Calorimetry Method

Differential scanning calorimetry (DSC) is a thermo-analytical technique in which the difference in the amount of heat required to increase the temperature of a sample and reference is measured as a function of temperature. Both the sample and reference are maintained at nearly the same temperature throughout the experiment. Generally, the temperature program for a DSC analysis is designed such that the sample holder temperature increases linearly as a function of time. The reference sample should have a well-defined heat capacity over the range of temperatures to be scanned.

The technique was developed by E.S. Watson and M.J. O'Neill [6], and introduced commercially at the Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy.

The basic principle underlying this technique is that when the sample undergoes phase transitions, more or less heat will need to flow to it than the reference to maintain both at the same temperature. Whether less or more heat must flow to the sample depends on whether the process is exothermic or endothermic.

The DSC method has been widely used in many aspects, which includes the safety screening, drug analysis, general chemical analysis and food science.

However, there are some limitations of using the DSC methods to determine the thermal physical properties of PCM-concretes. That is: (1) only small pieces of PCMs can be tested by the DSC methods, whose thermal physical properties may be different from the bulk materials including heterogeneous additives. Careful sampling of the material is required to obtain the representative property of the compound, particularly in a locally heterogeneous PCM which has a dependency of sampling point; (2) it is also a difficult thing to use the DSC methods to determine the thermal conductivity of phase change materials. Thus, the equivalent thermal physical properties of phase change materials integrated with concretes of bulk materials can’t been determined accurately through the DSC methods.

2.1.2. T-history Method

Zhang [5] et al. proposed a new method. T-history method, as an alternative way to DSC method, and the most important improvement of this method is that it can work with large representative samples of bulk PCM which includes several additives. The proposed T-history method is a fast and simple technique for the measurement of thermal physical properties in the bulk PCM. And the T-history method can test several samples at the same time; also it can derive the thermal conductivity of the PCMs.

Many improvements have also been proposed on this method. One of the improved procedures is the ‘‘thermal delay method’’ [7]. The suggested improvements refer to (a) the measurement arrangement; (b) the way of measurements processing, which is the most important part of the contribution, and (c) the kind and presentation format of the final results. The changes made increased accuracy and provided automation, convenience, quickness and results directly applicable to most calculations and in particular in numerical predictions.

However, it is necessary to meet several conditions to apply the T-history method. In order to apply the lumped capacitance method, when *Bi* should be less than 0.1, the temperature distribution in the sample can be regarded as uniform. It can be imaged that the length of the tube will be very large if the bulk material is needed to be tested, which is not feasible for engineering applications.

2.2. MEASUREMENT OF THERMAL CONDUCTIVITY OF PHASE CHANGE MATERIALS

2.2.1. Hot wire method

The hot-wire method was adopted by many researchers when they deal with the thermal conductivity measurement of phase change materials. This method allows measuring the thermal conductivity utilizing a particular heat conduction equation that is valid for a linear heat source in a homogenous and isotropic medium at uniform initial temperature. In particular, the method is established for an infinitesimal linear heat source and an infinite mass, as proposed by Carslaw and Jaeger’s theory [8]. According to this theory, the heat produced by means of an electric current flow, diffuses through the system along orthogonal direction respect to that of the hot-wire.

It can be derived that the thermal conductivity of the phase change material can be determined by the following equation [9]:

$$\mathrm{k} = \left(\frac{\mathrm{VI}}{4\pi\mathrm{L}}\right)/(\mathrm{dt}/\mathrm{d}(\ln\tau)) \tag{1}$$

where V is the tension, V, I is the current, A, L is the hot wire length, m, t is the temperature of the wire, ℃, and τ is the time, s.

The hot wire method is very easy to proceed with simple equipments. However, according to the national standards (GB/T 10297 - 1998), this method is suggested used to measure thermal physical properties less than 2 W m^{-1}℃$^{-1}$ of isotropy materials.

2.2.2. T-history method

The T-history method proposed by Zhang et al. [5] can also be used to determine the thermal physical properties of phase change materials. However, in order to ensure that the tube contained the melted PCM whose temperature is uniform, the ratio of the length to diameter of a tube should be larger than 15. And the *Biot* number should be less than 0.1 and the Stefan number should between 0 and 0.5. This method can only be applied to measure the thermal conductivity of the PCMs whose phase-change process there is one clear interface between two phases (in fact, for some salt hydrates, this condition cannot be met) [5].

It can be concluded from the above introductions that the disadvantages of conventional methods are: (1) it is impossible to use the conventional methods to measure thermal physical properties of bulk materials that just use a small piece of PCMs (like DSC methods); (2) the installments of the measurement using T-history method will not be feasible in order to meet some conditions; (3) the conventional methods (such as the DSC or T-history methods) can’t determine different thermal physical properties simultaneously. Thus, a new method should be put forward to deal with the accurate and fast measurement of PCMs mixed with concretes.

