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Porous silica matrices infiltrated with PCM for thermal protection purposes

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Abstract

In this work, numerical and experimental studies are proposed to predict and investigate the thermal absorption characteristics of porous silica infiltrated with phase change materials (PCM) for thermal protection applications. Several types of different solid–liquid phase change composites were introduced into a cylindrical enclosure while it was heated on the left of the enclosure. The numerical simulation was performed using a volume-averaging technique, and a finite volume modelling (FVM) was used to discretise the heat diffusion equation. The phase change process was modelled using the enthalpy–porosity method. The results are portrayed in terms of the temperature distribution and liquid fraction, and the numerical and experimental results showed good agreement. The results indicated that a higher latent heat storage capacity meant a more stable thermal performance of the phase change composite.

Keywords: Ceramic-matrix composites (CMCs); Differential scanning calorimeter (DSC); Finite volume modelling (FVM); Phase change materials (PCM)

1. Introduction

Controlling the temperature and/or heat transfer is of crucial importance in numerous technical processes and natural occurrences, including cooling of electronics and telecommunications equipment in defence industries and in aerospace applications. One method for protecting a surface subjected to a high heat flux is the use of a thermal barrier to keep its temperature under emergency operating conditions. Thermal management utilising solid–liquid PCMs is one of the most interesting passive thermal management techniques due to its simplicity and reliability. Latent heat absorption phenomena associated with melting of a suitable PCM may be effectively used to delay or modify the temperature rise of the surface subjected to high heat flux. Solid–liquid PCM including salt hydrates, paraffin waxes, certain hydrocarbons and metal alloys are often used for thermal protection applications.

Sari et al. [1–3] investigated some fatty acids and their eutectic mixtures used for latent heat storage, and Alkan et al. [4] investigated a novel material for thermal storage solid/liquid transitions in ethylene glycol distearate. The thermo-physical properties of three kinds of paraffin with different melting points were determined by the differential scanning calorimeter (DSC) method, and its heat transfer process was investigated [5]. In addition, the thermal properties and heat transfer characteristics of various sugars and sodium acetate as PCMs were studied by Kaizawa et al. [6].

Various geometric configurations have been considered for the phase change thermal management devices. Bain et al. [7] considered the configurations of a PCM-filled rectangular cavity for spacecraft thermal control while

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Ismail and Trullenque [8] analysed the use of electronic equipment. Sarier and Onder [9] proposed utilising polyurethane foams containing polyethylene glycol for preventing discontinuous thermal regulation when the external temperature increases or decreases. A numerical and experimental study on the melting of a spherical PCM was performed using transient numerical simulations by Assis et al. [10]. Kandasamy et al. [11] investigated a novel PCM package for thermal management of portable electronic devices, and they reported that a PCM-based design is an excellent candidate for transient electronic cooling applications.

Although organic PCMs like paraffin waxes exhibit desirable properties such as non-corrosiveness, low cooling and thermal stability, during the melting process they are mobile and will leech out. This property restricts the heat absorption applications of the thermal protection system; however, the problem of melted organic PCM leakage may be improved by many techniques, including embedding within a porous matrix. Wirtz et al. [12] developed a novel lamination that consists of aluminium heat spreader plates interspersed with a polymer-based thermal energy storage composite. The composite consists of a thermoplastic matrix that encapsulates paraffin such that it is immobilised when in the liquid phase. Using graphite foam impregnated with paraffin, Wirtz et al. [13] also developed a multifunctional lamination consisting of a paraffin-impregnated porous graphite core encapsulated between rigid graphite/epoxy composite skins. The performance of this lamination has been studied in the temperature control of sensors and electronic devices, including both thermal and mechanical analyses. The study showed that the graphite foam effectively immobilised the liquid paraffin.

The heat transfer modelling of the phase change composite materials may produce a workable design and lead to optimal design operation for thermal absorption applications. Bejan [14] defined the optimal thermal system as the least irreversible system using thermal design techniques that are based on minimisation of entropy generation. However, melting and solidification of PCMs inside a porous matrix is a very complicated phenomenon due to the existence of different phases: the solid phase of the porous matrix; and the PCM itself, which may be in a solid, liquid or mixed state. The analysis of heat transfer problems in melting and solidification process is that the solid–liquid boundary moves depending on the speed at which the latent heat is absorbed or lost at the boundary, so that the position of the boundary is hard to specify. Due to this complication, a volume-averaging method for the microscopic conservation equations might account for the complex interfacial structures of each of the constituents. A numerical model based on solving the volume-averaged conservation equations for mass momentum and energy with phase change process has been investigated by Mesalhy et al. [15]. Using this approach, the thermal characteristics of PCMs in saturated porous media for thermal protection purposes have been experimentally and numerically studied [16]. Recently, the thermal performance of porous media infiltrated with PCM for space applications was investigated [17]. Mesalhy' model was based on a volume-averaging technique, while a finite volume method was used to discretise the heat diffusion equation.

