Melting of a Nano-enhanced Phase Change Material (NePCM) in partially-filled horizontal elliptical capsules with different aspect ratios

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\textbf{A R T I C L E   I N F O}

Keywords:
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\textbf{A B S T R A C T}

Melting of a Nano-enhanced Phase Change Material (NePCM), i.e., n-octadecane paraffin dispersed with Cu nanoparticles, in partially-filled horizontal elliptical capsules for a Rayleigh number of $1.744 \times 10^6$ is investigated numerically using the collocated finite volume method. To accommodate the increase in the NePCM volume during melting, a 15% air void within the capsule is considered. The simulations are carried out using the enthalpy-porosity technique and the Volume of Fluid (VOF) model. In this work, three volumetric concentrations ($\Phi = 0$, 1 and 3 vol\%) of nanoparticles and various aspect ratios (AR = 2.0, 1.0 and 0.5) of the capsule are adopted. The accuracy of the numerical procedure is validated through the comparison of two test cases with those available in the literature. The results are demonstrated in terms of the isotherms, streamlines, melting interface and the air-NePCM interface. It is concluded that for a given AR, the presence of nanoparticles enhances the melting rate and decreases the volume change of NePCM as compared to the pure PCM case. In addition, the highest and the lowest melting rates are associated with the AR = 2.0 and AR = 1.0, respectively.

1. Introduction

Undoubtedly, the earth’s resources are not infinite and therefore, they should be replaced by suitable alternatives. Solar energy is one of the alternatives being currently under development. As the way of exploiting the solar energy not new, it needs further development to become as efficient as fossil fuel processes. Currently, there are two approaches to convert solar radiation into electrical energy, namely, Concentrating Solar Power (CSP) plants and making use of Photo-Voltaic (PV) cells. The latter converts the solar radiation into electrical energy directly. In contrast, CSP plants convert the solar radiation into thermal energy and subsequently, use the thermal energy via a power generation cycle to generate electrical energy. The main drawback of solar energy as most of renewable energies is the irregularity. This drawback of solar energy can be overcome by increasing the efficient operation hours of the plant. One choice is to use Thermal Energy Storage (TES). Depending on the energy storage principle, the TES is generally divided into three categories: sensible heat, latent heat, and chemical storage. The sensible TES has high storage capacity, although it needs a large amount of mass and/or volume to store a certain amount of heat [1]. In the latent TES, the charging and discharging processes are nearly isothermal and its ratio of volume to energy is low [2]. Finally, in the chemical storage, heat is released/absorbed using a reversible chemical reaction.

One of the widely studied techniques of latent TES is the use of Phase Change Materials (PCMs) due to their exceptional features such as high storage capacity, chemical stability and low temperature reduction during heat recovery. The PCMs have found many industrial applications including solar energy [3–5], electronic devices [6–9], thermal management of PV cells [10,11] and thermal management in buildings [12–14]. Dhadan and Khodadadi [15] presented an elaborated review of the studies performed on melting of PCMs in enclosures with different configurations. Despite the outstanding features of PCMs stated above, they have the drawback of low conductivity, causing the heat transfer rate to decrease during the charging/discharging cycles. In order to overcome this drawback, numerous methods have been proposed. These include using heat pipes [16,17], micro encapsulated PCMs [18,19], inserting metal foams [20], finned tubes with different configurations [21,22], multiple PCMs [23,24] and dispersion of particles with high conductivity in PCMs [25,26]. Nano-enhanced PCM (NePCM) was introduced by Khodadadi and Hosseinizadeh [27]. They numerically investigated the solidification of water-Cu nanofluid in a square cavity heated differentially. It was found that the presence of nanoparticles in the PCM could increase the heat release and, hence, be more suitable for thermal storage applications than the pure PCM. Kibria et al. [28] reviewed
the studies conducted on the variations of thermo-physical properties of different PCMs due to dispersion of nanoparticles. Sehti et al. [29] investigated numerically the heat transfer enhancement via addition of Cu nanoparticles to the PCM in a square enclosure. They found that the melting time decreased with the nanoparticles volumetric concentration. Ebrahimi and Dadvand [30] studied numerically the melting of a NePCM in a square cavity due to two pairs of heat source–heat sink on the side walls. They showed that the maximum melting rate was obtained for the volumetric concentration of 2 vol%. Ghalamzani et al. [31] investigated the melting of different NePCMs inside a square enclosure by Finite Element Method (FEM). They utilized hybrid nanoparticles with different nanoparticles volume fractions and combinations. They found that the hybrid nanoparticles composed of Mg–MgO gave rise to the best fusion performance. Chamkha et al. [32] studied the melting of a NePCM in a square enclosure involving a hot cylinder inside using Galerkin FEM. Both the single and hybrid nanoparticles are tested. They found that the liquid fraction and liquid-solid interface are strongly influenced by the thermal conductivity and the volume fraction of nanoparticles. Dadvand et al. [33] simulated melting of a NePCM due to a heated plate inside a square enclosure. They investigated the effects of different nanoparticles concentrations and different positions of the plate and concluded that the lowest melting time was corresponding to 5 vol% nanoparticles concentration and the bottom position of the plate. Recently, Dhaidian [34] presented an elaborated review on the numerical, experimental and analytical investigations studied the melting of NePCM inside enclosures having different configurations.