3. PROBLEM DESCRIPTION

3.1. METHODOLOGY DESCRIPTION

3.1.1. Heat transfer model

If the bulk material was heated symmetrically from the top and the bottom, half of the samples can be used to build the heat transfer model. And the middle of the sample can be regarded as thermal isolation because of the symmetry. This heat transfer process can be simplified by the one dimension conductive heat transfer model, which is schematically shown in Fig.1. Thus, the heat transfer process of the bulk material can be expressed as follows:

$$\rho c_p \frac{\partial \mathrm{T}}{\partial \mathrm{t}} = \frac{\partial}{\partial \mathrm{x}}\left(\mathrm{k}\frac{\partial \mathrm{T}}{\partial \mathrm{x}}\right) \quad \mathrm{t} > 0, 0 < x < \delta \tag{2}$$

The initial condition is:

T (x,0)=T_0, $0 \le \mathrm{x} \le \delta$

The boundary conditions are:

T(0,t)=T(t) $\mathrm{t} > 0$

$$-\mathrm{k}\frac{\partial \mathrm{T}}{\partial \mathrm{x}}\Big|_{\mathrm{x}=\delta} = 0$$

In order to deal with the numerical simulation of the heat transfer process, the heat equation is solved in a traditional manner-explicit finite difference method. The thermal properties: ρ-density, k-thermal conductivity and c_p(t)-specific heat in function of temperature and also temperature boundary conditions are given in order to solve the 1D unsteady heat conduction problem.

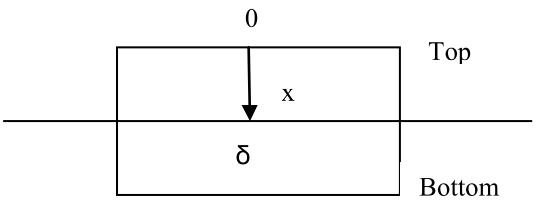


Figure 1 Schematic show of the 1-D heat transfer model

3.1.2. Determination of thermal conductivity and specific heat

Although the heat flux on the top and bottom of the bulk material and the temperature distribution can be measured through corresponding experimental installments, it's not an easy way to determine the thermal physical properties of the PCM-concretes. Because of the phase change process, it is a nonlinear problem. The equivalent specific heat and thermal conductivity can't be derived directly from these equations. Thus, a new method is proposed by us to deal with such problems-determine the key thermal physical properties in a nonlinear problem. Although the objective functions were different, a similar method has been proposed by Zeng et al. [11] to determine the ideal specific heat in passive buildings.

In order to extend the application scope of the proposed inverse problem method, the method is described in a general manner as follows.

The measured and calculated heat flux and temperature distribution can be achieved through experiments and numerical simulations, respectively. And only with the correct thermal physical properties, the calculated data can fit well with the measured ones, which means the correct thermal physical properties can be determined only when the difference between the measured and calculated data approaches zero. Thus, the nonlinear optimization method can be used to determine such thermal physical properties. In our problems, the optimization objectives and constraints can be described as follows:

$$\mathrm{Min}\ \omega_1(q_{\mathrm{mea}} - q_{\mathrm{cal}})^2 + \omega_2(T_{\mathrm{mea}} - T_{\mathrm{cal}})^2 \qquad (3)$$

$$\mathrm{s.t.}\begin{cases} c_{p,\mathrm{low}} \le c_{p,i} \le c_{p,\mathrm{high}} \\ k_{\mathrm{low}} \le k_i \le k_{\mathrm{high}} \end{cases}$$

where q_{mea}, q_{cal} are the measured and calculated heat flux, T_{mea}, T_{cal} are the measured and calculated temperature in different points, ω_1 and ω_2 are the relative weights of the difference of heat flux and temperature, which can be determined by the error transfer function, $c_{p,low}$ and $c_{p,high}$ are the lower and upper bound of the specific heat, k_{low} and k_{high} are the lower and upper bound of the thermal conductivities.

Then the problem of determining the thermal properties of PCM-concretes is transferred to a nonlinear multi-objective optimization problem with inequality constraints. The next step is to find a proper nonlinear optimization method to complete the optimization procedure.

Over the past decades, many numerical methods have been proposed to solve this problem, which include interior point methods, gradient projection methods, trust region techniques and sequential quadratic programming (SQP) methods. In addition, many intelligent evolutionary optimization algorithms have also been put forward to deal with different optimization problems for which the conventional methods may be ineffective.

