

# Optimizing the thermocapillary-driven melting of phase change materials in microgravity

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## Abstract

Organic phase change materials (PCMs) are used for energy storage and thermal management in numerous applications, including space missions. Their low thermal conductivity, however, has discouraged wider use. Recent studies showed that incorporating a free surface can significantly enhance heat transfer via thermocapillary convection and improve performance. Analysis of PCM melting in rectangular domains revealed the detrimental influence of a final conduction-dominated stage, which limits performance. Improvements based on trapezoidal and triangular containers have already been assessed. Here, we propose a new triangle-like shape with a curved "hypotenuse" that can achieve an additional enhancement factor of 1.2 in short containers.

## 1. Introduction

Phase change materials (PCMs) are characterized by their capacity to store and release substantial amounts of energy during a (usually solid/liquid) phase transition. This process is characterized by the melting temperature  $T_M$  and the latent heat  $c_L$ , which typically dominates the energy transfer/storage balance. A suitable choice of PCM can substantially improve performance in a broad range of systems by increasing thermal inertia and reducing temperature deviations away from  $T_M$ . PCMs form a part of numerous active and passive thermal control and energy storage systems, with notable applications in food storage, net-zero energy buildings, space conditioning,<sup>32,49</sup> renewable energies,<sup>5,21</sup> electronics,<sup>3,18</sup> exhaust gas waste heat recovery<sup>38</sup> and space applications,<sup>6,9,19</sup> among many others.

There is a wide variety of PCMs available in the market. Inorganic PCMs, such as salt hydrates, offer high energy storage capacity and thermal conductivity. However, they can suffer from chemical incompatibility with certain materials and their properties often deteriorate during their operational life. Metals are another class of inorganic PCMs that possess good thermal properties but are generally expensive and scarce. Organic PCMs, like alkanes and fatty acids, are typically non-corrosive, with good thermal and chemical stability, but have the disadvantage of relatively low thermal conductivity, which results in prolonged melting and solidification cycles. Furthermore, they may experience significant volume expansion associated with the solid/liquid transition.

There have been several recent studies aimed at improving heat transport within organic PCMs to reduce their melting time. Various approaches can be followed,<sup>42</sup> such as the incorporation of more conductive materials in the form of spheres<sup>13</sup> and fins,<sup>2,33,53</sup> for example. This leads to improved performance but comes at the cost of increased system mass or reduced PCM volume (and thus, energy storage capacity), which is not ideal for space applications where weight is a critical factor. An alternative is the dispersion of small, thermally conductive particles throughout the PCM to create a nano-enhanced PCM (NePCM).<sup>22,26,46</sup> Metals and metal oxides are suitable candidates for these particles.<sup>4</sup>

The separate and combined effects of conductive fins and nanoparticles were investigated in various PCM geometries including cases of circular, elliptical, square, triangular and trapezoidal cross-section.<sup>20</sup> The analysis considered the melting and solidification processes in these geometries using the same PCM volume. The inclusion of fins resulted in a maximum improvement of 46% for solidification and 24% for melting. Nanoparticles provided a maximum improvement of 15% for solidification and 48% for melting, and it was seen that particle density had minimal effect. The geometry itself had a significant impact, with melting and solidification times varying by up to 57% and 38%,

## OPTIMIZING THERMOCAPILLARY-DRIVEN MELTING IN MICROGRAVITY

respectively. A recent review<sup>37</sup> also compared the effects of geometry, fins and nanoparticles as well as the orientation with respect to gravity.

To quantify the heat transfer intensity during PCM melting in the liquid phase, where natural convection occurs, Huang et al.<sup>23</sup> introduced the coordination (Co) factor. This metric, which is the dot product of the temperature gradient and the velocity field, provides insights into the melting process in the presence of convection. It can be used to study the enhancement of melting times by optimizing the geometry. A recent study<sup>24</sup> compared melting in an "optimized" container (with an elongated teardrop-like shape) with that in a rectangular container based on the Co-factor. The elongated shape resulted in a reduction of more than 20% in the melting time. Similarly, Mohaghegh et al.<sup>31</sup> proposed a new pear-shaped geometry for thermal energy storage and Dhaidan<sup>10</sup> studied a triangular cavity for different orientations.

The Co-factor was introduced as a measure of heat transport due to natural convection, a mechanism that can accelerate melting via the fluid motion driven by the temperature-dependence of liquid density,<sup>11</sup> or buoyancy. While natural convection helps mitigate the problem of low thermal conductivity on Earth, it has no effect in weightless environments where fluids may behave in a dramatically different way.<sup>36,45</sup> An alternative mechanism that functions in either case is thermocapillary (Marangoni) convection driven by the temperature-dependence of surface tension.<sup>35</sup> This approach, which requires a free surface, was initially proposed by Madruga and Mendoza,<sup>27,28</sup> who conducted a numerical investigation of thermocapillary-driven melting dynamics in PCMs. It is worth noting that the presence of a free surface also helps alleviate the stresses associated with the volume change between solid and liquid phases.

