# Numerical simulations of energy storage with encapsulated phase change materials. Special emphasis on solid-liquid phase change CFD modelling.

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## 1. Introduction

Thermal energy storage systems are an essential feature to make a better use of various thermal energy facilities; e.g. low/medium temperature solar thermal systems (hour/s of storage), high temperature solar thermo-electrical generation plants (several hours of storage), ground source heat pumps (seasonal storage) or electrical heat pumps in buildings or districts. The aim is to reduce the mismatch between the energy supply and demand (e.g. where the energy source is the sun), or to optimize the use of the equipment (e.g. in HVAC applications).

Phase change materials (PCM) provide an effective way of accumulating thermal energy, due to their high capacity to store heat at a constant or near to constant temperature.

This paper deals with the numerical simulation of thermal energy storage systems with PCM. Numerical simulations are a powerful tool for predicting the thermal behaviour of thermal systems, as well as for optimizing their design.

In a previous work (Galione et al., 2011) the performance of a cylindrical container, filled with spheres containing paraffin wax (PCM) and water occupying the space left between the spheres was studied. Two different processes were analyzed: charging and discharging. In charging mode, hot water coming from the solar field passes through the container, delivering energy to the PCM spheres. In the discharging mode, cold water from supply comes through, extracting the energy previously stored in the PCM and leaving the tank at a higher temperature.

Transient one dimensional (1D) analysis was performed, where assumptions of 1D fluid flow and 1D heat transfer – in the flow and inside the spheres – were made. Furthermore, another model consisting of 1D transient analysis for the fluid flow coupled with a detailed CFD analysis for the PCM inside the capsules was developed (see fig. 1). Results showed that the introduction of the detailed computations did not modify substantially the overall system performance, although natural convection phenomenon was indeed observed, especially in the melting process. However, significant differences were observed between results obtained adopting constant or variable phase change temperature. Thus, there is an interest of being able to accurately simulate, within a CFD framework, the change of phase under a temperature range.

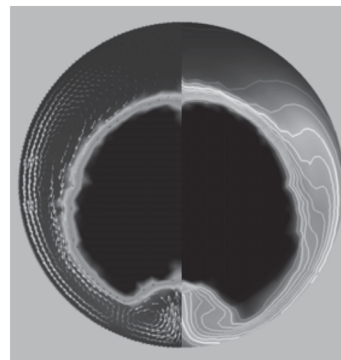In this work, the possibility of temperature variation during a



Fig. 1: Spherical capsule with PCM melting at a fixed phase change temperature (from Galione et al., 2011). Left half shows the enthalpy map and velocity vectors while right half shows the temperature map and contours.

melting/solidification process is introduced in our CFD model. Firstly, an extension of the classical and widely used formulation developed by Voller and Prakash (1987) to an explicit time scheme discretization is used. Secondly, a more refined formulation of the momentum equation – taken from porous media theory (Hsu and Cheng, 1990; Nield and Bejan, 2006) – is adopted.

Both formulations are compared by simulating a standard case study: the melting of Tin in a 2D square cavity (Wolff and Viskanta, 1987; Hannoun et al., 2003; Costa et al., 1991). These simulations have been run in a 2D in-house code which works with structured meshes. Presently, the inclusion of these formulations in an unstructured 3D parallel code called TermoFluids (Lehmkuhl et al., 2009) is being accomplished. The aim is to be able to obtain results similar to the observed in fig. 1, with PCMs changing phase at a temperature range.

## 2. Materials and method

When the PCM inside the spheres are changing phase, natural convection is produced due to the difference between solid and liquid densities and gravity action. To simulate this phenomenon, Navier-Stokes and energy equations are numerically solved. Some simplifying assumptions are made:

- Incompressible fluid.

- Boussinesq approximation (density is considered constant, except in the gravity forces term).

- Constant thermo-physical properties and equal between solid and liquid states.