Melting of PCMs in elliptical cylinders is of great importance due to its application in latent heat TES systems, casting and cooling of electronic devices. Melting in horizontal elliptical cylinders is categorized into constrained or unconstrained. In constrained melting, there exists no direct contact melting adjacent to the enclosure wall. However, in unconstrained melting, the solid phase can move up or down depending on its density with respect to density of the liquid phase. Knowing that the aspect ratio is a key factor in controlling the melting heat transfer in elliptical enclosures, there have been many analytical, numerical and experimental studies to optimize the horizontal elliptical tubes that might be used as thermal storage units. Alawadhi [35] studied the solidification of water in an elliptical enclosure utilizing the FEM along with the apparent heat capacity method. The effects of ellipse inclination, initial fluid temperature and aspect ratio on the solidification process were examined. It was concluded that total solidification time decreased as the ellipse aspect ratio was increased. Chen et al. [36] analytically studied the unconstrained melting of a PCM in an elliptical horizontal tube. It was concluded that the prolate tubes give rise to a higher melting rate as compared to the oblate and circular ones due to the influence of gravity in the direction of the tube’s vertical large diameter. Fomin and Wilchinsky [37] mathematically evaluated the effects of the aspect ratio of the capsule on the melting rate. They found that the prolate capsules lead to higher melting rates than the oblate ones. Also, Fomin et al. [38] indicated that the prolate ellipse gives rise to a higher melting rate as compared to the oblate one due to fact that the molten layer thickness of the prolate ellipse is thinner than that of the oblate enclosure, which exerts pressure on the solid portion. Hirose et al. [39] investigated both numerically and experimentally the natural convection heat transfer of water around horizontal elliptical containers combined with the constrained melting of ice inside the containers. Jourabian et al. [40] studied the melting of ice as a PCM saturated with and without a nickel-steel porous matrix in a horizontal elliptical tube. It was concluded that the melting rate increased as the aspect ratio of the circular tubes was changed. In addition, the melted PCM-induced natural convection could increase the melting rate merely in the tube with a circular cross-section.

All the above-mentioned studies have not considered the volume expansion of the PCM during the melting process. Assis et al. [41] analyzed numerically and experimentally the melting of PCM in an open spherical enclosure. They considered a combined PCM-air to account for the volume expansion of the PCM when melting in the enclosure. The air space was located in the upper part of the enclosure. They considered the natural convection in both the air and molten PCM and took into account the density difference between the liquid and solid PCM and thereby, the vertical motion of the solid PCM. For all the cases tested, the mass fraction changed almost linearly with time, showing a constant-rate heat transfer between the PCM and the surroundings. Assis et al. [42] also performed a combined numerical and experimental investigation on the solidification of PCM in various diameters of spherical shells. Hosseinizadeh et al. [43] numerically examined the unconstrained melting of NePCMs inside a spherical enclosure filled with RT27 dispersed with Cu nanoparticles. The computational domain they defined was identical to the one developed by Assis et al. [41]. The effects of nanoparticles volume fractions on the melting rate were evaluated. The results showed a melting rate augmentation of the NePCM compared to the pure PCM because of the higher thermal conductivity. Archibold et al. [44] utilized sodium nitrate as the PCM to extend the low temperature considered by Assis et al. [41] to higher temperatures. Hosseinizadeh et al. [45] performed numerical and experimental analyses on the unconstrained melting of n-octadecane as PCM inside a spherical container and examined the effects of Stefan number and container diameter on the melting process. The results showed that at the beginning of the melting process, the melting rate was high due mainly to the perfect contact between the solid PCM and the hot wall of the container, but it was decreased as part of the PCM was molten and located between the container wall and the solid PCM. Elmozoughi et al. [46] performed melting and solidification of high temperature PCMs considering a 20% void in a capsule and a sphere. They took into account the influences of volume expansion due to phase change and the thermal expansion on the melting and solidification processes. It was found that the presence of the air void caused the solidification and melting per unit mass of the PCM to be prolonged. Solomon et al. [47] investigated the effects of the initial position of an internal 20% air void inside encapsulated PCM capsule on the melting rate. They found that the highest heat transfer rate was achieved when the void was initially located at the center of the encapsulated PCM capsule. Li et al. [48] investigated numerically melting of paraffin blend RT27 inside a horizontal annulus with water as the heat transfer fluid. They considered 15% air void to account for density changes. They found that as the heating boundary temperature was increased, the melting time became shorter. In addition, the different eccentricity and diameters of the inner tube resulted in different melting rates. Ehms et al. [49] simulated the solidification process of a PCM in spheres with different diameters under wall temperatures below the phase change temperature. About 98.5% of the sphere volume was initially filled with liquid and the remaining part was filled with air. They found S-curve pattern of solidification. They also found that the total solidification time was dependent on both the temperature difference and the diameter of the sphere.

A literature review reveals that there is a scarce study on the melting of NePCM in horizontal elliptical capsules in the presence of air void. The thermal expansions of the liquid NePCM is taken into account. In order to examine the effects of thermal expansion of the NePCM on the heat transfer as well as to avoid high pressure in the capsule, an internal void space of 15% is considered. The results of the present work would help the engineers in the design of latent heat thermocline storage systems. It should be highlighted that the main novelty of the present work is the study of the effects of nanoparticles which change the fundamental properties of PCMs in a geometry with different aspect ratios that has potential industrial applications.

2. Physical model

The physical model is demonstrated in Fig. 1. The geometry is a horizontal elliptical capsule with vertical and horizontal semi-axes, a and b, so that the surface curve of the ellipse is described by the equation \(\left(\frac{x}{a}\right)^2 + \left(\frac{y}{b}\right)^2 = 1\). The ellipse Aspect Ratio (AR) is defined as \(AR = \frac{b}{a}\).
Three different aspect ratios are examined: AR = 0.5 (oblate capsule), AR = 1.0 (circular capsule) and AR = 2.0 (prolate or elongated capsule). In order to preserve the quantity of NePCM (n-octadecane paraffin + Cu nanoparticles), the cross-section area of the enclosure (\(a \times b\)) is kept fixed. Initially, the solid NePCM fills 85% of the enclosure and the remainder is filled with air (i.e., 15% air void fraction). The air void fraction is considered to accommodate any increase in the volume of NePCM during the phase change, due to the difference in density between the solid and liquid NePCM. Three different nanoparticles volume fractions of \(\Phi = 0, 1\) vol\% and 3 vol\% are considered. Part of the capsule surface, which is adjacent to the NePCM is subject to constant heat flux of 250 [W m\(^{-2}\)] (\(Ra = 1.744 \times 10^6\)). The value of the heat flux is determined based on the melting temperature of the PCM employed. With this value, the melting process of the NePCM occurs slowly and smoothly and that the flow of the melted NePCM remains within the laminar flow regime. In contrast, part of the capsule wall adjacent to the air is thermally insulated to prevent the capsule from failure due to the rise in internal pressure [50]. In fact, heating the air void part would not affect the melting rate significantly due to the low thermal conductivity of air (see Elmozuzhi et al. [46] for more details), but it increases the pressure inside the capsule and leads to the problems due to the wall thermo-mechanical stresses. It is worth mentioning that almost all of the previous works have used a constant temperature boundary condition. In practice, the constant temperature boundary condition is not easy to enforce as it often requires a phase-change process such as evaporation, condensation, etc. In addition, the constant heat flux is more realistic and more practical than the constant temperature. Particularly, when the solar energy is used as the heat source, it would not impose a constant temperature boundary condition but rather a constant (or a piecewise constant) heat flux.