Ezquerro et al.<sup>14,15</sup> then conducted parabolic flight experiments to investigate the thermocapillary effect during the melting of n-octadecane in a cuboidal container. The results confirmed numerical predictions and revealed a melting rate approximately twice that of the purely conductive case, providing experimental evidence for thermocapillary convection as a PCM enhancement mechanism. Salgado Sánchez et al.<sup>43</sup> validated a numerical model using this experimental data and a subsequent numerical analysis provided a more detailed understanding of the dynamics of thermocapillary-driven melting for both small and large aspect ratio containers.<sup>40</sup> Oscillatory instabilities<sup>34,44,47</sup> within the liquid phase were observed and the critical Marangoni number was calculated. The enhancement of thermocapillary convection with respect to the diffusive case was significant with both small and large aspect ratios.<sup>39</sup> Additionally, the impact of heat exchange across the free surface was investigated to better predict the melting dynamics in real experiments.<sup>29,30</sup>

The numerical model was further extended to study a liquid bridge configuration, where the ratio of free surface to volume is larger,<sup>50,51</sup> and to include the combined effects of natural and thermocapillary convection.<sup>8,50</sup> These studies demonstrated that Marangoni convection can be advantageous as well in the presence of gravity. The behavior of different PCMs, including n-alkanes and gallium, were also compared.<sup>17</sup>

To further reduce the melting time and improve PCM performance, Borshchak Kachalov et al.<sup>7</sup> combined thermocapillary convection with the selection of an optimal trapezoidal container. By increasing the area where thermocapillary convection dominates and reducing the area where diffusion dominates, the melting rate was improved by a factor of up to 3 for the limiting case of a right triangle. The aim of the current work is to enhance the melting rate still further by deforming the hypotenuse of this right triangle into a curved shape that better accommodates the form of the solid/liquid front during thermocapillary-driven melting.

This manuscript is structured as follows. Section 2 describes the novel geometry of the PCM container, along with the mathematical and numerical model. Section 3 provides background information and motivation for the study. The results of the geometric optimization are presented in Section 4 and conclusions are given in Section 5.

## 2. Problem statement and formulation

We investigate the thermocapillary-driven melting of n-octadecane in microgravity when held in an open triangle-like container, as described in Sec. 2.1 and illustrated in Fig. 1. The phase transition occurs due to the application of distinct constant temperatures ( $T_H$  and  $T_C$ ) at the lateral boundaries of the PCM, while the associated temperature gradient along an open interface with air generates thermocapillary convection within the liquid phase.

Inspired by experimental<sup>14,15,36,43</sup> and numerical work<sup>7,39,40,50,51</sup> on heat and mass transport during PCM melting with thermocapillary flows in microgravity, we explore the optimization of the container shape as a means to enhance the overall PCM performance. This study departs from the right triangular geometry put forward by Borshchak Kachalov et al.<sup>7</sup> and introduces a novel triangle-like shape with a curved "hypotenuse". The additional improvement with respect to right triangular geometry is analyzed.

More details of the mathematical and numerical models employed, including mesh convergence tests, can be found in the above references.

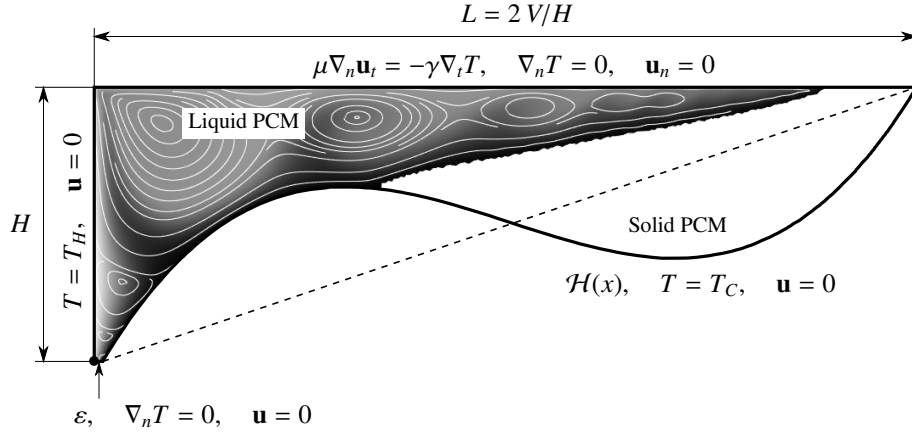


Figure 1: Sketch of the two-dimensional triangle-like container with a curve  $\mathcal{H}(x)$  in place of the hypotenuse. Boundary conditions are indicated.

## 2.1 Geometry of the container

The geometry of the container is defined as follows:

1. The PCM volume  $V$  is selected to match that of a rectangular container of length  $L_0 = 22.5$  mm and height  $H_0 = 10$  mm analyzed by Salgado Sánchez et al.<sup>39,40</sup> The value  $V = L_0 \times H_0 = 225 \text{ mm}^2$  is fixed in the remainder of this paper.
2. Following the work of Borshchak Kachalov et al.,<sup>7</sup> we define the reference right triangular geometry. This preserves  $V$ , so that the triangle length  $L$  and height  $H$  satisfy

$$L \times H = 2V. \quad (1)$$

3. The reference right triangle is modified by deforming its hypotenuse using a third-order polynomial function:

$$\mathcal{H}(x) = a + bx + cx^2 + dx^3, \quad (2)$$

where  $a$ ,  $b$ ,  $c$ , and  $d$  are constant, linear, quadratic, and cubic coefficients, respectively.

