Effect of microstructure on melting in metal-foam/paraffin composite phase change materials

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ABSTRACT

The performance of phase change materials (PCM) as energy storage units are often limited by their low thermal conductivities that constrain the rates of melting or solidification. Highly porous metal foam composite PCMs are increasingly being used to abate this limitation and enable greater control over the thermal and phase change characteristics of the system. In the present study, a pore-scale computational analysis is carried out to characterize the performance of an n-eicosane-aluminium-foam composite PCM with a porosity of 0.94, over varying microstructural properties including strut, pore and cell sizes, and specific surface area. The simulations are carried out using OpenFOAM by employing the enthalpy-porosity formulation for modeling phase change during melting. The foam geometries are generated computationally using tools developed by the authors, published recently (Abishek et al., 2017, Ref. [1]). The statistics of the pore-scale structures of the virtual foam geometries and the numerical methodology employed for the modeling were validated against theoretical and empirical data from the literature. The simulations reveal that the presence of metal foam significantly enhances the melting rate as compared to pure PCM. It is also found that the melting rates are strongly correlated to the specific surface of the foam – highlighting a vital parameter that can be used to optimize the performance of the composite PCM for a given application. An empirical relationship correlating the dimensionless melt fraction with the Fourier number, Stefan number and dimensionless specific surface area is also presented for the range of parameters considered in this study.

1. Introduction

Phase change materials (PCM) such as paraffin or salt hydrates are widely used for thermal energy storage and temperature control in several applications including renewable power, heat recovery, HVAC, health care and electronics. PCMs have also found widespread uptake in the building and construction industry, in order to provide low cost thermal management of buildings [2]. Melting and solidification are the most common physical phase change processes which are essential to be understood and controlled in order to optimize such products for specific applications. PCMs are advantageous due to their favorable properties including high energy density, chemical stability and availability over wide temperature ranges [3]. However, the low thermal conductivity of most commercially used PCMs restricts their use in applications which require high rates of melting or solidification (or high heat transfer rates) [4]. Many early-to-market products in the building and construction industry consisted of a PCM in a matrix with poorly conducting materials such as cellulose or calcium carbonate [3]. This was because many PCMs were designed to also function as structural or cosmetic cladding. However PCM-composites using a highly conductive substrate material appear much more promising for the entire spectrum of applications. Experimental works combining a PCM with a high thermal conductivity substrate have proven promising [5], thereby spawning a significant research effort in this field. PCM-filled highly porous metal foams aid in abating the limitations in pure PCMs by significantly increasing the effective thermal conductivities of the composites for a fractional increase in the size of the energy storage unit. Similar to other phase change phenomena in a porous medium, it is a serious challenge to experimentally observe or measure the interstitial or micro-scale properties, which have a pivotal role in gaining a complete understanding of the melting/solidification and associated pore-scale convective processes. Specific surface area of the porous medium

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Nomenclature

A_f	specific surface area of foam, 1/m
A_i	specific interfacial area, 1/m
c_p	specific heat capacity, J/kg-K
d	strut diameter, m
Fo	Fourier number ($k_f t / \rho_f c_{p,f} L_z^2$), –
h	enthalpy, J/kg
k	thermal conductivity, W/m-K
K	specific kinetic energy, m^2/s^2
$L_{x,y,z}$	size of the geometry, m
p	pressure, Pa
$S_{m,e}$	momentum or energy sources, Pa/m or Pa/s
Ste	Stefan number ($c_{p,l}[T_h - T_m]/L$), –
t	time, s
T	temperature, K
u	velocity, m/s
$\tilde{x}, \tilde{y}$	local position and diameter of strut, m
x, y, z	length along x/y/z-axes, m

Symbols

α	volume fraction, –
ϵ	porosity, –
ψ_p	polydispersity of foam, –
λ	dimensionless temperature ($[T - T_m]/[T_h - T_m]$)
μ	dynamic viscosity, Pa-s
ρ	density, kg/m^3

Subscripts

c	cold (or bottom) wall
f	foam
h	hot (or top) wall
l	liquid paraffin
m	melting point
s	solid paraffin

is, for instance, one such parameter which significantly determines the phase exchange rate and varies markedly between different microstructures for any given porosity.