The thermo-physical properties of the PCM and nanoparticles employed in the present work are given in Table 1. The properties of the NePCM except the density are assumed constant. The variation of density with temperature in the buoyancy term of the momentum equation in y-direction is modeled by the Boussinesq approximation.

The initial temperature of the system is 295.65 K (i.e., the NePCM is 5.5 K sub-cooled). According to Assis et al. [41], the following density-temperature relation is used for air

\[
p_{air} = 1.2 \times 10^{-5} T^2 - 0.01134 T + 3.4978
\]

Although there is buoyancy force because of the difference in the density of the solid and liquid of the NePCM that can move the solid phase, however, following Elmozuzhi et al. [46], it is assumed that the solid phase will remain fixed without sinking (i.e., constrained melting). Had we considered the motion of the solid NePCM, we would have had to use its dynamic equation. In practice, sinking of the solid NePCM can be avoided by adhering it to a rake of thermocouples that may also serve as sensors for measuring the instantaneous temperature of the liquid and solid NePCM.

The liquid NePCM is assumed to be Newtonian and incompressible and its flow is considered unsteady. As stated by Xuan and Roetzel [51], when the nanoparticles diameter is about 100 nm (80 nm in this study), they can be fluidized. In addition, the nanofluid is supposed to behave as a continuous medium in thermodynamic equilibrium and no velocity slip occurs between the PCM and nanoparticles in this range. Based on these assumptions, in the present study, the NePCM is reasonably treated as a single phase, i.e., the PCM-nanoparticles mixture is considered homogenous with effective properties.

### Table 1

<table>
<thead>
<tr>
<th>Property</th>
<th>NePCM, n-octadecane paraffin [76]</th>
<th>Solid Cu nanoparticles</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting temperature (solidus-liquidus) [K]</td>
<td>300.15–302.15</td>
<td>N/A</td>
</tr>
<tr>
<td>Density (solid-liquid) (\left[ \frac{\text{kg}}{\text{m}^3} \right])</td>
<td>865 / 770</td>
<td>8954</td>
</tr>
<tr>
<td>Specific heat (solid-liquid) (\left[ \frac{\text{J}}{\text{kg} \cdot \text{K}} \right])</td>
<td>1954 / 2196</td>
<td>383</td>
</tr>
<tr>
<td>Thermal conductivity (solid-liquid) (\left[ \frac{\text{W}}{\text{m} \cdot \text{K}} \right])</td>
<td>0.358 / 0.148</td>
<td>400</td>
</tr>
<tr>
<td>Viscosity (\left[ \frac{\text{Pa}}{\text{s}} \right])</td>
<td>0.00385</td>
<td>N/A</td>
</tr>
<tr>
<td>Latent heat (\left[ \frac{\text{J}}{\text{kg}} \right])</td>
<td>243500</td>
<td>N/A</td>
</tr>
<tr>
<td>Thermal expansion coefficient (\left[ \frac{1}{\text{K}} \right])</td>
<td>(9.1 \times 10^{-4})</td>
<td>(1.67 \times 10^{-5})</td>
</tr>
</tbody>
</table>

3. Mathematical formulation and numerical implementation

A finer unstructured mesh is used near the wall of the capsule and near the air-NePCM interface while a coarser mesh is employed in the other parts of the domain to decrease the computational cost. It must also be emphasized that due to the symmetry of the computational domain with respect to y-axis, only half of the domain is considered in the simulations. The liquid NePCM-air interface can be handled by the well-known Volume of Fluid (VOF) method introduced originally by Hirt and Nichols [52]. To allow for the NePCM expansion, the air is considered as a compressible gas. In addition, the enthalpy-porosity technique [53] is employed to model the phase change occurring in the NePCM during the melting process and track the motion of the solid-liquid interface. The system is an air-NePCM multiphase problem that involves a moving interface without inter-penetration of phases. In any specified cell, the volume fraction of each phase is applied to the governing equations based on the parameter \(\alpha_q\) which is defined as,

\[
\alpha_q = \frac{\text{Volume of phase } q \text{ in a cell}}{\text{Volume of the cell}}
\]

For a cell which is empty of the \(q\)th fluid \(\alpha_q = 0\) and a value of \(\alpha_q = 1\) implies that the cell is full of the \(q\)th fluid. For a cell containing the interface between the two fluids (here air and NePCM), \(0 < \alpha_q < 1\). The kinetic and thermodynamic properties of the cell are calculated as volume-fraction-average of the corresponding properties of each phase. For example, density is calculated as,

\[
\rho = \alpha_{gp} \rho_p + (1 - \alpha_{gp}) \rho_{air}
\]
According to the aforementioned assumptions, the continuity, momentum and energy equations can be written respectively as,

\[
\frac{\partial \alpha}{\partial t} + u_i \frac{\partial \alpha}{\partial x_i} = 0
\]  
(4)

\[
\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \mu \left( \frac{\partial^2 u_i}{\partial x_j \partial x_j} \right) + \rho g_i + S_i
\]  
(5)

\[
\frac{\partial}{\partial t} (\rho h) + \frac{\partial}{\partial x_j} (\rho u_i h) = \frac{\partial}{\partial x_j} \left( \kappa \frac{\partial T}{\partial x_j} \right)
\]  
(6)