Porous silica ceramics filled with organic PCMs are introduced as thermal barriers or carriers to protect a surface subjected to heat flux followed by our recent work about preparation and thermal properties of silica ceramic matrix composite (CMCs) [18]. The thermal characteristics of the proposed systems were investigated experimentally and numerically in a simulated environment. A detailed temperature distribution and liquid fraction were obtained via the modelling of solidification/melting using Fluent 6.3 software package, demonstrating heat transfer evolution in the system as the phase change material melts.

2. Experimental

Three porous silica cylindrical disks with three different solid–liquid PCMs (two kinds of paraffin: C58$^{\sharp}$ and 64$^{\sharp}$ and one kind of xylitol: X98$^{\sharp}$) were fabricated as the solid matrices of the silica-PCM composites according to our recent study [18–20]. The porous silica ceramic matrix was heated in a molten PCM to prepare the phase change composites. Phase change point and heat storage capacity of the composites were measured by DSC (NETZSCH STA449C) calibrated with an indium standard in the range from 30 °C to 200 °C at a scan rate of 5 °C/min. The conductivity and specific of heat of the composites were measured by a hot disk conductivity instrument (TPS 2500S). The thermo-physical data for these samples are given in Table 1.

The composites (100 mm in diameter and 10 mm thick) were then introduced into the experimental setup (see Fig. 1). A 2 mm thick steel plate was glued to left side of the sample using a silicon layer and tightened by screws. A second steel plate of the same thickness was used to press the sample from the right side. A j-type thermocouple was installed on the right steel plate in order to measure the temperature of the samples (cold face). The temperature was recorded as it varied with time. The composite sample was heated from the left side using a heater installed on the furnace, and its temperature was recorded.

Table 1
The thermo-physical parameter of the porous silica matrix composites.

Thermo-physical parameter	C58$^{\sharp}$	C64$^{\sharp}$	X98$^{\sharp}$
Phase change point(K)	324	329	363
Heat storage capacities (kJ kg^{-1})	172	165	198
Thermal conductivity at 300 K(Wm^{-1}K^{-1})	0.38	0.38	0.46
Specific heat (kJ(kg)$^{-1}$K^{-1})	2.4	2.4	3.8

The top and bottom walls of the container were insulated by adiabatic materials.

For the sake of validation of the numerical model and assumptions, the temperature of the cold face of composite X98$^{\#}$ as a function of time was deduced by the numerical simulation.

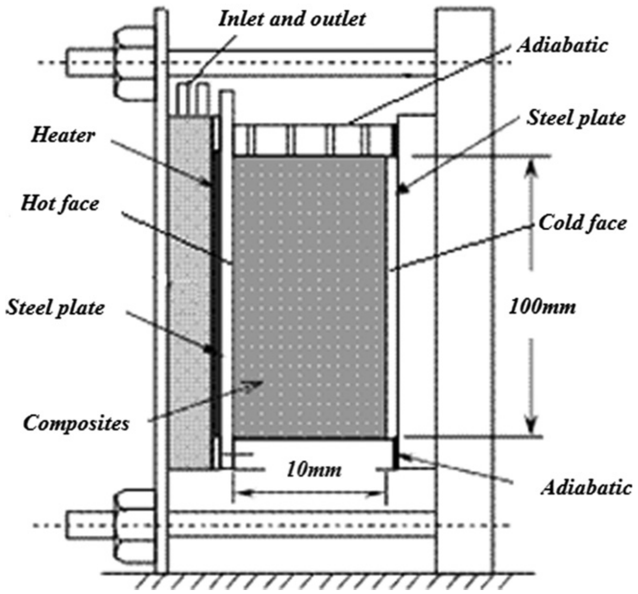

Fig. 1. Experimental setup for heat transfer of phase change composite (100 mm in diameter and 10 mm thick).