It is well known that the traditional SQP methods generate a sequence $\{x_k\}$ converging to the desired solution by solving the quadratic programming problem [12]

$$\mathrm{Min}\ g(x)^T d + \frac{1}{2} d^T H d \qquad (4)$$

$$\mathrm{s.t.}\{C(x) + A(x)^T d \le 0$$

where $H \epsilon R^{n \times n}$ is an approximate Hessian of the Lagrangian function of the objective function, which is usually obtained by quasi-Newton techniques.

For the current iteration point x_k, let d_k be the solution of (5), the SQP method generates the next iteration point by

$$x_{k+1} = x_k + \lambda_k d_k \qquad (5)$$

where $\lambda_k > 0$ is a step length obtained by some line search techniques.

Evolutionary Algorithms (EAs) are good candidates for multi-objective optimization problems due to their abilities, to search simultaneously for multiple Pareto optimal solutions and perform better global search of the search space. Among all the evolutionary algorithms, the well known one is the Genetic Algorithms (GA). GA is a stochastic search procedure based on the mechanics of nature selection, genetics and evolution. Since this type of algorithm simultaneously evaluates many points in the search space, it is more likely to find the global solution of a given problem. In addition, it uses only a simple scalar performance measurement that does not require or use derivative information, so methods classified as GA are easy to use and implement.

PSO algorithm is an adaptive algorithm based on a social–psychological metaphor [13]; individuals in a population adapt by returning stochastically toward previously successful regions in the search space, and are influenced by the successes of their topological neighbors. Each individual in particle swarm, called as a "particle", represents a potential solution; each particle moves its position in search space and updates its velocity according to its own flying experience and neighbors' flying experience, aiming at a better position for itself.

The particles are manipulated according to the following equations (the superscripts denote the iteration):

$$v_i^{k+1} = \omega v_i^k + c_1 r_1 (p_i - x_i^k) + c_2 r_2 (p_g - x_i^k) \tag{6}$$

$$x_i^{k+1} = x_i^k + v_i^{k+1} \tag{7}$$

where i = 1, 2, . . . , N, and N is the size of the population; w is the inertia weight; c_1 and c_2 are two positive constants, called the cognitive and social parameter respectively; r_1 and r_2 are random numbers uniformly distributed within the range [0, 1]. Eq. (6) is used to determine the i-th particle's new velocity v_i^{k+1}, in each iteration, while Eq. (7) provides the new position of the i-th particle x_i^{k+1}, adding its new velocity v_i^{k+1}, to its current position x_i^k. Figure 2 shows the description of velocity and position updates of a particle for a two-dimensional parameter space.

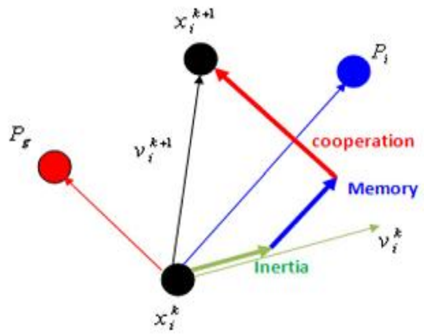


Figure 2 Schematic of velocity and position updates in PSO for a two dimensional parameter space

3.2. EXPERIMENTAL MEASUREMENT

3.2.1. Measuring equipment

The commercially available hot plate apparatus type EP500 manufactured by Lambda Messtechnik consists of lower "cold" plate and upper "hot" plate consisting of two plates-the hot plate and the cold plate (Figure 3). The sample tested is inserted between lower and upper plate. The dimensions of the plates are 50 x 50 cm. However, the measurements on the samples are performed on a core square of 15 x 15 cm only. More information regarding steady-state thermal conductivity measurements with use of hot plate apparatus can be found in [10]. Firstly, the upper and lower plate should be kept at 18 ℃ for at least 5 hours in order to ensure that the whole sample reaches the same temperature. Then the sample should be symmetrically heated by both upper and lower plate from 18 ℃ to 32 ℃ (in order to see the whole phase change process) more than 10 hours and finally is kept at 32 ℃, which was shown in Figure 4.