In Eq. (5), \( S_i = -A(f)\phi_i \) denotes the momentum source vector \([49,50]\). Here, \( A(f) = \frac{C(1-f^2)}{f^3} \) is the porosity function \([54,55]\), \( C \) is the mushy zone constant and \( f \) is a small computational constant. According to Shmueli et al. \([56]\), both the liquid fraction and solid shape evolution depend highly on \( C \), and an optimum value of \( C \) exists for each problem. Therefore, suitable determination of \( C \) is necessary. In the present study, we consider a value of \( 10^8 \) [kg m\(^{-3}\)s\(^{-1}\)] for \( C \). In addition, \( \epsilon \) is a small value (0.0001) introduced to prevent the numerical singularity at \( f = 0 \) \([53]\). The porosity function \( A(f) \) is used to reduce the velocity to zero at a solid region and converts the momentum equation to the Kozenny-Carman equation being applicable for laminar flow in porous media. The total enthality \( h \) is defined as,

\[
h = h_{Sat} + \int_{T_{ref}}^T C_p \, dT + f \int L
\]  
(7)

where \( f \) denotes the liquid fraction, which is a function of temperature,

\[
\begin{align*}
\begin{bmatrix}
 f = 0 & \text{Solid} & T < T_{Solidus} \\
f = 1 & \text{Liquid} & T > T_{Liquids} \\
f = \frac{T-T_{Solidus}}{T_{Liquids}-T_{Solidus}} & \text{Mushy Zone} & T_{Solidus} < T < T_{Liquids}
\end{bmatrix}
\end{align*}
\]  
(8)

The density, specific heat at constant pressure, thermal expansion coefficient and the latent heat of NePCM are respectively evaluated as follows \([57]\):

\[
\rho_{np} = \phi \rho_h + (1 - \phi) \rho_p
\]  
(9)

\[
(\rho C_p)_{np} = \phi (\rho C_p)_h + (1 - \phi) (\rho C_p)_p
\]  
(10)

\[
(\rho \beta)_{np} = \phi (\rho \beta)_h + (1 - \phi) (\rho \beta)_p
\]  
(11)

\[
(\rho L)_{np} = (1 - \phi) (\rho L)_h
\]  
(12)

The following effective viscosity for the NePCM introduced by Brinkman \([58]\) is used,

\[
\mu_{np} = \frac{\mu_h}{(1 - \phi)^{1/2}}
\]  
(13)

The thermal conductivity of NePCM is considered to be composed of two parts, namely, the static part (Maxwell’s model) and the dynamic part (Brownian motion). Therefore, the following correlation proposed by Vajjha et al. \([59]\) is employed in the present work,

\[
k_{np} = \frac{k_h + 2k_p - 2(k_h - k_p)\phi}{k_h + 2k_p + (k_h - k_p)\phi} k_p + f B \gamma \phi \rho_p C_p \sqrt{\frac{\kappa T}{\rho_a d_a}} F(T, \phi)
\]  
(14)

where,

\[
\gamma = 8.4407(100\phi)^{-1.07304}
\]  
(15)

\[
F(T, \phi) = \left( 28.217 \times 10^{-3} \phi + 3.917 \times 10^{-3} \right) \frac{T}{T_{ref}} + \left( -30.669 \times 10^{-3} \phi - 3.91123 \times 10^{-3} \right)
\]  
(16)

Here, \( B \) is the Brownian motion constant taking the value of 5 \times 10\(^5\), \( \kappa \) denotes the Boltzmann constant (1.381 \times 10\(^{-23}\) [J K\(^{-1}\)], \( d_{np} \) stands for the nanoparticle diameter (80 \times 10\(^{-9}\) [m]) and \( T_{ref} \) refers to the reference temperature (298.15 [K]).

The governing equations are solved using the collocated Finite Volume Method (FVM) \([60]\) by the commercial software Ansys Fluent 14.0. The existence of the nanoparticles is taken into account by calculating the effective physical properties using Eqs. (9)–(14) for the NePCM. Therefore, the NePCM is treated as a single phase solid (before melting) and/or a single phase liquid (after melting). Then, the governing equations are solved for this new single phase material having effective properties. The power-law differencing scheme is utilized to discretize the advection terms in the governing equations, while the PISO algorithm is employed for velocity-pressure coupling. The convergence criteria are based on the residuals chosen less than 1 \times 10\(^{-4}\), 1 \times 10\(^{-5}\) and 1 \times 10\(^{-7}\) for the continuity, momentum and energy equations, respectively.

4. Validation

The accuracy of the present numerical procedure is verified through the comparison of two test cases with the data available in literature.

4.1. Melting of a PCM (Gallium) in a rectangular enclosure

The accuracy of the present work is substantiated via the comparison of the results associated with the melting of a pure metal (Gallium) in a rectangular cavity to the experimental results of Gau and Viskanta \([61]\) and the numerical results of \([27,54,62]\) as shown in Fig. 2. The height/width ratio of the cavity is equal to 0.714 and \( Ra = 6 \times 10^5 \), \( Pr = 0.0216 \). The top and bottom walls are thermally insulated, while the right and left walls are kept respectively at cold and hot constant temperatures. It is clearly evident that the results of the present study are in good agreement with those available in the literature. The difference between the current results and those of Gau and Viskanta \([61]\) may be due to the method of melting interface evaluation utilized in \([61]\). Notably, this problem is also simulated numerically by Kashani et al. \([63]\), Tiari et al. \([64]\) and Arici et al. \([65]\).
paraffin as PCM for a circular capsule of 30 mm in diameter. The instantaneous liquid fraction for different grid sizes is investigated. A grid size with 7958 cells is adequately fine to guarantee a grid independent solution. In addition, the influence of time step on the melting process for this unsteady problem is investigated. The simulations are carried out until St.Fo = 0.586 is reached. The time step of 0.05 s is chosen for all the simulations carried out in the present work. A computer unit with two 2.2 GHz Intel® processors each with five cores and 10GB RAM is used for simulations. Using this system, full melting with 7958 grid cells and time step of 0.05 s requires about 8 days of CPU time.