Table 2
The experimental data of the porous silica matrix composites.

	C58$^{\#}$	C64$^{\#}$	X98$^{\#}$
Sample volume (m^3)	3.05E–3	3.05E–3	3.05E–3
Mass before infiltration (kg)	7.20E–1	7.20E–1	7.20E–1
Mass after infiltration (kg)	2.79	2.83	4.16
Density (kg m^{-3})	914.75	927.87	1363.93
PCM (paraffin or xylitol) mass rate (%)	74.19	74.56	82.69

3. Numerical model

Modelling of the phase change processes presents a significant challenge due to the complexity and conjunction of the involved physical phenomena, such as volumetric expansion due to the phase change, convection in the liquid phase, and motion of the solid in the melt due to density differences. In order to overcome these limitations and solve the complete conservation equations allowing for PCM expansion, convection in the fluid media, and solid motion in the liquid, detailed temperature and phase fields contours have been obtained with time. These contours demonstrate the heat transfer evolution in the system as the phase change materials melt.

The composites (180 mm in diameter and 120 mm thick) were then introduced into the numerical analysis. The mean mass of the composites before/after the infiltration was measured and the mass infiltration rate of PCM in composites was calculated. The experimental data of the porous silica matrix composites are given in Table 2. A schematic diagram of the composite and two-dimensional grids are given in Fig. 2. Due to the symmetry and regularity, the samples were formulated with two-dimensional axis-symmetric coordinates and uniformly split quadrangle grids in all 19,481 nodes by Gambit 2.2.30, and the boundary conditions were specified.

3.1. Assumptions and governing equations

The mathematical formulations have been made based on the following assumptions:

The properties of each composite are homogeneous and isotropic.

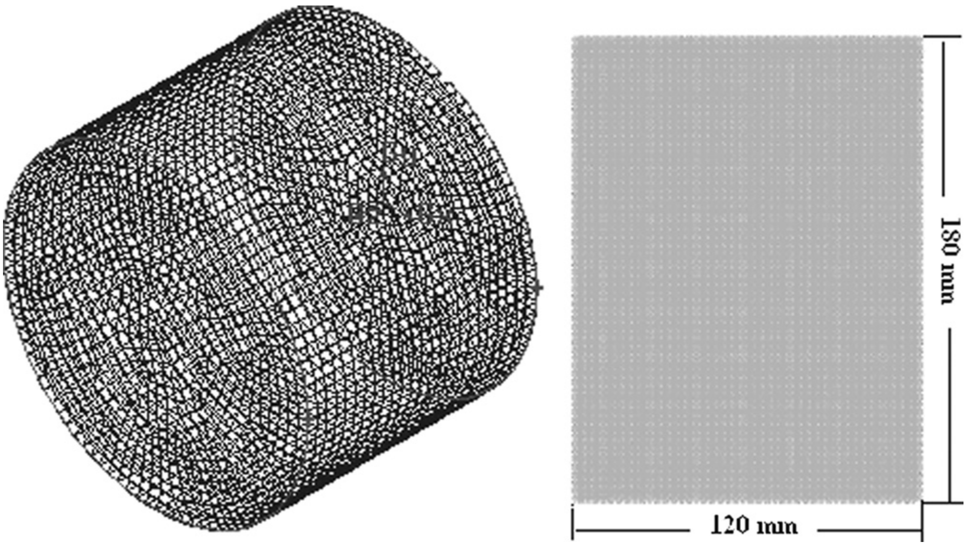

Fig. 2. Modelling and grids for the composite (180 mm in diameter and 120 mm thick).

The thermo-physical properties are different for the solid and liquid phases but are dependent on temperature.

Heat loss from the container to its surroundings is negligibly small.

Based on these assumptions, the enthalpy–porosity method [21] was used for the phase change region in the PCM. Thus, the porosity in each computational cell is set equal to the liquid fraction in that cell. Accordingly, the two-dimensional governing equations used here for the setup model are given below.

$$\frac{\partial \rho}{\partial t}+\frac{\partial(\rho u)}{\partial x}+\frac{\partial(\rho v)}{\partial y}=0 \tag{1}$$

where ρ is the density, u is velocity in x direction, t is the time, and v is velocity in y direction.

