Cement and Concrete Composites 65 (2016) 214–226

Contents lists available at ScienceDirect

Cement and Concrete Composites

journal homepage: www.elsevier.com/locate/cemconcomp

Figure of merit for the thermal performance of cementitious composites containing phase change materials

Alexander M. Thiele [a], Zhenhua Wei [b], Gabriel Falzone [b], Benjamin A. Young [a], Narayanan Neithalath [d], Gaurav Sant [b, c, **], Laurent Pilon [a, *]

[a] Mechanical and Aerospace Engineering Department, University of California, Los Angeles, Henry Samueli School of Engineering and Applied Science, United States
[b] Laboratory for the Chemistry of Construction Materials (LC^2), Department of Civil and Environmental Engineering, University of California, Los Angeles, CA, United States
[c] California Nanosystems Institute (CNSI), University of California, Los Angeles, CA, United States
[d] School of Sustainable Engineering and the Built Environment, Arizona State University, United States

ARTICLE INFO

Article history:
Received 15 June 2015
Received in revised form
25 September 2015
Accepted 29 October 2015
Available online 3 November 2015

Keywords:
Phase change materials
Microencapsulated
Energy efficient building
Cracking
Cement
Characterization

ABSTRACT

This paper presents a novel method to quantitatively characterize the thermal performance of composite materials containing phase change materials (PCM) based on a figure of merit we termed the energy indicator. The method features (i) commonly used specimen geometry, (ii) straightforward experimental implementation, and (iii) sensitivity to relevant design parameters including PCM volume fraction, enthalpy of phase change, composite effective thermal conductivity, and specimen dimensions. The experimental method and the concept of energy indicator were demonstrated on PCM-mortar composites using various volume fractions of two commercial microencapsulated PCMs. This was supported by transient two-dimensional heat transfer simulations. The energy indicator was shown to increase linearly with increasing microencapsulated PCM volume fraction and latent heat of fusion and quadratically with the specimen radius. This figure of merit can be used to rapidly screen and select microencapsulated PCM composite materials for energy efficient buildings or crack-resistant concretes.

1. Introduction

The embedment of microencapsulated phase change materials (PCMs) has been shown to be an effective means of enhancing the effective thermal inertia of concrete [1–5]. PCMs store and release heat by undergoing reversible phase transitions between the solid and liquid states [6]. The associated latent heat greatly increases the volumetric thermal storage of traditional building materials, which otherwise only demonstrate sensible heat storage and release [7]. Recently, the incorporation of PCMs has also been demonstrated as a means to mitigate thermal cracking in restrained concrete elements including pavement and bridge decks [8].

Cementitious composites containing PCMs (henceforth referred to as PCM-mortar composites) utilized for reducing building energy needs or for mitigating thermal cracking may feature a wide variety of cement compositions and microencapsulated PCMs with a wide range of thermophysical properties. In both applications, the amount and thermal properties of PCM within the composite must be chosen to achieve the desired augmentation in thermal energy storage and/or decrease in effective thermal conductivity. In spite of significant research, performance-based design criteria for such composites have not been defined. For example, typical experimental research highlights that thermal performance of PCM-composite materials improves as PCM is added, but does not quantify how much a unit increase in PCM volume fraction alters such performance. To address these limitations, this study introduces a novel, and easy to implement, experimental method to quantitatively compare the thermal behavior of PCM-mortar composites with various constituent volume fractions and thermal properties. This method reveals the thermal benefits, or lack thereof, inherent in any combination of PCM-composite materials.

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* Corresponding author. Engineering IV, 420 Westwood Plaza, Los Angeles, CA, 90095-1597, United States.
** Laboratory for the Chemistry of Construction Materials (LC^2), Department of Civil and Environmental Engineering, University of California, Los Angeles, CA, United States.
E-mail addresses: gsant@ucla.edu (G. Sant), pilon@seas.ucla.edu (L. Pilon).

http://dx.doi.org/10.1016/j.cemconcomp.2015.10.023
0958-9465/

Nomenclature

$c_{p,j}$	specific heat of component “j”, J/(kg K)
d_i	specimen diameter, mm
d_o	outer cylindrical mold diameter, mm
D_o	microcapsule diameter, μm
D_{50}	median outer microcapsule diameter, μm
EI	energy indicator, °C h
E_r	energy flux reduction, %
h	convective heat transfer coefficient, W/(m^2 K)
h_{sf}	latent heat of fusion, kJ/kg
k_j	thermal conductivity of material “j”, W/(m K)
L	cylindrical specimen height, mm
q_r'', q_z''	heat flux in the $r-$ and $z-$ directions, W/m^2
r	radial coordinate, mm
r_i	specimen radius, mm
r_o	outer cylindrical mold radius, mm
t	time, s or h
$T(r,t)$	local temperature, °C
T_c	centerpoint temperature, °C
T_∞	chamber temperature, °C
T_{max},T_{min}	maximum and minimum outdoor temperatures, °C
T_p	peak hydration temperature, °C
T_{pc}	PCM phase change temperature, °C
w/c	water to cement ratio
z	vertical coordinate, mm
z_b	bottom thickness of cylinder mold, mm