A sketch of the container is provided in Fig. 1.

The objective is to determine the optimal container shape that minimizes (maximizes) the melting time (rate). We formulate the optimization problem in terms of the coefficients of  $\mathcal{H}$ , subject to volume conservation:

$$V = \int_0^L \int_{\mathcal{H}}^H d\Omega, \quad (3)$$

and the boundary conditions:

$$\mathcal{H} = 0, H, \quad \text{at } x = 0, L. \quad (4)$$

These are complemented by the following inequality constraints:

$$0 \leq \mathcal{H} \leq H, \quad \forall x \in [0, L]; \quad (5)$$

and

$$d\mathcal{H}/dx \geq \Gamma^{-1}, \quad \text{at } x = 0, L, \quad (6)$$

which ensure that no topological changes occur in the shape of the container. Here,  $\Gamma = L/H$  is the aspect ratio of the container.

The constraints described by Eqs. (3) and (4) allow us to reduce the degrees of freedom of  $\mathcal{H}(x)$  to one. Thus, the cubic coefficient  $d$ , properly bounded by inequalities (5) and (6), can be used to parameterize the geometry of the new container.

## OPTIMIZING THERMOCAPILLARY-DRIVEN MELTING IN MICROGRAVITY

## 2.2 Governing equations

The phase change is modeled using the enthalpy-porosity formulation of the Navier-Stokes equations<sup>52</sup> describing the conservation of mass, momentum, and energy:

$$\nabla \cdot \mathbf{u} = 0, \quad (7a)$$

$$\rho \left( \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = -\nabla p + \nabla \cdot (\mu \nabla \mathbf{u}), \quad (7b)$$

$$\rho c_p \left( \frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) + \rho c_L \left( \frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla f \right) = \nabla \cdot (k \nabla T), \quad (7c)$$

where the velocity, pressure, temperature field and local liquid fraction are denoted by  $\mathbf{u}$ ,  $p$ ,  $T$  and  $f$ . The density, dynamic viscosity, heat capacity at constant pressure, thermal conductivity and latent heat appear as  $\rho$ ,  $\mu$ ,  $c_p$ ,  $k$  and  $c_L$ , respectively.

During melting, the quantity of absorbed heat is measured by the product  $\rho c_L f$ . The local liquid fraction  $f$  depends on  $T$  and is defined as a function that smoothly transitions from 0 to 1 (i.e., solid to liquid) over an interval  $\delta_T$  centered at the melting temperature  $T_M$ :

$$f(\widehat{T}) = \begin{cases} 0 & \widehat{T} < -\delta_T/2, \\ \frac{1}{2} + \frac{\widehat{T}}{\delta_T} + \frac{1}{2\pi} \sin\left(\frac{2\pi\widehat{T}}{\delta_T}\right) & |\widehat{T}| \leq \delta_T/2, \\ 1 & \widehat{T} > \delta_T/2. \end{cases} \quad (8)$$

where  $\widehat{T} = T - T_M$ . The transition interval characterized by  $\delta_T$  is known as the  *mushy region* .<sup>12</sup> We select a value of  $\delta_T = 1$  K in accord with previous work.<sup>17,43</sup>

This formulation considers the solid and liquid phases of the PCM, denoted by the subscripts ‘s’ and ‘l’, as a single continuous phase whose physical properties depend on  $T$  and can be written as

$$(\rho, \mu, c_p, k) = (\rho_s, \mu_s, c_{ps}, k_s)(1 - f) + (\rho_l, \mu_l, c_{pl}, k_l)f, \quad (9)$$

where  $\mu_s$  is a virtual solid viscosity that satisfies  $\mu_s \gg \mu_l$  so that  $\mathbf{u}$  vanishes in the solid phase. As in earlier studies,<sup>39,40,43</sup> we choose  $\mu_s = 10^3$  Pa s.

## 2.3 Boundary conditions

The thermocapillary effect is captured using a linear approximation for the dependence of surface tension  $\sigma$  on  $T$ :

$$\sigma = \sigma_0 - \gamma(T - T_M), \quad (10)$$

where  $\sigma_0$  and  $\gamma = |\partial\sigma/\partial T|$  refer to the surface tension and the thermocapillary coefficient at  $T_M$ , respectively.

At the free surface, which is assumed flat,<sup>16,43,48</sup> the momentum balance between viscous stress and surface tension is

$$\mu \nabla_n \mathbf{u}_t = -\gamma \nabla_t T, \quad (11)$$

where the subscripts ‘n’ and ‘t’ indicate the normal and tangential components. The remaining conditions along the free surface are

$$\nabla_n T = 0, \quad \mathbf{u}_n = 0. \quad (12)$$

At the left lateral wall (see Fig. 1), isothermal and no-slip boundary conditions are imposed for temperature and velocity:

$$T = T_H = T_M + \Delta T, \quad \mathbf{u} = 0. \quad (13)$$

A similar combination of isothermal and no-slip boundary conditions is applied along the curve  $\mathcal{H}(x)$ :

$$T = T_C = T_M, \quad \mathbf{u} = 0. \quad (14)$$

Note that it is the temperature difference  $T_H - T_C = \Delta T$  between these boundaries that drives the melting process. In this work, we select the constant value of  $\Delta T = 30$  K.

