Contents lists available at ScienceDirect



International Journal of Heat and Mass Transfer

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

Heat transfer performance and melting dynamic of a phase change material subjected to thermocapillary effects



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ARTICLE INFO

Article history: Received 12 September 2016 Received in revised form 26 January 2017 Accepted 8 February 2017

Keywords: Marangoni Phase Change Material Microgravity Energy storage Melting

ABSTRACT

We carry out extensive numerical simulations on the melting of the *Phase Change Material* n-octadecane subjected to thermocapillary driving at a free surface on geometries with the form of circular sections of radius in order of centimeters. Simulations employ Stefan numbers Ste = 0.22 and Ste = 0.67. We compare the heat transfer performance with melting induced only by conduction and find a reduction of melting times by thermocapillarity up to a factor five for semicircular geometries. As a consequence, we propose the use of this mechanism in applications of thermoregulation in microgravity that require fast charge and discharge cycles. We show how a longer free surface enhances the effect of thermocapillarity on the heat transfer performance due to a greater contact area of solid PCM with regions of melted PCM dominated by thermocapillary flows. The length of the free surface has more impact on the heat transfer performance than the contact area between PCM and heat source in the geometries studied in this work. Besides, we observe as well how greater thermal gradients for higher Stefan number augment the importance of thermocapillary effects on the heat transfer performance.

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1. Introduction

The high latent heat involved in the solid/liquid phase change is the key feature that allows Phase Change Materials (PCM) to store or release a large amount of thermal energy during melting or solidification, barely changing the temperature. Chemical composition allows to classify them in organic such as paraffins, inorganic such as salt hydrates, and eutectic mixtures [34,33]. Many technological applications take advantage of this stability on temperature changes and thermal storage capacity to use these materials in electronic cooling, air conditioning in buildings, waste heat recovery, to compensate the time offset between energy production and consumption in solar power plants, or combining with construction materials to increase the thermal energy storage capacity of construction elements in light structures [3,24,32,46].

In addition to ground applications, the usual cycles of operation of devices onboard spacecrafts suit well with the heat storage and discharge cycles of PCMs. Thus thermal control using PCMs in microgravity has been widely used in space systems for low and high temperature applications to avoid temperature peaks coming from electronic devices, power electrical components, control bat-

* Corresponding author. E-mail address: santiago.madruga@upm.es (S. Madruga). tery temperature in lunar and Mars rovers, or even to refrigerate food and biological waste samples in manned spacecrafts [28]. Furthermore, PCMs involve technology with high potential in many proposed future missions that require very tight and stable temperature (± 1 °C), deep cryogenic temperatures, high flux acquisition (> 100 W/cm²) and minimization of mass and power use [16].

Nowadays, hundredths of natural and synthetic PCMs are known at a broad range of operating temperatures. However, a major issue in thermal regulation with these materials is their low conductivity, specially in paraffins at room temperatures. This leads to very long times during the heat storage and discharge phases and reduces their usability and performance on heat control. The natural trend for lower conductivity with higher latent heat exacerbates this problem [43,10].

On ground applications, the main choice to reduce the problem of low conductivity is to promote convective motions within the liquid phase of the PCM. Convective motions driven by gradients of density induced by differences of temperature can enhance the heat transfer rate about an order of magnitude with respect to conductive heat transfer [11,26,42]. However, this strategy is not applicable in microgravity. Another approach to accelerate the heat transfer is to place a large area of PCM in contact with high conductivity materials such as metallic fins or metallic foams [2,25,15]. Whereas this solution is applicable as well under microgravity con-

Nomenclature				
PCM ρ σ T α f_1	Phase Change Material density specific heat surface tension temperature volume expansion coefficient liquid fraction	t Dimensior Ra Pr Ma Ste	time nless numbers Rayleigh number Prandtl number Marangoni number Stefan number	
$ \begin{array}{l} \Gamma \\ \mu \\ \lambda \\ \gamma \\ \mathbf{L} \\ \mathbf{u} = (u, w) \end{array} $	Darcy coefficient dynamic viscosity thermal conductivity surface tension with respect to the temperature latent heat	Subscripts l, s h		

ditions, it increases the mass and size of the devices and convective driving is reduced or even suppressed.