3.1.1. u -Momentum

$$\rho\left(\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}\right)=\mu\left(\frac{\frac{\partial^2 u}{\partial x^2}+\partial^2 u}{\partial y^2}\right)-\frac{\partial p}{\partial x}+S_u \tag{2}$$

where the source term is $S_u=\left((1-f_l)^2/\left(f_l^3+\varepsilon\right)\right)A_{mush}u$, μ is the dynamic viscosity, ε is constant, f_l is the liquid fraction and A_{mush} is the solid–liquid mushy region number, range from 10^4 to 10^7.

3.1.2. v–Momentum

$$\rho\left(\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}\right)=\mu\left(\frac{\frac{\partial^2 v}{\partial x^2}+\partial^2 v}{\partial y^2}\right)-\frac{\partial p}{\partial y}+S_v \tag{3}$$

where the source term is $S_v=\left((1-f_l)^2/f_l^3+\varepsilon\right)A_{mush}v+\left(\rho_{ref}g\beta\left(h-h_{ref}\right)/c_p\right)$, β is the thermal expansion coefficient, h is the sensible enthalpy, and $c_p$is the specific heat.

3.1.3. Energy

$$\rho\left(\frac{\partial H}{\partial t}+u\frac{\partial H}{\partial x}+v\frac{\partial H}{\partial y}\right)=\frac{k}{c_p}\left(\frac{\frac{\partial^2 H}{\partial x^2}+\partial^2 H}{\partial y^2}\right)+S_k \tag{4}$$

where the source term is $S_k=\frac{\rho}{c_p}\frac{\partial(\Delta H)}{\partial t}$,and

$$H=h+\Delta H$$
$$h=h_{ref}+\int_{T_{ref}}^{T}c_p\mathrm{d}T \tag{5}$$

where, H is the enthalpy, T is the temperature, and $\Delta H$is the specific enthalpy.

The density and dynamic viscosity of the liquid PCM depend on its temperature. The density can be expressed as

$$\rho=\rho_{ref}\left[1-\beta\left(T-T_{ref}\right)\right] \tag{6}$$

where$\beta=0.001$ can be used as presented by Humphries and Griggs [22].

The dynamic viscosity of the liquid PCM can be expressed as

$$\mu=0.001\times\exp\left(A+B/T\right) \tag{7}$$

where $A=-4.25$ and $B=1760$ following Reid et al. [23]

3.1.4. Boundary conditions

Given the constant temperature of the cold face and the adiabatic top and bottom wall,

$$T(x,y,t)\big|_{x=d}=T_{cold}$$
$$\frac{\partial T}{\partial y}\big|_{y=0,t}=0 \tag{8}$$

3.1.5. Initial conditions

Assuming initial temperature conformity and a fixed temperature of the hot face,

$$T(x,y,t)\big|_{t=0}=T$$
$$T(x,y,t)\big|_{x=0,t>0}=T_{hot} \tag{9}$$

The numerical solution was carried out using the Fluent 6.3 software package [21]. The PISO algorithm was used for pressure–velocity coupling. The number of computational grids was ~19,200 for the 2D model after grid-independence tests. After a careful examination of the preliminary calculations, the time step in the simulations was as small at $\Delta t=0.1$ s. The convergence was also checked at each time step, with convergence criteria of 10^{-4} for velocity components and 10^{-7} for energy equation.

4. Results and discussion

4.1. Experimental results and discussion

The composites had different thermo-physical data owing to the three types of organic PCMs used during the preparation of the porous silica-PCM composites (see Table 1). The varying heat storage capacities of the composites have an influence on the experimental melting process. Experiments are required to determine the suitable silica-PCM for the service conditions.

The thermal protection characteristics of three types of porous silica-PCM were experimentally studied (Fig. 3) through the experimental setup (Fig. 1). Fig. 3a compares the temperature of the cold face of the composites when they are subjected to same hot face temperature; Fig. 3b represents their temperature of cold face varies with time as they are subjected to hot face temperature, 600 °C. As can be seen in the Fig. 3, the X98$^{\#}$ composite shows the best heat absorption properties among the three composites. Firstly, the temperature of the cold face of the X98$^{\#}$ composite subjected to same hot face temperatures is lower than the other two composites. The temperature of the cold face of the composite X98$^{\#}$ is 45 °C while one of the