Figure 3 Hot plate apparatus EP 500

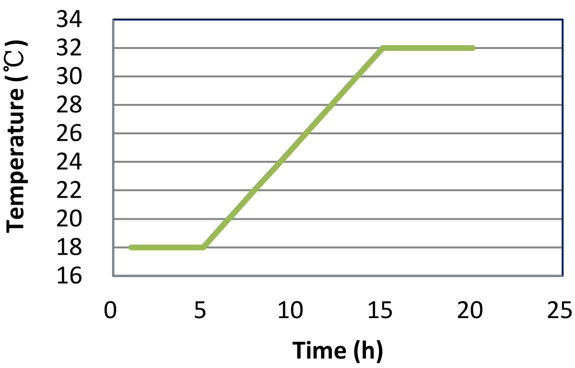


Figure 4 Dynamic temperatures boundary on top and bottom of the sample

3.2.2. Material preparation

A set of PCM-concrete samples were prepared with 0%, 1%, 4%, and 6% by weight of incorporated PCM. Each sample has an area of 15 x 15 cm^2 and height of approximately 8 cm. Specification of the concrete can be found in [10]. When preparing mixtures the total volume for each concrete mixtures was 0.025 m^3. The prepared PCM-concrete samples of dimensions of 15 cm x 15 cm x 8 cm were dried in the oven at 65-70 ℃ until they stopped changing weight. The constant weight signalized that the measured thermal conductivity is independent of moisture content in the samples.

3.3. MEASUREMENT OF TEMPERATURE AND HEAT FLUX

The samples were cut into two equal pieces of dimensions 15 x 7.5 x 8 cm^3 and the surfaces along the cut were carefully polished. Afterwards, 9 parallel grooves of depth and width of 0.3 mm and distance between them of 8 mm were cut as presented in Figure 5. Calibrated thin thermocouples, type K, were inserted in the specially prepared PCM-concrete samples with grooves. Then, the two parts of previously cut sample were assembled with inserted in-between thermocouples. At the end, visual check was performed to see whether there are air gaps along the assemblage where the thermocouples were inserted and whether samples fit well to each other. The procedure was repeated for all investigated samples. Furthermore, the methodology to insert thermocouples in the concrete sample used in the presented experiment was validated with use of plaster sample.

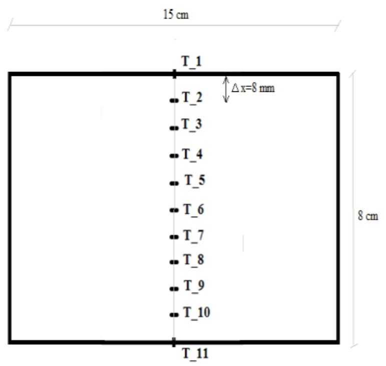
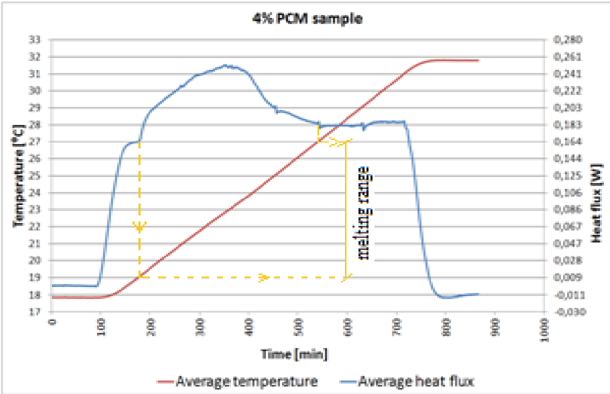


Figure 5 Location and thermal couples in the sample

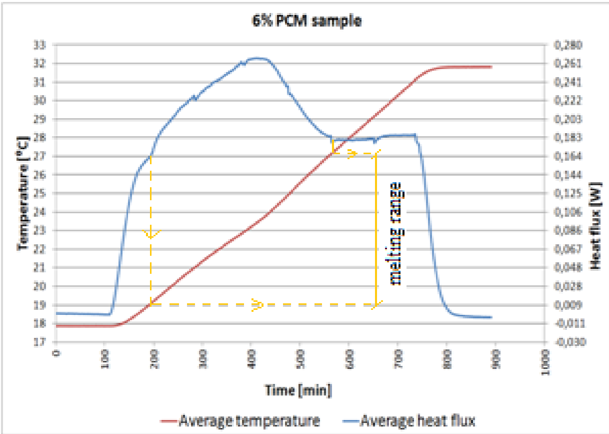
In order to perform measurements of only 1D heat flux provided from the apparatus plates and that is free of side heat flux from the frame, the heat flux sensor has to have a smaller area than the total area of the sample of dimensions of 15 x 15 cm and has to be located at the center of the sample. In order to calculate the percentage ratio of the side heat flux to the sample with regards to the heat flux applied from the hot plate apparatus, the numerical investigation has been performed in COMSOL multiphysics program. The result from that investigation indicated that, if the heat flux film has square size of 8 x 8 cm^2, then side heat flux is of maximum only 0.6 % of the total heat flux provided from the bottom and top plate of the apparatus. It was assumed that the error at this level can be accepted. The heat flux film used in the experiment is the square heat flux sensor produced by Captec and has sensitivity of 23.4 $\mu Vm^2 W^{-1}$. Because the PCMs have been encapsulated and integrated with the concretes. And its relative ratio is little compared with that of concretes in the mixtures (4 wt% and 6 wt %), the thermal conductivity of whole sample measured when it is in low temperature range from 2.5 to 17.5 ℃ (all PCM is solid), from 12.5 to 27.5 (some PCM is melted and some solid), and from 32.5 to 47.5 ℃ (all PCM is melted) are nearly a constant (1.29 for 4 wt% mixtures and 1.08 for 6 wt% mixtures) [10].