To avoid a double-valued boundary condition for  $T$  at the lower vertex of the right triangle or triangle-like domain, a short straight segment of length  $\varepsilon = L/100$  is introduced along the bottom boundary where adiabatic and no-slip conditions are enforced:

$$\nabla_n T = 0, \quad \mathbf{u} = 0. \quad (15)$$

This means that the geometric constraints imposed at  $x = 0$  in Section 2.1 are actually applied at  $x = \varepsilon$ .

Table 1: Physical properties of n-octadecane, reproduced from Salgado Sánchez et al.<sup>43</sup>

|                                       |                                         |
|---------------------------------------|-----------------------------------------|
| Melting temperature, $T_M$            | 28 °C                                   |
| Liquid density, $\rho_l$              | 780 kg/m <sup>3</sup>                   |
| Solid density, $\rho_s$               | 865 kg/m <sup>3</sup>                   |
| Latent heat, $c_L$                    | 243.5 kJ/kg                             |
| Liquid heat capacity, $c_{pl}$        | 2196 J/(kg K)                           |
| Solid heat capacity, $c_{ps}$         | 1934 J/(kg K)                           |
| Liquid thermal conductivity, $k_l$    | 0.148 W/(m K)                           |
| Solid thermal conductivity, $k_s$     | 0.358 W/(m K)                           |
| Dynamic viscosity, $\mu_l$            | $3.54 \times 10^{-3}$ Pa s              |
| Thermocapillary coefficient, $\gamma$ | $8.44 \times 10^{-5}$ N/(m K)           |
| Liquid thermal diffusivity, $\chi$    | $8.64 \times 10^{-8}$ m <sup>2</sup> /s |

## 2.4 Dimensionless parameters

Length, time and temperature are nondimensionalized using the characteristic values of  $L$ , the thermal diffusion timescale  $L^2/\chi$ , and  $\Delta T$ :

$$\begin{bmatrix} \mathbf{x} \\ t \\ T - T_M \end{bmatrix} \rightarrow \begin{bmatrix} \tilde{\mathbf{x}} L \\ \tau (L^2/\chi) \\ \Theta \Delta T \end{bmatrix}, \quad (16)$$

where  $\chi = k_l/(\rho_l c_{pl})$  is the liquid thermal diffusivity.

The physical properties of the PCM are scaled with the values for the liquid phase, which defines the solid/liquid ratios:

$$\tilde{\rho} = \frac{\rho_s}{\rho_l}, \quad \tilde{\mu} = \frac{\mu_s}{\mu_l}, \quad \tilde{k} = \frac{k_s}{k_l}, \quad \tilde{c}_p = \frac{c_{ps}}{c_{pl}}. \quad (17)$$

With these scalings, the dynamics of the system depend on the Marangoni and Stefan numbers,

$$\text{Ma} = \frac{\gamma L \Delta T}{\mu_l \chi}, \quad \text{Ste} = \frac{c_{pl} \Delta T}{c_L}, \quad (18)$$

which quantify the thermocapillary effect and the relative importance of specific and latent heats, respectively, on the Prandtl number,

$$\text{Pr} = \frac{\mu_l}{\rho_l \chi}, \quad (19)$$

which compares the diffusion of momentum and heat, on the aspect ratio,

$$\Gamma = \frac{L}{H}, \quad (20)$$

which characterizes the slenderness of the container, the (dimensionless) coefficients of  $\mathcal{H}(aL^{-1}, b, cL, dL^2)$ , and the ratios  $\tilde{\rho}$ ,  $\tilde{\mu}$ ,  $\tilde{k}$ ,  $\tilde{c}_p$  defined above.

The numerical analysis is performed for the PCM n-octadecane because of its relevance for recent and future microgravity research.<sup>15,35,39–41</sup> The pertinent physical properties are presented in Table 1, from which one obtains the following constant values:

$$\text{Pr} = 52.53, \quad \tilde{\rho} = 1.11, \quad \tilde{k} = 2.42, \quad \tilde{c}_p = 0.88. \quad (21)$$

The fixed value of  $\Delta T = 30$  K also determines  $\text{Ste} = 0.271$ .

The results below are obtained with containers of  $\Gamma = 3, 4.5$  and  $8$  that preserve  $V$ , meaning that  $L$  and  $H$  vary. The problem is restricted to two-dimensional dynamics, a simplification supported by the large  $\text{Pr}$  of n-octadecane.<sup>25,34,47</sup>