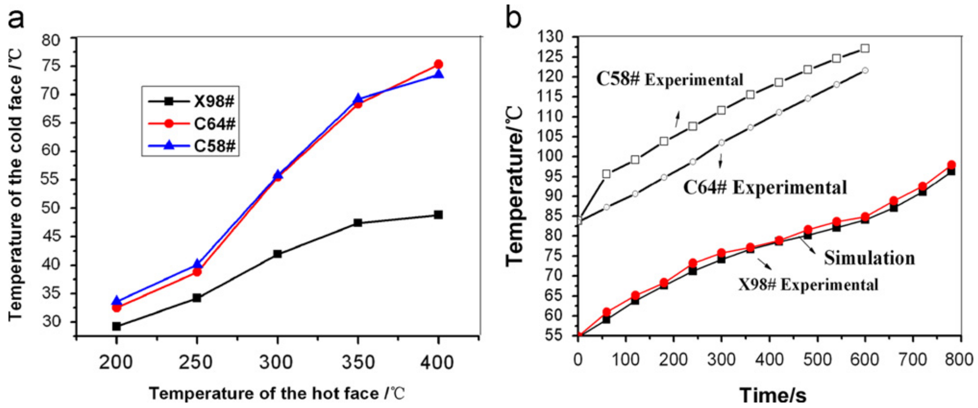

Fig. 3. (a) Comparison of cold face and hot face temperature of three types of composites and (b) cold face temperature varied with time as hot face temperature is 600 °C.

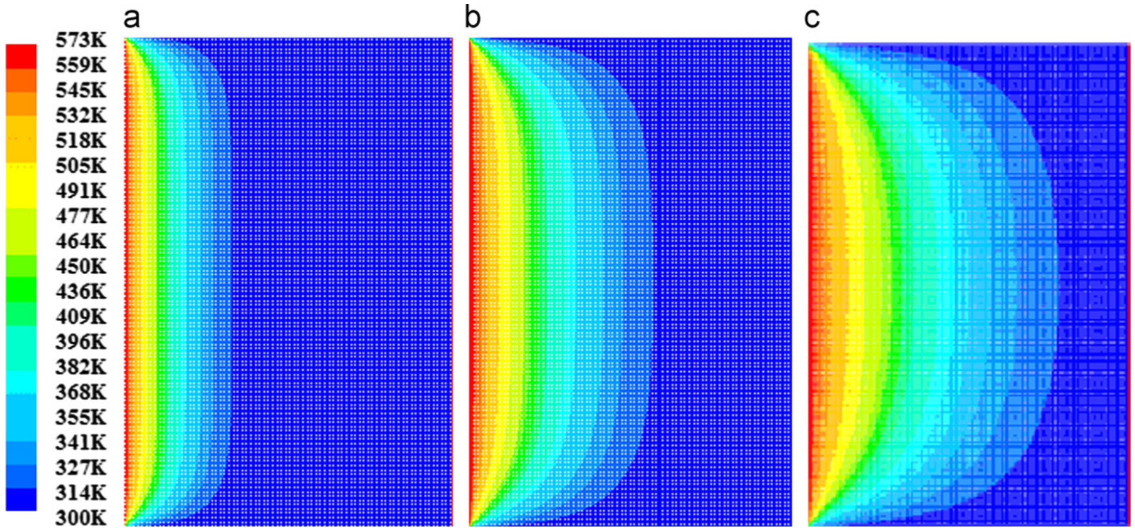

Fig. 4. Contours of temperature of the composite C58#. Time intervals=(a) 10 s, (b) 30 s and (c) 60 s.

other two composites is 75 °C as the three types of composites subjected to same hot face temperature, 400 °C (see Fig. 3a). Secondly, the slope of the time–temperature curve of the X98# composite decreases at a temperature ~80–90 °C, which is close to the phase transition range of the X98# composite and does not vary substantially with time. This trend is obvious at the melting temperature of the X98# composite, and it did not appear for the other two composites 58# and C64#, as they are above their phase change temperature and had already melted (see Fig. 3b).

For the cold face of composite X98#, good agreement is obtained when comparing the temperature as a function of time to the numerical simulation results (Fig. 3b), which indicates the assumptions are acceptable.