Prompted by the above considerations, a mechanism to enhance the heat transfer on PCMs in microgravity, without increasing mass and volume, is to benefit from the Marangoni flow induced by thermal gradients of surface tension. The study of the influence of thermocapillarity on PCM melting is the main goal of this work. This requires selecting a PCM with a phase change temperature complying with design limits, high latent heat and the best possible thermal conductivity in liquid and solid phases. As a case of interest, we aim at studying the melting dynamic of noctadecane, which exhibits a solid/liquid phase change within the temperature range of spacecraft payloads, and belongs to the PCM group of paraffins widely used due to their stability and no undercooling.

Whereas melting of a solid in the presence of thermocapillary effects has been subjected to intense scrutiny on crystal growth or laser processing of materials [37], the focus on PCMs for terrestrial applications has diverted attention from PCM heat transfer dynamics under microgravity conditions and few works haven been published [19,20,23,41,45]. In addition, a large number of experiments in simple and complex geometries have been dedicated to tracking the advance of the solid/liquid interface under microgravity conditions have not been carried out. It is worth mentioning that the interplay between Marangoni flow induced by thermal gradients and phase change in PCMs under microgravity has only been specifically studied by Giangi et al. [19] to the best of our knowledge.

Along with the type of PCM, the geometry of the enclosure is a very influential factor in the dynamic and heat transfer properties of PCMs. Most of the studies have focused in regular geometries, such as square, rectangular [17,18,7] or with circular symmetry [9,27,42,22]. However, modern software facilitates the analysis of the dynamics of PCMs for non-symmetric or irregular geometries, closer to many engineering applications in thermoregulating systems in power plants, waste energy recovery, etc. [13]. The loss of spatial symmetries, such as rotational, has been studied in the melting between two eccentric cylinders with shifted centers between inner and outer cylinders, where it has been shown that the progressive shift leads to an increased melting rate [12]. Trapezoidal geometries produce a higher heat transfer rate compared to a square geometry of the same area in nano-enhanced materials [36].

We use in this work two bi-dimensional geometries in the form of circular sections with a conductive curved boundary and adiabatic flat upper surface. These exhibit a broken mid-plane symmetry and are relevant in microgravity. This is because the differences in density between the liquid and solid phases generate empty spaces in the container. Although at microgravity the location of the void is not necessarily at the top of the container, and a distribution of small voids can be created we consider for simplicity the formation of a void on the top with our geometry. This generates unfilled spherical geometries which have been studied within the PCM literature under gravity [5,22,40]. The void breaks the midplane symmetry of the geometry and complicates the thermal boundary conditions because the upper free surface is open to the air and the curved part is in contact with the enclosure.

In Section 2 we present the governing equations of the PCM model, emphasizing the effect of the dependence of the surface tension with the temperature in the boundary conditions, and the geometries selected to study the melting process under thermocapillary effects. Section 3 explains the algorithms we follow to solve the equations and how our code is validated with experimental and numerical results available in the literature of PCMs and Marangoni convection. The results of our simulations are discussed in Section 4, where we present the melting dynamic when the phase change is combined with thermocapillarity. This section includes a comparative of the melting process for (i) conductive transport, (ii) thermocapillarity driven convection, (iii) natural convection and (iv) combined thermocapillary and natural convection. Finally, conclusions of our work are provided in Section 5.

2. Governing equations and geometry

We have chosen for our simulations the PCM n-octadecane. This is a typical viscous paraffin with Prandtl number Pr = 60.3 and latent heat usual as well in these type of materials $L = 243.5 \cdot 10^3$ J kg⁻¹. The thermophysical properties of the liquid and solid phases used in the simulations are listed in Table 1. We have employed two geometries with axial symmetry in this work

Table 1

Thermophysical properties of n-octadecane. Values for the solid and liquid states are listed for the cases distinguished in the equations of the PCM model used in this work.

$\rho (\text{kg m}^{-3})$ [21]	776
μ (N s m ⁻²) [21]	$3.6 \cdot 10^{-3}$
$c_{\rm s} c_{\rm l}~({\rm J~kg}^{-1}~{\rm K}^{-1})$ [4]	1934 2196
$\lambda_s \lambda_l (W m^{-1} K) [21]$	0.358 0.13
$\gamma (N m^{-1} K^{-1})$ [29]	$8.4\cdot 10^{-5}$
$T_{s} T_{l}(K)$ [21]	298.25 299.65
<i>L</i> (J kg ⁻¹) [21]	$243.5\cdot10^3$
α (K ⁻¹) [14]	$9.1 \cdot 10^{-4}$

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