## OPTIMIZING THERMOCAPILLARY-DRIVEN MELTING IN MICROGRAVITY

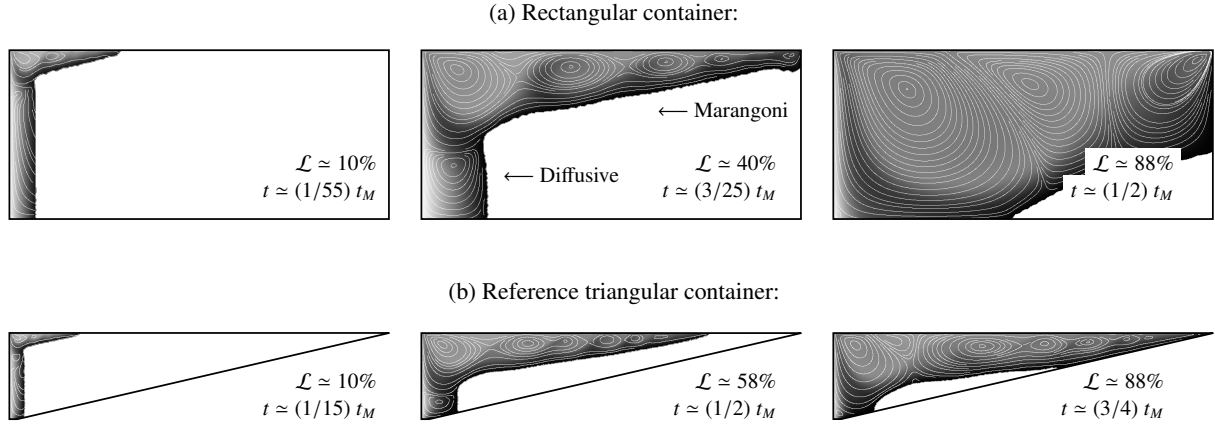


Figure 2: Snapshots of melting dynamics with  $\Delta T = 30$  K for (a) rectangular container with  $L_0 = 22.5$  mm,  $H_0 = 10$  mm ( $\Gamma_0 = 2.25$ )<sup>39,40</sup> and (b) triangular (reference) container with  $L = 45$  mm,  $H = 10$  mm ( $\Gamma = 4.5$ ).<sup>7</sup> The dimensionless temperature field is indicated by a grayscale map (black, white for  $\Theta = 0, 1$ ) with streamlines of the flow superimposed. The values of  $\mathcal{L}$  and  $t$  are shown in each snapshot.

## 2.5 Numerical model

We solve the formulation presented above using the finite-element-based software COMSOL Multiphysics.<sup>1</sup> An initial temperature  $T_0 = 25$  °C is assumed at which n-octadecane is a solid and, thus,  $\mathbf{u} = 0$ . Note that there is a mismatch between  $T_0$  and the imposed boundary conditions for  $T$ . This problem is handled by taking the first time step with the backward Euler method. The rest of the melting process is resolved using a Backward Differentiation Formulae scheme with a time step  $\Delta t = 0.01$  s that satisfies the Courant-Friedrichs-Lewy convergence condition.

The mesh used is the same as in the previous work of Borshchak Kachalov et al.<sup>7</sup> and consists of triangular elements with a maximum element size  $h = 1/3$  mm, with mesh refinement in the vicinity of the free surface where thermocapillary convection develops. Details of the mesh convergence tests and other relevant information can be found in previous publications.<sup>7,39,40,43</sup>

## 3. Background and motivation

As stated above, the aim is to optimize the geometry of the container to minimize (maximize) the melting time (rate) in microgravity by improving the convective transport associated with thermocapillary flows. For the sake of clarity and to permit direct comparison between containers of different shape, (melting) times are given in dimensional values.

Earlier related studies analyzed the melting process in rectangular geometry<sup>39,40</sup> over a wide range of  $Ma$  and  $\Gamma$ . As illustrated in Fig. 2(a), three general melting stages were distinguished according to the advancement of the solid/liquid front and the associated melting rate.<sup>8</sup> To quantify this rate and the overall heat transport, the (global) liquid fraction is defined as

$$\mathcal{L} = \frac{1}{V} \int_V (T > T_M) d\Omega, \quad (22)$$

which measures the volume of liquid PCM with respect to the total volume  $V$ . Each snapshot of Fig. 2 has labels indicating the value of  $\mathcal{L}$  (in percent) and of the time  $t$  relative to the full melting time, which is  $t_M = 3200$  s in (a) and  $t_M = 1069$  s in (b).

In the initial melting stage, the solid/liquid front is largely parallel to the hot vertical wall, which reflects the dominance of conductive transport; see the first snapshot of Fig. 2(a). Despite the low conductivity of n-octadecane, there is a large effective thermal gradient. As the solid/liquid front moves inwards and melting progresses, thermocapillary convection develops and accelerates heat transport near the free surface, while the relative strength of conductive transport decreases. This description applies to the second melting stage where two regions, characterized by the dominance of convective or conductive transport, can be identified. The second snapshot of Fig. 2(a) shows how thermocapillary convection prevails close to the free surface, along the entire container, while approximately vertical isotherms can be observed in a region near the bottom wall, as in the initial conduction-dominated stage.