The measured average heat flux and average temperature of the 4% and 6% PCM-concrete were shown in Figure 6. Presented results are the average results of 3 series of measurements that were performed on each of the investigated sample. The average temperature presented in Figure 6 is calculated as average temperature from all thermocouples inserted in the sample and from all 3 series of measurements for each investigated sample.

In graphs for 4 wt % and 6 wt % PCM-concrete, where peak is very distinct, the melting range has been marked. The highest peak of the heat flux occurs at approximately 23°C, which is also the melting point of the used PCM. The measured temperature profile in the sample and the heat flow to the sample in function of time are the outputs of the experiment. These outputs will be used to calculate the specific heat capacities of the PCM-concrete samples in function of temperature.



(a)



(b)

Figure 6 Temperature and heat flux results from the dynamic experiment (a) 4% (b) 6%.

4. RESULTS AND DISCUSSION

4.1. Determination of thermal physical properties through SQP algorithm

4.1.1 Determination of the weights in the objective function

Now the weights should be determined through the error transfer function. The heat transfer equation (Eq.(2)) can be linearized through the difference method.

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right)$$

The difference form of the above equation can be simplified as follows:

$$\rho c_p \frac{T_{n,t+1}-T_{n,t}}{\Delta t}=k\frac{1}{\Delta x}\left(\frac{T_{n+1,t}-T_{n,t}}{\Delta x}-\frac{T_{n,t}-T_{n-1,t}}{\Delta x}\right)$$
$$=k\frac{T_{n+1,t}-2T_{n,t}+T_{n-1,t}}{\Delta x^2} \quad (8)$$

The total heat obtained by the surface can be derived by summing the heat transferred by each layer per unit area in time △t.

$$\sum_{n=1}^{9}\rho c_p \frac{L}{9}\frac{T_{n,t+1}-T_{n,t}}{\Delta t}=q\Delta t \quad (9)$$

Using the total differential form of the both sides, the following equation can be derived:

$$dc_p\sum_{n=1}^{9}\rho\frac{L}{9}\frac{T_{n,t+1}-T_{n,t}}{\Delta t}+dT_{n,t+1}\sum_{n=1}^{9}\rho c_p\frac{L}{9\Delta t}-$$
$$dT_{n,t}\sum_{n=1}^{9}\rho c_p\frac{L}{9\Delta t}=dq\Delta t \quad (10)$$

Finally, the error transfer equation of the calculated specific heat and its sensitivity to the error of the surface heat flux and temperatures of each measured layer can be derived as follows:

$$\Delta c_p=\frac{\Delta t^2}{\rho L\left|T_{n,t+1}-T_{n,t}\right|_{min}}\Delta q+\frac{2c_p}{\left|T_{n,t+1}-T_{n,t}\right|_{min}}\Delta T_{n,t} \quad (11)$$

Similarly, Eq.(2) can be rewritten as follows in order to determine the error transfer equation of thermal conductivity.

$$k\frac{T_{n+1,t}-2T_{n,t}+T_{n-1,t}}{\Delta x^2}=\rho c_p\frac{T_{n,t+1}-T_{n,t}}{\Delta t} \quad (12)$$

The error transfer function of the thermal conductivity to the surface heat flux and temperatures of each measured layer can be derived based on the total difference form and simplification, which is

$$\Delta k=\frac{\rho L^2\left|T_{n,t+1}-T_{n,t}\right|_{\max}}{81\Delta t\left|T_{n+1,t}-2T_{n,t}+T_{n-1,t}\right|_{\min}}\frac{\Delta t^2}{\rho L\left|T_{n,t+1}-T_{n,t}\right|_{\min}}\Delta q$$
$$+\left(\begin{array}{c}\dfrac{\rho L^2\left|T_{n,t+1}-T_{n,t}\right|_{\max}}{81\Delta t\left|T_{n+1,t}-2T_{n,t}+T_{n-1,t}\right|_{\min}}\dfrac{2c_p}{\left|T_{n,t+1}-T_{n,t}\right|_{\min}}+\\ \dfrac{2L^2\rho c_p+324k\Delta t}{81\Delta t\left|T_{n+1,t}-2T_{n,t}+T_{n-1,t}\right|_{\min}}\end{array}\right)\Delta T_{n,t} \quad (13)$$

Because the thermal conductivity of the problem presented in this paper is already measured by the hot plate method and it can be regarded as a constant. Thus, the main purpose of this paper is to determine the dynamically changed specific heat. And the relative weight of the surface heat flux and temperatures of each layer to the error of specific heat determination can be derived through the error transfer function as shown in Eq.(11).