6. Results and discussion

In the following, the melting of n-octadecane dispersed with Cu nanoparticles in a partially-filled horizontal elliptical capsule is investigated. Three different aspect ratios of 2.0, 1.0 and 0.5 each with three different nanoparticles volume fractions (i.e., $\Phi = 0$ vol%, 1 vol% and 3 vol%) and, hence, a total number of nine different test cases are examined. Initially, 85% of the capsule volume is filled with solid NePCM and the rest of its volume (15%) is filled with air. The results are presented and discussed below.

6.1. Evolution of streamlines, isotherms, solid NePCM and air-NePCM interface for $\Phi = 1$ vol %

The evolution of the calculated isotherms [K], streamlines, solid and liquid NePCM and air-NePCM interface at different dimensionless times (St.Fo numbers) of 0.064, 0.117, 0.181, 0.266, 0.346 and 0.650 for the three cases distinguished by aspect ratios of 2.0, 1.0 and 0.5 are respectively depicted in Figs. 5–7. These times are chosen so that the important events happening during the melting process can be captured. All the results given in this section are associated with the melting of n-octadecane dispersed with 1 vol% of Cu nanoparticles. The isotherms are presented in the right side of the capsule, while the left side depicts simultaneously the streamlines associated with molten NePCM, the net solid (grey region) and mushy NePCM and the air-NePCM interface. It may be noted that those parts of the left half of the capsule which are left blank and do not involve any streamlines, are mushy region. In addition, the minimum temperature of the NePCM in contours legends is fixed at 300.15 K during the melting process.

At early stages of the melting process (0.0 < St.Fo < 0.1), the buoyancy forces are unable to overcome the resistance due to the viscous forces. Hence, the conduction heat transfer is dominated and the supplied heat flux is used merely to compensate for the initial subcooling. The isotherms of the NePCM near the capsule shell form a nearly-perfect concentric ring, and are parallel to the shell curvature (see Figs. 5–7 at St.Fo = 0.064). Immediately after, a net energy imbalance at the solid-liquid interface is established that leads to melting (see Webb [66] for more details). As the melting process progresses, the temperature of the molten NePCM increases rapidly, while that of the solid NePCM remains almost constant. Since the heat transfer process within the NePCM is controlled by diffusion, melting is inceptioned in the peripheral portion of the NePCM. As a result, a thin layer of molten NePCM is produced in close proximity to the shell of the capsule. At early stages of the melting process, the melting rate is high. This is because the thin liquid layer enforces a lower thermal resistance to the heat flux that is transferred to the solid NePCM by conduction. Then, the liquid layer will become thicker, the ensuing thermal resistance increases and consequently, the conduction heat transfer is degraded (second stage is started). Meanwhile, a buoyancy-driven convection develops that is able to compensate the reduction of conduction and hence, the melt fraction is less steep than the previous periods. This is consistent with the findings of Dhaidan et al. [67] who investigated experimentally and numerically the constrained melting of a NePCM (Octadecane + CuO) in a horizontal capsule subjected to a constant heat flux.

4.2. Melting of a PCM (RT27 paraffin wax) exposed to air in a spherical shell

In the second test case, we simulate unconstrained melting of RT27 (Rubitherm GmbH) as the PCM in a spherical shell with the diameter of 40 mm. The wall-temperature is kept constant at $6 \degree C$ (St = 0.06), which is above the mean melting temperature of the PCM. Initially, 85% of the shell volume is filled with the solid PCM and the remainder 15 % of its volume is filled with air. The results are represented at different times and compared with those reported by Assis et al. [41], Figs. 3 and 4 show the liquid fraction versus time diagram and melting fronts, respectively. It can be observed that the solid fraction sinks in the molten PCM (see Fig. 4), which is consistent with the findings in [41]. In addition, a reasonable agreement is observed between the current liquid fraction and that reported in [41] (see Fig. 3).

5. Grid and time step independence study

The grid and time step independence tests are conducted using four different non-uniform unstructured grids respectively with 3840, 5268, 7958 (chosen) and 11, 000 cells and four different time steps of 0.01, 0.025, 0.05 (chosen) and 0.075 s. The results are associated with $Ra = 6.9775 \times 10^6$ and 3 vol% of Cu nanoparticles in n-octadecane.
As time advances (second stage, St.Fo > 0.1), the natural convection will become more significant and the role of conduction will gradually diminish. During the second stage, the applied heat flux is used for phase change without a considerable temperature rise (isothermal process) and this feature is the key advantage of utilizing NePCM in thermal storage where a large amount of energy is absorbed and/or released at about constant temperature. In comparison with the previous stage, the second stage extends for a longer period. As the molten portion is more extended, the density of the liquid NePCM adjacent to the capsule shell decreases due to the higher temperature gradient, it moves upward due to the lower density, reaches the top stagnation point, and covers the top region of the solid NePCM. In the meantime, the molten NePCM flows downward alongside the liquid-solid interface, where it loses heat that contributes directly to melting of the solid NePCM. The denser cold liquid NePCM ultimately reaches the lower part of the capsule and absorbs heat from the lower shell heat flux. This process is repeated resulting in expansion of high- and low-temperature zones in the upper and lower parts of the capsule, respectively. As a result, an unsteady, clockwise recirculating flow (clockwise vortex) is formed between the capsule shell and the liquid-solid interface (see Figs. 5–7 at St.Fo > 0.1). This progresses the melting in this region by enhancement of the heating rate towards the solid NePCM. The dimension of the vortex will increase as the NePCM melts further. In addition, according to Fig. 8, a clockwise vortex (left hand side) is generated in the air region (for AR = 1.0 at...
Fig. 6. Streamlines and liquid fraction contours and solid NePCM (grey region) with air-NePCM interface (left Side) and isotherms (K) (right Side) at St.Fo = (a) 0.064, (b) 0.117, (c) 0.181, (d) 0.266, (e) 0.346 and (f) 0.650 respectively for AR = 1.0 attained at Φ = 1 vol%.