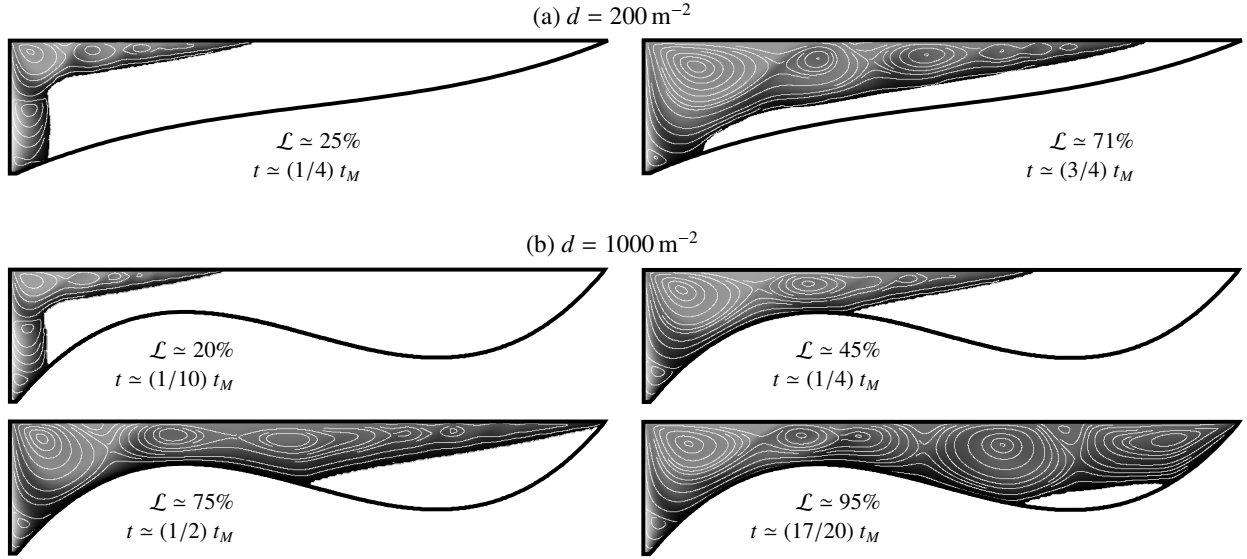


Figure 3: Snapshots of the melting process for  $\Gamma = 4.5$  and different  $\mathcal{H}(x)$ : (a)  $d = 200 \text{ m}^{-2}$  ( $\mathcal{G} \approx 1.2$ ) and (b)  $d = 1000 \text{ m}^{-2}$  ( $\mathcal{G} \approx 0.6$ ).

The third melting stage begins at some point after the solid/liquid front reaches the cold wall and the influence of convective flow diminishes. The melting rate decreases significantly as heat transfer again relies predominantly on conduction. As demonstrated in the third snapshot of Fig. 2(a), it takes approximately  $(1/2) t_M$  to melt 88% of the PCM, which corresponds to an average melting rate of  $\Delta\mathcal{L}/\Delta t \approx 0.055 \text{ \%}/\text{s}$ . During the second half of melting, this average rate is reduced to approximately  $0.008 \text{ \%}/\text{s}$ , which is an order of magnitude smaller. The maximum instantaneous melting rate occurs during the second melting stage when thermocapillary flow has fully developed near the free surface and dominates the melting process.

Despite this slow final stage, recent investigations have shown that thermocapillary flows can accelerate melting with respect to the purely diffusive case by a significant factor — up to 20 in rectangular containers.<sup>39</sup> It makes sense to pursue further reduction in  $t_M$  by diminishing the influence of the slow final stage on the overall melting process. The recent work of Borshchak Kachalov et al.<sup>7</sup> proposed using right triangular containers generated by inclining the cold wall; see Fig. 2(b). This reduces the relative quantity of PCM that must be melted in this final stage and shortens  $t_M$  for the same volume  $V$ . In short containers, the reduction in  $t_M$  is substantial — up to a factor of 3. This is illustrated in the third snapshot of Fig. 2(b), which shows that melting the last 12% of the PCM only requires  $(1/4) t_M$  (compared to  $(1/2) t_M$  for the rectangular case). The average melting rate during that final stage is approximately  $0.045 \text{ \%}/\text{s}$ , an order of magnitude larger than the average rate of  $0.008 \text{ \%}/\text{s}$  measured in the rectangular case.

It is reasonable to attribute the improvement in triangular geometry to the fact that the inclined lower boundary is a better match to the shape of the solid/liquid front during the melting process. Pursuing this idea further, one could speculate that  $t_M$  would be reduced even more if the cold wall perfectly matched the shape of the solid/liquid front as it reached the right boundary, allowing melting to finish just at that time, without the need for a final conduction-dominated stage. This observation provides the motivation behind the present study, which replaces the hypotenuse of the right triangle by a parameterized curve  $\mathcal{H}(x)$  that can more accurately match the shape of the advancing solid/liquid front.

#### 4. Results

The main results of the optimization are presented in this section. A constant PCM volume of  $V = 225 \text{ mm}^2$  is used in order to compare with the work of Borshchak Kachalov et al.<sup>7</sup> Note that the reference right triangular geometry corresponds to a null cubic coefficient ( $d = 0$ ). A parametric study is conducted by varying  $d$  within the interval of admissible values consistent with the geometrical constraints given in Sec. 2; this range depends on  $\Gamma$ .