4.1.2 Determination of the thermal physical properties through the SQP algorithm

It can be inferred from the above description that the proper temperature range of the PCM-concretes should be within 18 to 32 ℃.In this problem, because the PCMs have been encapsulated and thermal conductivity of the mixtures of PCM-concretes changes very small during the phase change process according to the steady state measurement. The thermal conductivity in our problem is regarded as a constant and determined through the steady state measurements, which is 1.29 W/mK for the 4% mixtures of PCM and concretes and 1.08 W/mK for the 6% mixtures of PCM and concretes. How to determine the dynamic specific heat during the phase change process is the main task in our problem. Firstly, the temperature was divided into 15 segments, and specific heat is regarded as a constant in each segment (Figure 7). In Figure 7, the function f(t) can be c_p(t). Then the upper and lower limits of the specific heat were assumed to be 0-3000 J kg^{-1}℃$^{-1}$. In the numerical simulation program, the space and time size were 8 mm and 10 seconds, respectively. The space step size was chosen in order to match the experimental results well. The time step size was chosen to ensure the stability of this explicit finite difference method. The distribution of specific heat will change automatically through the SQP optimization method by lowering the absolute difference, the equivalent thermal physical properties can be got when the objective function can't be lowered any more.

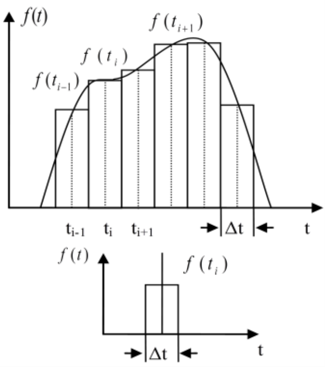


Figure 7 Schematic of the distribution of c_p and k with temperature

Firstly, the above mentioned methods are used to determine the equivalent thermal physical properties of 6% PCM-concrete.

The specific heat distribution with temperature is derived through the above mentioned methodology, which is shown in Figure 8.

The relative error of the heat flux RE_{flux} and temperature $RE_{temperature}$ are defined as:

$$RE_{flux} = |q_{cal} - q_{mea}| / |\frac{q_{cal}+q_{mea}}{2}| \quad (8)$$

$$RE_{temperature} = |T_{cal} - T_{mea}| / |\frac{T_{cal}+T_{mea}}{2}| \quad (9)$$

The average relative error of the heat flux, RE_{flux}, and temperature, $RE_{temperature}$, are 1.44 % and 1.42 % of all the calculated points. Thus, the accuracy of the calculated thermal physical properties is good enough for engineering application.

The measured and calculated heat fluxes on the top are shown in Figure 9(a) and the measured and calculated temperatures in the eleven layers are shown in Figure 9(b).

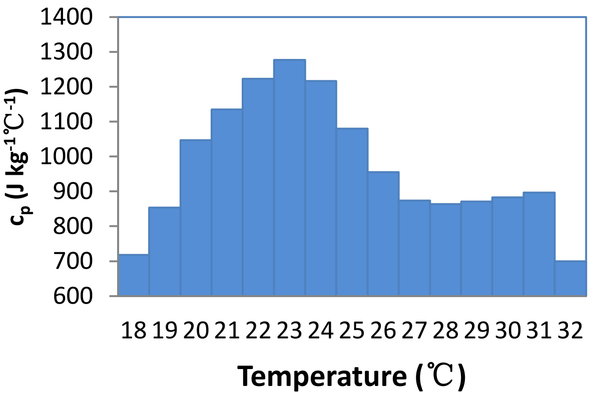
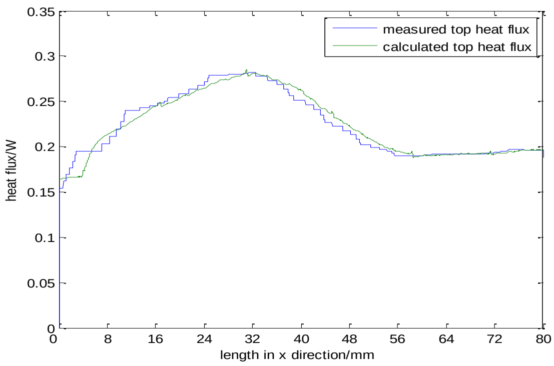
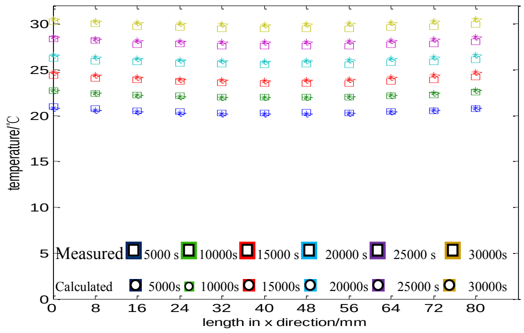