4.2. Simulation results and discussion

Numerical studies have been carried out for the three types of composites under identical conditions. In the numerical model, the input temperature was modelled as a uniform heat generation source inside the heater material. The temperature contours for the composite C58# at a constant hot face temperature (573 K) and different time intervals (10, 30, and 60 s) are shown in Fig. 4. The temperature rises quickly at the beginning of the heating process and propagated as time goes on, as the melting of the composites started at the hot face in direct contact with the heating surface and the solid–liquid interface moved gradually in the axial direction over time. For the composite C64#, the heat transfer numerical studies showed the same melting process compared with the composite C58# because of their approximate thermo-physical data including heat storage capacities (approximate mass infiltration rate) and phase change point. For the composite X98#, the temperature contours at different time intervals (10, 30, 60, and 120 s) are shown in Fig. 5 under identical conditions (a constant hot face temperature, 573 K), and liquid fraction contours of the composites X98# at 180 s are shown in Fig. 6, which indicated the more stable thermal performance during the melting process due to higher heat storage capacities and phase change point as compared with the composites C58# and C64#.

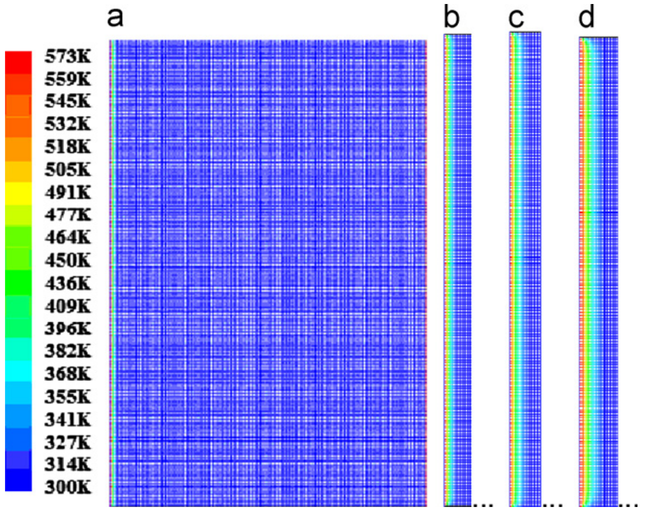

Fig. 5. Contours of temperature of the composite 98# Time intervals = (a) 10 s, (b) 30 s, (c) 60 s and (d) 120 s.

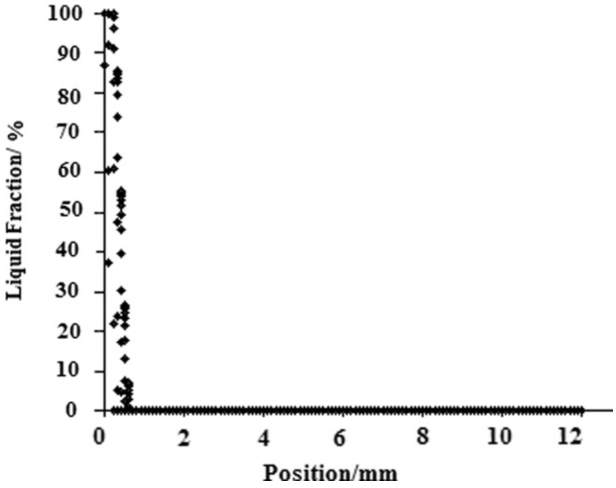

Fig. 6. Liquid fraction of the composite 98# at 180 s.

The objective of using this porous silica composite is to control the temperature and absorb heat from any surface subjected to a certain heat flux. The heat absorbed by the composites and the temperature of the cold–hot face were taken as indicators for this study. The experimental results indicated the suitable silica-PCM for the service conditions is the composite X98#. In addition, the composite X98# showed the more stable thermal performance during the melting process based on numerical results for the temperature and liquid contours of the composites. From the experimental data of the porous silica matrix composites (Table 2), the mass infiltration rate of PCM (xylitol) in the porous silica matrix composite X98# is more than the other two composites C58# and C64#. The X98# type composite has both high heat storage capacity and a high phase change point. Thus, it may be concluded that controlling the surface temperature depends mainly on these two main parameters. In addition, a higher heat storage capacity means a longer heating process, and the phase change point of the composite determines the suitable service conditions.

5. Conclusions

The effects of the heat storage capacity and thermal properties of porous silica filled with different PCMs were studied numerically and experimentally. The experimental and numerical results showed a good agreement, which indicates the proposed assumptions and numerical model procedures are acceptable. It has been shown that the heat storage capacity and phase change point of the composites play important roles in their thermal performance. It has been illustrated that a higher heat storage capacity leads to more stability in the thermal performance of the composite. On the other hand, the phase change point of the composite determined its service conditions.

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