Figure 3 illustrates the melting process for  $\Gamma = 4.5$ , comparing small and large values of  $d$ :  $200 \text{ m}^{-2}$  in (a) and  $1000 \text{ m}^{-2}$  in (b). The melting times for these cases are  $t_M = 918 \text{ s}$  and  $1871 \text{ s}$ , respectively. The first snapshot in (a) is quite similar to that of the right triangle in Fig. 2(b). Indeed, the melting process is generally similar to that of

## OPTIMIZING THERMOCAPILLARY-DRIVEN MELTING IN MICROGRAVITY

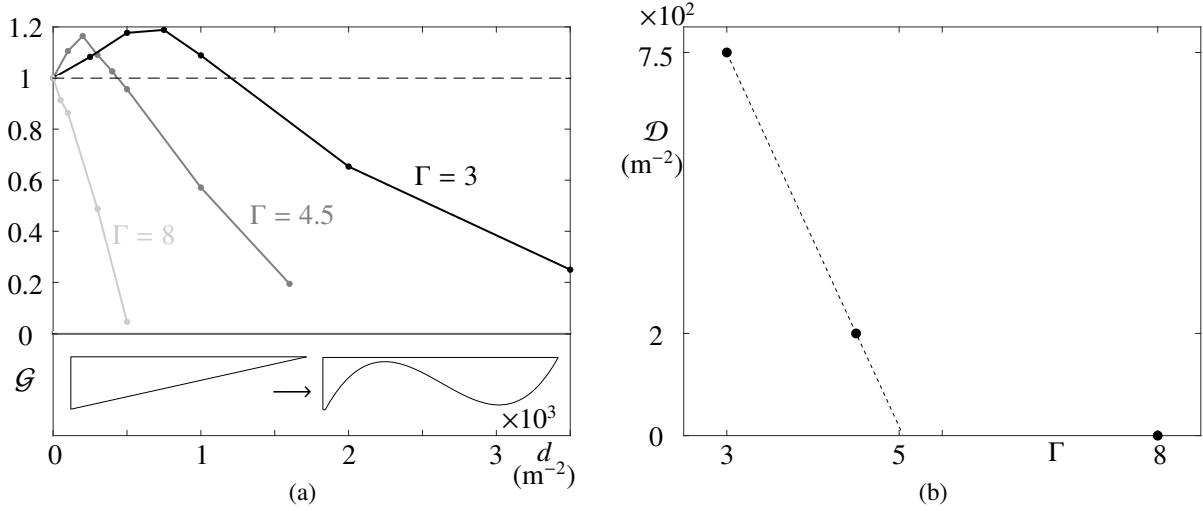


Figure 4: (a) Enhancement ratio  $\mathcal{G}$  as a function of  $d$  for  $\Gamma = 3, 4.5$  and  $8$ . The  $d = 0$  (reference) case corresponds to a right triangle; sketches at the bottom of the figure provide a visual indication of the geometry as  $d$  increases. (b) Optimal value  $\mathcal{D}$  that maximizes  $\mathcal{G}(d)$  as a function of  $\Gamma$ . The dashed line is a linear interpolation between the first two data points.

the triangular (reference) case. However, toward the end of the melting process, the shape of the solid/liquid front is more aligned with the curved boundary  $\mathcal{H}(x)$ . This can be quantified by comparing the values of  $\mathcal{L}$  at  $t \approx (3/4)t_M$ : approximately 88% for the triangular and 71% for the  $\mathcal{H}$ -curve containers. The last quarter of the melting process for the modified container has a faster average melting rate of roughly 0.126 %/s, approximately three times that of the right triangular container.

If the value of  $d$  is large, as in Fig. 3(b),  $\mathcal{H}(x)$  exhibits a local maximum and minimum with a corresponding constriction followed by an extended ("belly") region. The dynamics of the initial conduction-dominated stage are again similar. As melting progresses, however, the shape of  $\mathcal{H}(x)$  exerts a significant influence. The second stage, which is dominated by thermocapillary flow, finishes more rapidly as the solid/liquid front passes through the constriction and advances quickly along the free surface. Once it reaches the cold wall, as in the third snapshot of Fig. 3(b), the third melting stage begins and thermocapillary flow has a diminishing effect on the remaining process, which is increasingly controlled by conduction; this is reflected in the significant increase in  $t_M$ . It is clear that larger values of  $d$  increase the quantity of PCM that needs to be melted near the lower boundary during that final stage, reducing average melting rate and penalizing PCM performance. The fact that the curved hypotenuse can either improve or reduce performance suggests that there is an optimal value of  $d$ , which is analyzed below.

In order to quantify the improvement of the new triangle-like geometry, we compare melting times  $t_M$  and define the enhancement ratio

$$\mathcal{G} = \frac{t_{\text{ref}}}{t_M}, \quad (23)$$

measured with respect to the right triangular (reference) case, denoted by the subscript 'ref'. Figure 4(a) illustrates  $\mathcal{G}$  as a function of  $d$  for  $\Gamma = 3, 4.5, 8$ . For small  $\Gamma$  (3, 4.5) and  $d \sim \mathcal{O}(10^2) \text{m}^{-2}$ , melting is accelerated since  $\mathcal{H}(x)$  better matches the shape of the solid/liquid front. The values of  $t_M$  are reduced by a factor of up to 1.2. For  $\Gamma = 8$ , however, there is no observed enhancement with finite  $d$ . This large  $\Gamma$  limit has similar dynamics to those discussed by Borshchak Kachalov et al.,<sup>7</sup> where the melting in slender trapezoidal geometries was detrimentally affected by viscous effects, resulting in larger  $t_M$ .