St.Fo = 0.117) that slightly increases the heat transfer to the NePCM. This, however, results in negligibly small increase in the pressure and temperature of the air and hence in the thermo-mechanical stresses of the capsule shell due to the adiabatic condition of part of the shell that is in direct contact with air.

The (cyclic) motion of the liquid NePCM is repeated in conjunction with deformed melt front and increase of the volume occupied by the molten liquid (as shown in the left side of Figs. 5–7). Thus, the air is compressed, which increases the pressure inside the capsule. The motion of the air-NePCM interface is tracked by drawing a horizontal line on the left side of all the presented plots of Figs. 5–7. The positions of the solid-liquid and air-NePCM interfaces are distinguished by the density of each phase. Table 2 shows the change of NePCM volume inside the

<table>
<thead>
<tr>
<th>Situation</th>
<th>ΔV (%)</th>
</tr>
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<tbody>
<tr>
<td>AR = 0.5, Φ = 0 vol%</td>
<td>2.121</td>
</tr>
<tr>
<td>AR = 0.5, Φ = 1 vol%</td>
<td>1.744</td>
</tr>
<tr>
<td>AR = 0.5, Φ = 3 vol%</td>
<td>1.508</td>
</tr>
<tr>
<td>AR = 1.0, Φ = 0 vol%</td>
<td>1.666</td>
</tr>
<tr>
<td>AR = 1.0, Φ = 1 vol%</td>
<td>1.433</td>
</tr>
<tr>
<td>AR = 1.0, Φ = 3 vol%</td>
<td>1.066</td>
</tr>
<tr>
<td>AR = 2.0, Φ = 0 vol%</td>
<td>1.225</td>
</tr>
<tr>
<td>AR = 2.0, Φ = 1 vol%</td>
<td>1.084</td>
</tr>
<tr>
<td>AR = 2.0, Φ = 3 vol%</td>
<td>0.777</td>
</tr>
</tbody>
</table>
Fig. 7. Streamlines and liquid fraction contours and solid NePCM (grey region) with air-NePCM interface (left Side) and isotherms (K) (right Side) at St.Fo = (a) 0.064, (b) 0.117, (c) 0.181, (d) 0.266, (e) 0.346 and (f) 0.650 respectively for AR = 0.5 attained at Φ = 1 vol%.

Fig. 8. eneral vortex in the air region depicted on liquid fraction contour (for AR = 1.0 at St.Fo = 0.117).

capsule for all the nine cases. The dimensionless volume change $\Delta V^*$ is defined as,

$$\Delta V^* = \frac{(H_2 - H_1)}{2a} \times 100$$

where $H_1$ and $H_2$ are the heights of the NePCM inside the capsule before melting and after the melting is completed, respectively and $2a$ is the vertical diameter of the capsule. It is observed from this table that the amount of change in the volume of NePCM decreases with both the nanoparticles volume fraction (this can also be justified from Eqs. (9) and (11)) and aspect ratio.

The patterns of natural convection result in an asymmetric melting rate in the capsule so that the melting rate in the upper portion of the capsule is high compared to its counterpart in the lower section (see Figs. 6 and 7). Indeed, the molten NePCM is divided into two zones: (i) the thermally-stable zone located in the upper section of the molten NePCM. In this zone the hot liquid is located above the cold liquid and involves the main, larger and clockwise vortex as stated in the above paragraphs; (ii) the thermally-unstable zone, appearing only in AR = 1.0 & 0.5 (Figs. 6 and 7), is located in the lower section of the molten NePCM. In this zone the cold liquid is located above the hot liquid and consequently a secondary counterclockwise vortex is generated. This, in turn, would expedite the melting process due to the penetration of multi-cellular roll structures and forms a wavy liquid-solid interface in this zone (see Figs. 6 and 7 at St.Fo > 0.117). The vortices formed at the upper and lower sections of the molten zone are of dif-
different directions. They preserve their direction during the melting process and normally do not combine. These observations of the chaotic convection are consistent with those reported by Khodadadi and Zhang [68] and Tan et al. [69] for constrained melting in spherical enclosures and with those reported in horizontal cylindrical enclosures without air [70–72]. As time elapses, the size of the solid NePCM becomes smaller and smaller, the vortices formed at the upper section of the molten zone expand and gradually additional vortices will develop. These growing vortices move downwards and combine with the newly formed vortices to produce larger and stronger vortices.

The contours depicted in Fig. 5 show that for AR = 2.0, the thermally unstable zone with counterclockwise vortices and wavy liquid-solid interface is not formed in the lower section of the molten zone. This may be attributed to the dominance of conduction rather than convection heat transfer in this case as compared to the other two capsules studied in the present work. This result is quite similar to the findings reported by Jourabian et al. [73] associated with the constrained melting in circular cross-section capsules at low Ra numbers of $10^4$ and $10^5$. The number of unstable flow vortices formed in the bottom section of the capsule depends on the geometry of the cross-section of the capsule so that the number of vortices associated with AR = 2.0, AR = 1.0 and AR = 0.5 are equal to zero, one and three, respectively (Rayleigh-Bénard instability [74]). Therefore, it is concluded that as the aspect ratio is decreased the tendency of the molten NePCM to induce unstable vortices becomes more appreciable.

One of important features of the melting of NePCMs in enclosures is the shape of the solid-liquid interface. For example, the interface is circular for melting of NePCM in a circular cross-section capsule without air void, while it is mushroom-like when air void is involved (see Elmouzghi et al. [46]). A similar feature is observed in our work for AR = 1 (see Fig. 6 at St.Fo = 0.117). In the present work, the interface is a function of both the heat transfer rate (i.e., Ra number) and the air void (see also Solomon et al. [47] for more details) inside the capsule. The rate of heat transfer to the solid NePCM varies the shape and number of thermal plumes produced at the capsule’s bottom surface. Therefore, the interface is wavy for AR = 1.0 and 0.5 due to the presence of the thermal plumes and it is not wavy for AR = 2.0 since there are no thermal plumes.