Open cell metal foams are gaining significant interest for use as PCM substrates due their high (substrate) thermal conductivities and the ability to produce them with high porosities. Such structures are relatively recent in development, and production methods (and hence costs) are still being optimized. Besides macroscopic properties such as the porosity, the pore-scale morphology of a typical open cell foam can be characterized by the pore and cell sizes, shapes of the nodes, shape and length of connecting 'struts' (Plateau edge) [6] which are either cylindrical or tri-lobed in shape [7], and in some cases, spatial isotropy. Several recent studies [3,5,8] have focused on understanding and enhancing the performance of composite PCMs through investigations into the influence of material (copper, aluminium, carbon) and macroscopic properties (porosity and isotropy) [3,9] of the foams, or characterizing foams based on their effective thermal conductivities [10]. However, it is well known that such metal foams can be manufactured with a multitude of the outlined microstructural properties for any given porosity. Thorough knowledge of the influence of these microstructural properties on the melting/ solidification process is necessary for efficient design optimization.

Computational analysis involving foam/porous substrates in PCMs have predominantly been either with approximated homogeneous media models [3,11] that often do not adequately encapsulate the microstructural properties, or with geometries extracted from micro-CT scans [12] of real media, which limit possibilities for any parametric optimization studies. One reason for such approaches being adopted can be the complexity in the virtual generation of scalable realistic foam geometries for analysis. Recent studies have also considered simulations using idealized three dimensional foams derived from structures such as the voids in a lattice of spheres [13,14] with arrangements representing body- or face-centered structures [15], or regular Tetrakaidecahedrons [9,16,17]. However, the pore-structure of real foams are far from such simplified geometries which provide less accurate estimates of the pore-scale properties such as specific surface area, and void/ strut shapes. In a recent work, Abishek et al. [1] provided a computational methodology for the generation of realistic foams with customizable micro-scale properties – a technique that is used to produce the substrate geometries for this study. In contrast, homogeneous porous media approaches typically use macroscopic

properties of the foam to characterize its performance, and employ either thermal equilibrium [3,11,8] non-equilibrium [8,18] based models for the interaction between the solid foam and paraffin. While such simplified modeling techniques are preferable for reduced design lead times, a critical parameter that couples the energy exchange between the foam and the paraffin (solid or liquid) in such an approach is the energy source term (crudely a function of specific surface area and foam-paraffin heat transfer coefficient), which is largely modeled empirically. The development of more comprehensive correlations involving the pore-scale properties of the porous media is essential for fully reliable computational design of such composite energy storage systems.

In the present study, a spectrum of virtual metal foams are systematically generated using open-source tools [1] in Gmesh, Blender, with similar porosities, polydispersity and strut shapes but with varying strut and pore sizes (and hence, specific surface area). Fully resolved (pore-scale) computational analysis is carried out to study the isolated effect of the microstructure on the melting characteristics of the composite PCM. All simulations for the conjugate heat transfer problem employ the enthalpy-porosity formulation for modeling melting, and are carried out on high performance computing infrastructure using OpenFOAM.

2. Geometry and computational domain

The foam geometries were generated computationally according to a validated procedure reported in an earlier study [1], and subsequently meshed using the snappyHexMesh tool within Open-FOAM. In contrast to Abishek et al. [1], both, the internal (foam) and external (paraffin) meshes were retained as separate regions in the simulations for the conjugate thermal analysis. Representative geometry of the foam and computational mesh generated for this study are shown in Fig. 1(a) and (b); only surface mesh is shown for clarity. In this study, the axial variation in the diameter of a strut between two junctions is defined according to Jang et al. [6] as follows:

$$-0.5 < \tilde{x}/l_e < 0.5: \quad \tilde{y}/d = 36(\tilde{x}/l_e)^4 + (\tilde{x}/l_e)^2 + 1 \quad (1)$$

which was an empirical relationship developed for aluminium foams. In Eq. (1), d is the diameter at the centre ($\tilde{x}/l_e = 0$) of the strut, $\tilde{y}$ is the local diameter of the strut, $\tilde{x}$ is the position along the strut ($l_e/2 \leqslant \tilde{x} \leqslant l_e/2$) and l_e is the length of the strut. Another