Figure 8 Equivalent c_p of 6% PCM-concretes during the phase change process



(a)



(b)

Figure 9 Measured and calculated heat flux (a) and temperature (b) distribution with optimized thermal physical properties (6 wt% PCM)

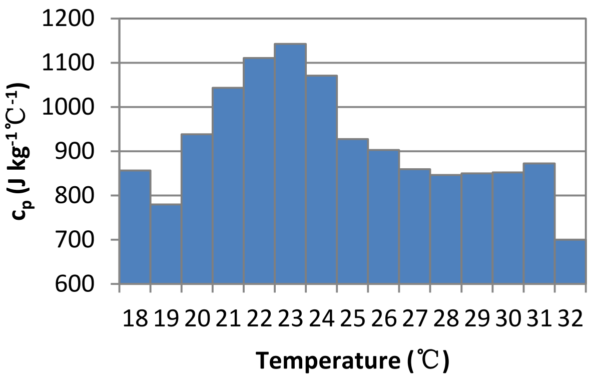
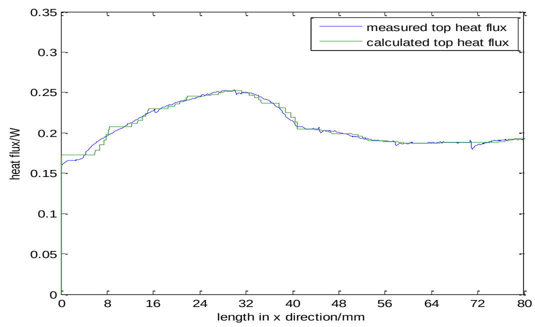
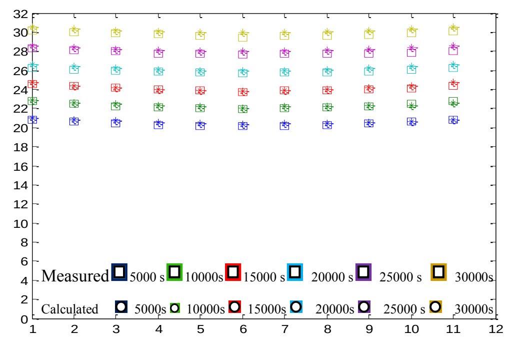


Figure 10 Equivalent c_p of 4% PCM-concretes during the phase change process



(a)



(b)

Figure 11 Measured and calculated heat flux (a) and temperature (b) distribution with optimized thermal physical properties (4 wt%)

It can be inferred from Figure 9 that the measured and calculated heat flux and temperature match very well with each other. Thus, the calculated thermal physical properties should be close enough to the real ones.

It can be concluded from Figure 8 that the specific heat of the PCM-concretes without phase change is about 700 J $kg^{-1}℃^{-1}$, and the largest specific heat appears at 23℃, which corresponding to the melting point of the PCM used in this research. When the temperature is higher than 23 ℃, its specific heat starts to decrease.

The equivalent specific heat distribution of 4% PCM-concrete is also determined by using the aforementioned inverse problem method. It can be seen in Figure 10 that the equivalent specific heat of 4% PCM-concretes is lower than that of 6% PCM-concretes. However, the phase change point is the same (i.e. 23 ℃). That is because less PCM is mixed with concretes.

4.2. Different temperature segment methods

The temperature segment methods will directly determine the variables in the optimization problem. It can be inferred that the relative errors of the heat flux and temperature both decrease with smaller temperature difference in each segment. However, the computation time and complexity will also increase with smaller temperature difference in each segment. Thus, the changes of accuracy and calculation speed with different temperature segments of the mixture with 6 wt% PCMs are analyzed, which are shown in Table 1.

Although the relative errors of heat flux improve absolutely, there are no absolute improvements to the relative error of temperature if the temperature segments increase. The accuracy with temperature segment of 2 ℃ is already good enough for engineering application. However, the SQP algorithm should calculated the numerical simulation program for n times to determine the next direction and step size (n is the number of variables). Thus the computation complexity will be seriously increased with more variables.