The temperature and liquid fraction evolutions on air-NePCM interface ($\alpha_{\text{d}} = 0.5$) for a volume fraction of 1 vol% at different times are depicted in Figs. 9–11 are associated with AR = 2.0, 1.0 and 0.5, respectively. The diagrams are depicted for the left half-section of the enclosure where the vertical symmetry line is located at $x = 0$. These diagrams show that the temperature in the air-NePCM interface increases with AR. Therefore, the enclosure with a smaller AR is more desired from the viewpoint of design and critical temperature considerations.

The variations of temperature with time along the capsule surface from its bottom point ($\theta = 0$) to the air-NePCM interface ($\theta = 0.7\pi$) for the case with AR = 1.0 are depicted in Fig. 12. It is observed that at St.Fo = 0.064 the temperature increases continuously along the capsule surface due to the fact that the natural convection is dominated in the molten zone and the temperature in the upper section of the molten zone is higher than its lower section. This trend holds until St.Fo = 0.1. After this time, a sudden decrease in the temperature of the capsule surface slightly before $\theta = 0.1\pi$ takes place. This is mainly due to the unstable vortices and hence, thermal plumes formed at the bottom of the capsule (see Fig. 6). As time progresses, the minimum point of the temperature diagram is displaced towards the upper section of the capsule. In addition, the slope of the temperature diagram versus time increases because the hot liquid region is extended.

6.2. Nusselt number

Figs. 13–15 depict the variations of the average Nusselt (Nu) number with time for aspect ratios of 2.0, 1.0 and 0.5, respectively. Each figure involves three different nanoparticles volume fractions of 0, 1 and 3 vol%. The slope of the average Nu number diagram characterizes the intensity of the effect of natural convection. Indeed, the average Nu number comprises two parts: conduction and convection. In the beginning, the Nu number is very high due to the low thermal resistance owing to the thin layer of the molten NePCM. Once the first layer of the molten NePCM forms, the Nu number decreases at a rate proportional to $1/\sqrt{t}$ due to the thermal resistance of this layer. At this stage, the conduction heat transfer mechanism is dominated. The salient feature of this stage is that there observed a very steep reduction in the value of Nu number and that the Nu number diagrams for different nanoparticles volume fractions coincide. As the thickness of the molten NePCM layer increases and in the meantime the contribution of natural convection heat transfer becomes important, the reduction in the value of Nu number gradually diminishes until it reaches a constant value. In fact, in this transient region, the competition between the conduction and natural convection heat transfer mechanisms restricts the reduction in the Nu number. Again, the Nu number diagrams for different nanoparticles
volume fractions coincide. This would suggest that temperature difference is unable to accelerate the conduction heat transfer mode. After this stage, the average Nu number experiences a uniform reduction during the melting process, because the heat transfer rate decreases due to the mass reduction of the NePCM solid phase. At this stage, the average Nu number decreases as the nanoparticles volume fraction increases. This is attributed the fact that thermal conductivity of the NePCM increases with the nanoparticles volume fraction but at the same time the temperature gradient decreases (see Feng et al. [75] for more details). However, the conductivity increment is not as much of the decrease in the temperature gradient and hence, the local Nu number defined as $\text{Nu} = \frac{\alpha}{\beta^*} V T^*$, which $T^*$ is the dimensionless temperature, decreases [75].

6.3. Melting rate

The diagrams of the liquid fraction versus time for different aspect ratios are depicted in Figs. 16-18. The slope of each diagram represents the melting rate. It is observed that the melting rate is high at the initial stages of the melting process since the solid NePCM is (almost) in direct contact with the capsule’s hot wall where the molten NePCM layer is thin and the conduction plays an important role in melting. As time progresses, the melting rate will decrease gradually due to the thermal resistance of the thick liquid layer. It is observed that at early stages of the melting process ($0.0 < \text{St.Fo} \leq 0.1$) the liquid fraction versus the dimensionless time diagram is identical for all the three examined nanoparticles volume fractions because conduction is the dominant heat transfer mechanism. As time passes, the nanoparticles contribution becomes more effective and as the nanoparticles volume fraction increases, both the liquid fraction and the melting rate increase. This may be deduced from Eqs. (14) and (12) which show that an increase in the nanoparticles volume fraction leads to an increase in the conductivity and a decrease in the latent heat of the NePCM. This would imply that NePCM requires less energy per mass and hence, a shorter time for melting than that for a pure PCM. It is important to note that the variations of the liquid fraction with time are (almost) linear for all the three capsules because the
presence of air void in the capsules imposes no resistance against volume change of the molten NePCM. It shows a constant-rate heat transfer between the NePCM and the capsule shell.

It should be emphasized that the melting ends at different times for the different capsules. Table 3 shows the dimensionless time required to complete melting of solid NePCM for all the nine cases studied in the present work. Notably, St.Fo and St.Fo_0 denote the corresponding dimensionless times of full melting associated respectively with the pure PCM and NePCM. In order to elucidate the effects of nanoparticles on melting, the melting efficiency (η) showing the superiority of NePCM in melting over the pure PCM is defined as,

$$\eta = \frac{\text{St.Fo}_0 - \text{St.Fo}_p}{\text{St.Fo}_p} \times 100\%$$

(18)

It can be seen from Table 3 that among the three configurations studied here the melting time of pure PCM is highest and lowest for AR = 1.0 and AR = 2.0, respectively. In addition, for all the three configurations, the melting time decreases and hence the melting efficiency (η) increases with the volume fraction of nanoparticles. The increment in the melting efficiency (η) is more considerable for AR = 0.5 compared to the other two cases.

Thus far in the present study, it is shown that the melting performance of the capsules with AR ≠ 1 is higher than the capsule with AR = 1. This may be due to the fact that in the former a larger area of the capsule is exposed to heating. This finding is consistent with those of Chen et al. [36] and Fomin and Wilchinsky [37] associated with uncon-
strained melting and with the constrained melting reported by Jourabian et al. [40]. This reveals that the melting performance of elliptical capsules is better than the circular ones irrespective of whether air void is present or not. This is even the case for solidification in the elliptical enclosures studied by Alawadhi [35].