Figure 4(b) shows the optimal value,  $\mathcal{D}$ , of the cubic coefficient  $d$  that maximizes  $\mathcal{G}$  for each  $\Gamma$  considered. A linear interpolation of the two data points with lowest  $\Gamma$  would suggest an upper limit of  $\Gamma \approx 5$  beyond which the new curved containers provide little or no enhancement. A simulation performed with  $d = 100 \text{m}^{-2}$  at  $\Gamma = 5$ , however, yielded an enhancement of  $\mathcal{G} = 1.1$ . Although the value of  $d$  was not optimized for this case, it does establish that melting can still be enhanced, which means the true upper limit, where  $d > 0$  is no longer beneficial, is higher (it has not been determined due to computational cost).

Although the enhancement ratio achieved with the present cubic-order "hypotenuse" optimization is relatively small, the combined effects of this and the use of a right triangle-like container instead of a rectangular one<sup>39,40</sup> can significantly improve the performance of the PCM. This overall enhancement can be visualized in Fig. 5, where the



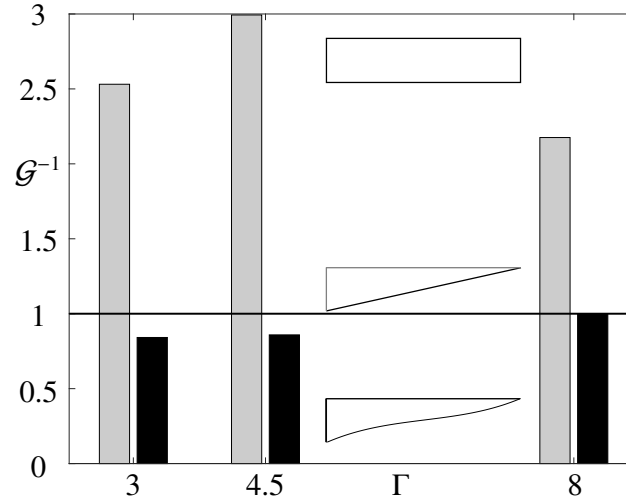


Figure 5: Inverse of the enhancement factor,  $\mathcal{G}^{-1}$  (i.e., the melting time scaled by the right triangle case), as a function of  $\Gamma$  for optimal  $\mathcal{H}$  (black bars). The associated ratios for rectangular containers of equal volume and height are included for reference (light gray bars, indicating slower melting). Sketches of the containers are included for visual reference.

inverse of  $\mathcal{G}$  (melting time relative to the right triangular case) is shown for the three aspect ratios considered here along with the same factor for rectangular containers of equal volume and height; note that the rectangular aspect ratio  $\Gamma_0 = L_0/H_0 = \Gamma/2$ .

The best reduction in melting time achieved with the new container proposed here is observed for  $\Gamma = 3$ , which corresponds to a gain factor of  $\mathcal{G} \approx 1.2$ . This value decreases with  $\Gamma$  and becomes 1 in the large aspect ratio limit where the right triangular geometry with  $d = 0$  is optimal. Note as well that, in this limit, the admissible values of  $d$  are very constrained.

Comparing rectangular and triangular geometries, the greatest reduction in  $t_M$  is observed for  $\Gamma = 4.5$ . This is also the aspect ratio where the maximum combined reduction of  $t_M$  is found; the total enhancement factor is  $3 \times 1.2 \approx 3.5$ . Moreover, for values of  $\Gamma > 8$ , it is expected that the optimal melting time is attained with rectangular geometry.<sup>7</sup>

## 5. Conclusions

Recent investigations of PCM melting in rectangular containers demonstrated that thermocapillary flows can significantly increase the melting rate.<sup>39,40</sup> However, the phase change process includes a final stage where heat absorption slows notably as the last portion of PCM in the lower, cooler part of the container melts and the thermocapillary flow, which is concentrated near the surface, is less effective. A subsequent study revealed that the use of triangular geometry can significantly limit the detrimental effects of this final stage, reducing the melting time  $t_M$  by a factor of up to 3 in short containers.<sup>7</sup>

We used this right triangular configuration as a starting point and reference case for the present optimization study, which relied on numerical simulations using an enthalpy-porosity formulation of the phase change and the Navier-Stokes equations. A class of triangle-like containers with a curved "hypotenuse" described by a third-order polynomial curve  $\mathcal{H}(x)$  was considered. The melting process was analyzed in these modified containers as a function of the cubic coefficient  $d$  for three values of the aspect ratio:  $\Gamma = 3, 4.5$  and 8.

The optimal configuration was found for small  $\Gamma$  and small values of  $d \sim \mathcal{O}(10^2) \text{ m}^{-2}$ . In this range, the curve  $\mathcal{H}$  closely approximates the shape of the solid/liquid front and leads to improved performance. An enhancement ratio of up to 1.2 is observed, highlighting the importance of the shape of the solid/liquid front relative to the shape of the container. However, for large  $\Gamma$ , a right triangular container remains the optimal choice within the scope of the present analysis.

## 6. Acknowledgments

This work was supported by the Ministerio de Ciencia e Innovación under Project No. PID2020-115086GB-C31, and by the Spanish User Support and Operations Centre (E-USOC), Center for Computational Simulation (CCS).

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## OPTIMIZING THERMOCAPILLARY-DRIVEN MELTING IN MICROGRAVITY

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