Greek symbols

α_j	thermal diffusivity of material “j”, m^2/s
ΔT_{pc}	PCM phase change temperature window, °C
ϕ_j	volume fraction of material “j” in composite
ρ_j	density of material “j”, kg/m^3

Subscripts

c	refers to core material (PCM)
$c+s$	refers to core–shell microcapsule
eff	refers to effective properties
exp	refers to experimental
f	refers to final
i	refers to initial
l	refers to liquid phase
m	refers to matrix material (cement paste)
s	refers to solid phase or shell material melamine formaldehyde (MF)
PVC	refers to polyvinyl chloride

2. Background

2.1. Performance metrics of PCM-composite materials

Evola et al. [9] proposed two metrics to quantify the effectiveness of gypsum wallboards containing PCM for improving the thermal comfort of building occupants during summer months. They offered two other metrics to quantify how often and to what extent the PCM latent heat storage was utilized. First, the intensity of thermal discomfort for overheating ITD$_{over}$ (in °C h) was defined as the time integral, over the room occupancy period, of the difference between the operative room temperature and the upper limit of thermal comfort temperature range. Second, the frequency of thermal comfort FTC was defined as the percentage of time, within the room occupancy period, during which the operative room temperature fell within the thermal comfort temperature range. Third, the frequency of activation FA was defined as the percentage of time, over an entire day or a given occupancy period, during which the PCM was experiencing phase change. Finally, the PCM energy storage efficiency η_{PCM} was defined as the ratio of the thermal energy stored by the PCM, over one day, to the PCM latent heat of fusion. In order to maximize the thermal comfort within the room, ITD should be minimized and FTC should be maximized. Additionally, FA and η_{PCM} should both be maximized in order to take full advantage of the PCM.

Castell and Farid [10] tested the methodology proposed by Evola et al. [9] using experimental measurements of the air temperature within enclosures made of concrete, brick, or timber walls containing PCM and located in Spain or New Zealand. They proposed two modifications to the metrics proposed by Evola et al. [9]: (i) ITD could include periods when the indoor temperature fell below the thermal comfort temperature range ITD$_{under}$, such as at night time so that ITD = ITD$_{over}$ + ITD$_{under}$ and (ii) FTC could be evaluated over the entire day rather than only during the occupancy period. With these modifications, Castell and Farid [10] evaluated the thermal comfort of the enclosures over three occupancy profiles: (i) between 9:00 am and 5:00 pm, (ii) between 6:00 pm and 8:00 am, and (iii) over the entire day. For all types of enclosures considered, ITD decreased as PCM was added to the wall and also depended strongly on the occupancy profile. In general, the FTC increased as PCM was added to the wall. Lastly, the FA provided contradictory and misleading indication of PCM performance. Castell and Farid [10] concluded that the ITD was the most relevant indicator suggested by Evola et al. [9] and that it should be evaluated during periods both when the indoor temperature exceeded (ITD$_{over}$) and when it fell below (ITD$_{under}$) the thermal comfort temperature range.

Overall, these metrics were useful to assess the thermal comfort within large-scale PCM-building envelopes subjected to realistic operating conditions. However, characterization using these metrics is costly both in terms of time and materials. In fact, they cannot be readily applied to a simple experimental setup to assess the thermal performance of novel PCM-composite materials. As such, there is a need for metrics to compare the attractiveness of different PCM-composite materials using straightforward experimental tests on relatively small samples. Such performance metrics should be sensitive to relevant design parameters such as the volume fractions and thermal properties of constituent materials, the phase change properties of the PCM, and the sample dimensions.

2.2. Numerical modeling of phase change in three-component composites

Recently, we showed that transient heat transfer through three-component composite materials consisting of ordered monodisperse PCM microcapsules and of either monodisperse or polydisperse PCM microcapsules randomly distributed in a continuous matrix can be accurately described by simulating a homogeneous material with some effective thermal conductivity and heat capacity [5,11]. The effective thermal conductivity k_{eff} of the three-component composites was predicted by the Felske model [12]. On the other hand, their effective volumetric heat capacity $(\rho c_p)_{eff}(T)$ was estimated based on simple thermodynamic arguments [5]. The effective thermal conductivity and effective volumetric heat capacity depended only on the constituent phase properties and on their volume fractions and were independent of the microcapsule spatial arrangement and polydispersity, as established numerically [5,11].

Two of the most common methods of simulating phase change