7. Conclusions

Melting of a NePCM in partially-filled horizontal elliptical capsules for Ra number of $1.744 \times 10^6$ is investigated numerically. The main results are summarized as below:

I. At early stages of the melting process ($0.0 < \text{St.Fo} \leq 0.1$), the heat transfer process within the NePCM is controlled by diffusion and the melting is incepted in the peripheral portion of the NePCM. As a result, a thin layer of molten NePCM is produced in close proximity to the capsule wall. As the molten portion increases, the liquid NePCM adjacent to the capsule wall rises upward due to its lower density and cover the top region of the solid NePCM. In the meantime, the molten NePCM flows downward along the solid–liquid NePCM interface. The denser cold liquid NePCM eventually reaches the lower section of the enclosure and absorbs thermal energy from the heat flux from the lower shell wall. As a result, an unsteady clockwise vortex is formed between the capsule surface and the liquid-solid NePCM interface.

II. It was found that the shape of the solid-liquid NePCM interface is a function of both the heat transfer rate (i.e., Ra number) and the air void inside the capsule. In addition, the amount of change in the volume of NePCM decreases with both the nanoparticles volume fraction and aspect ratio of the capsule.

III. The diagrams of the Nu number versus time show that once the first layer of the molten PCM forms, the Nu number decreases at a rate proportional to $1/\sqrt{\text{t}}$ due to the thermal resistance of this layer. Initially, there is a very steep reduction in the value of Nu number and the Nu number diagrams for different nanoparticles volume fractions coincide. Then, the reduction in the value of Nu number gradually diminishes until it reaches a constant value. Finally, the Nu number decreases as the nanoparticles volume fraction increases.

IV. At early stages of the melting process, the liquid fraction-time diagram is identical for all the three nanoparticles volume fractions examined because conduction is the dominant heat transfer mechanism. As time passes, the convection and hence, the nanoparticles contribution become more effective and both the liquid fraction and the melting rate enhance as the nanoparticles volume fraction increases.

V. Finally, it was shown that the melting performance of the capsules with $AR \neq 1$ is higher than the capsule with $AR = 1$.

This model can straightforwardly be extended to other cavity configurations, nanoparticles and PCMs. In addition, the model is applicable for a solidification process of NePCMs, which will be part of our future work.
Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>a, h</td>
<td>Vertical semi-axes of the capsule [m]</td>
</tr>
<tr>
<td>b, h</td>
<td>Horizontal semi-axes of the capsule [m]</td>
</tr>
<tr>
<td>f</td>
<td>Brownian motion constant</td>
</tr>
<tr>
<td>C</td>
<td>Mushy zone constant [kg m^-3 s^-1]</td>
</tr>
<tr>
<td>CP</td>
<td>Specific heat at constant pressure [J kg^-1 K^-1]</td>
</tr>
<tr>
<td>D</td>
<td>Diameter [m]</td>
</tr>
<tr>
<td>fL</td>
<td>Liquid fraction</td>
</tr>
<tr>
<td>FT</td>
<td>Fourier number</td>
</tr>
<tr>
<td>g</td>
<td>Gravitational acceleration [m s^-2]</td>
</tr>
<tr>
<td>n</td>
<td>Total enthalpy [J kg^-1]</td>
</tr>
<tr>
<td>H</td>
<td>Height of the NEPCM inside the capsule [m]</td>
</tr>
<tr>
<td>H'</td>
<td>Shell heat transfer coefficient [W m^-2 K^-1]</td>
</tr>
<tr>
<td>k</td>
<td>Thermal conductivity [W m^-1 K^-1]</td>
</tr>
<tr>
<td>L</td>
<td>Latent heat [J kg^-1]</td>
</tr>
<tr>
<td>Nu</td>
<td>Nusselt number</td>
</tr>
<tr>
<td>P</td>
<td>Pressure [Pa]</td>
</tr>
<tr>
<td>Pr</td>
<td>Prandtl number</td>
</tr>
<tr>
<td>q</td>
<td>Surface heat flux [W m^-2]</td>
</tr>
<tr>
<td>Ra</td>
<td>Rayleigh number</td>
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<tr>
<td>R</td>
<td>Equivalent radius of the ellipse</td>
</tr>
<tr>
<td>S</td>
<td>Source term</td>
</tr>
<tr>
<td>St</td>
<td>Stefan number</td>
</tr>
<tr>
<td>t</td>
<td>Time [s]</td>
</tr>
<tr>
<td>T</td>
<td>Temperature [K]</td>
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<tr>
<td>U</td>
<td>Velocity [m s^-1]</td>
</tr>
<tr>
<td>V</td>
<td>Volume [m^3]</td>
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<tr>
<td>x, y</td>
<td>Cartesian coordinates [m]</td>
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Greek symbols

<table>
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<th>Symbol</th>
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<tr>
<td>α, β</td>
<td>Thermal diffusivity [m^2 s^-1]</td>
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<td>Phase volume fraction</td>
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<td>β, γ</td>
<td>Thermal expansion coefficient [K^-1]</td>
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<tr>
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<td>Brownian motion parameter</td>
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<td>k</td>
<td>Boltzmann constant [J K^-1]</td>
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<tr>
<td>μ</td>
<td>Dynamic viscosity [Pa s]</td>
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<tr>
<td>ρ</td>
<td>Density [kg m^-3]</td>
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<tr>
<td>Φ</td>
<td>Nanoparticle volume fraction</td>
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<tr>
<td>ρ</td>
<td>Kinematic viscosity [m^2 s^-1]</td>
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<tr>
<td>ρ</td>
<td>Melting efficiency of nanoparticles</td>
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Subscripts

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<td>Direction index</td>
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<td>ini</td>
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<td>NEPCM</td>
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<td>Base PCM</td>
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<tr>
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<td>Reference</td>
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<tr>
<td>s, s'</td>
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<td>1, 2</td>
<td>Before and after melting</td>
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</table>

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References