Table 1 Relative error of heat flux and temperature with different temperature segments (SQP method) (6 wt% PCM)

Temperature difference in each segments	RE_{flux}	$RE_{temperature}$
2 ℃	3.25%	1.43%
1 ℃	1.44%	1.42%
0.5 ℃	0.61%	1.40%

4.3. Comparison of different optimization algorithms

In order to compare the accuracy and speed of different optimization algorithms applied to this nonlinear problem. Three typical optimization algorithms are compared, i.e. the above mentioned Sequential Quadratic Programming algorithm, the Particle Swarm Optimization algorithm and the Genetic Optimization algorithm.

Normally, an optimization algorithm is usually evaluated from two angles: the one is the accuracy of the final results, and the other is the time complexity. These algorithms are applied to determine the thermal physical properties of the 6% PCM-concretes. And the temperature difference in each segment is 0.5 ℃. The relative error of the optimization and the time complexity are shown in Table 2.

Table 2 Accuracy and time complexity of different optimization methods

Algorithms	RE_{flux}	$RE_{temperature}$	Time complexity (s)
SQP	0.61%	1.40%	336
GA	0.64%	1.42%	3216
PSO	0.97%	1.41%	2816

It can be figured out from Table 2 that the accuracies of SQP and GA methods are little better than that of the PSO method. However, time complexity of the SQP method is the least among these three algorithms. So that it can be concluded in our problem that the SQP method is the best optimization algorithm compared with GA and PSO method. It is with the highest accuracy and least time complexity. And GA has higher accuracy than the PSO method. However, the time complexity of GA is higher than that of the PSO method.

In can be found in Figure 12 that the objective function begins to fluctuate after 500 generations, which leads to higher time complexity of the Genetic Algorithms, this is because of the nature of our objective function. It can be seen from Figure 13 that the optimized specific heat distributions with temperatures through these three optimization algorithms are very similar to each other, which justified the calculated specific heat distributions.

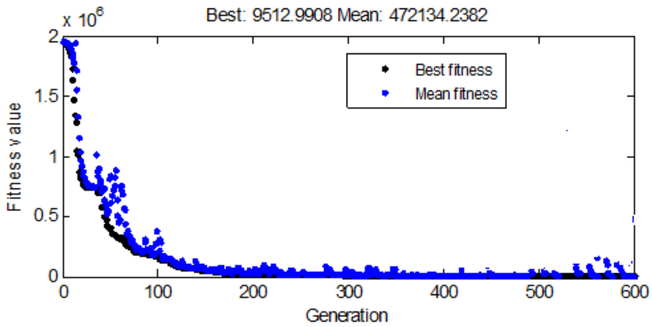


Figure 12 Optimization histories of the Genetic Algorithm

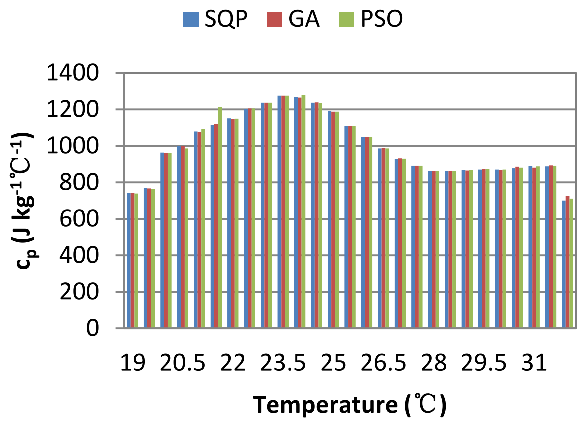


Figure 13 Optimized specific heat distribution with various optimization algorithms

5. CONCLUSIONS

A novel method to determine the equivalent thermal conductivity and specific heat of PCM-concretes is proposed in this paper. The input data needed is only the top heat flux and the temperature distribution in different layers and there is no need for complex installments to be used. The dynamic change of thermal physical properties can be clearly presented by using the proposed method, which is very difficult to be measured by using the conventional methods.

The accuracy of the SQP optimization is good enough for engineering applications (maximum relative error <4%), and it is very fast. Influences of different temperature segment methods and optimization algorithms are analyzed. It is showed that the SQP method is with the highest accuracy and least time complexity, which is the best optimization method for our problem compared with Genetic Algorithm and Particle Swarm Optimization method. It is found that the optimized specific heat distribution will nearly not be influenced by various optimization methods.

The proposed method can also be used to determine key parameters of other similar nonlinear heat and mass transfer problems, which are not easy and feasible to be determined through conventional methods. The only necessary thing is that solution can be determined from theoretical analysis and the system of equations is closed. With the application scope of PCM-concretes becomes larger and larger, the method to determine thermal physical properties of PCM-concretes will be more and more important than ever before.

ACKNOWLEDGEMENT

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