Based on the above mentioned hypotheses and adopting the enthalpy-porosity model to account for the phase change phenomenon (Voller and Prakash, 1987; Brent et al., 1988), mass, momentum and energy equations can be written in the following form:

$$\nabla . \vec{u} = 0 \tag{Eq. 1}$$

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla . \left( \rho \vec{u} \vec{u}^* \right) = -\nabla p_d + \mu \nabla^2 \vec{u} - \rho \vec{g} \beta (T - T_0) - S\vec{u} \tag{Eq. 2}$$

$$\frac{\partial \rho h}{\partial t} + \nabla . \left( \rho \vec{u} C_{pl} (T - T_0) \right) = \nabla . \left( k \nabla T \right) \tag{Eq. 3}$$

where the enthalpy $h$ includes both sensible and latent components. The source term $-S\vec{u}$ is added in order to account for the presence of solid in the control volumes (nodes). The final form of coefficient $S$ depends on the approximation adopted for the behavior of the flow in the "mushy zone", i.e. where mixed solid and liquid states are present. However, in the case of constant phase change temperature, the solid-liquid interface should be of infinitesimal width (Brent et al., 1988) (although it cannot be thinner than the width of one control volume in our simulations); therefore, the formulation used for the source term does not follow any physical law, and it is just required to manage bringing the velocity to zero in mostly solid control volumes and to vanish if the volume contains pure liquid. In our previous work (Galione et al., 2011) we adopted an own formulation of S in order to have a smooth variation of the velocity from almost liquid to almost solid control volumes.

However, in this work we are intended to simulate phase change in a temperature range, i.e. the solid-liquid interface width will not be infinitesimal but a "mushy zone" will develop. Thus, the formulation adopted for the source term will have an effect on the flow configuration in this "mushy zone".

Voller and Prakash (1987) assumed that the "mushy zone" behaves like a porous medium and suggested the following formulation for coefficient $S$:

$$S = \frac{C(1-\varepsilon)^2}{(\varepsilon^3 + q)}$$

where $C$ depends on the morphology of the porous media, and is assumed to be constant. $q$ is just introduced to avoid division by zero and should be a very small value. A higher value of $C$ will produce a higher opposition to the flow.

This formulation has been widely adopted by many authors in the simulation of solid-liquid phase change (e.g. see Hannoun et al., 2003).

However, in the field of flow simulation in porous media, different formulations have been (and are being) developed for the momentum equation (Nield and Bejan, 2006). Here we will adopt the one proposed by Hsu and Cheng (1990), mentioned in Nield and Bejan (2006), obtained by using the Volume Averaging Theory (Whitaker, 1969).

Momentum equation for porous media (Hsu and Cheng, 1990) with Boussinesq approximation can be written as:

$$\rho\left[\frac{\partial \vec{u}}{\partial t} + \nabla\cdot\left(\frac{\vec{u}\vec{u}^*}{\varepsilon}\right)\right] = -\nabla(\varepsilon p_d) + \mu\nabla^2\vec{u} - \rho\varepsilon\vec{g}\beta(T-T_0) - \frac{\mu\varepsilon\vec{u}}{K} - \rho\frac{F\varepsilon|\vec{u}|\vec{u}}{K^{1/2}} \qquad \text{(Eq. 4)}$$

where $K = \dfrac{d_p^2\varepsilon^3}{a(1-\varepsilon)^2}$, $F = \dfrac{b}{\sqrt{a\varepsilon^3}}$, $a$=150 and $b$=1.75 are the Ergun constants and $d_p$ the pore diameter. It is important to indicate that the velocity appearing in the above equation corresponds to the seepage velocity (or Darcy velocity), i.e. the average fluid velocity over a representative volume that may contain both liquid and solid phases (Nield and Bejan, 2006).

Substituting the expressions of $K$ and $F$ in the above equation results in:

$$\rho\left[\frac{\partial \vec{u}}{\partial t} + \nabla\cdot\left(\frac{\vec{u}\vec{u}^*}{\varepsilon}\right)\right] = -\nabla(\varepsilon p_d) + \mu\nabla^2\vec{u} - \rho\varepsilon\vec{g}\beta(T-T_0) - \frac{\mu a(1-\varepsilon)^2\vec{u}}{d_p^2\varepsilon^2} - \rho\frac{b(1-\varepsilon)|\vec{u}|\vec{u}}{\varepsilon^2 d_p} \qquad \text{(Eq. 5)}$$

which has several differences with eq. 2. Apart from the addition of a new term (Forcheimer term) this last equation differs from eq. 5 since the convective term includes the factor $\varepsilon^{-1}$, the pressure gradient includes $\varepsilon$ and the Darcy term (fourth term of the right side of the equation) has $\varepsilon^2$ as a denominator instead of $\varepsilon^3$. Therefore, it is expected that the results obtained with this formulation will be different from the obtained with eq. 2.

As a first approximation, the Forcheimer term in eq. 5 has been dropped in order to simplify computations (it involves finding the modulus of the velocity, which can be time consuming). This approximation is also based on the fact that this term is negligible compared to the Darcy term at Reynolds numbers of 1 or less (based on the pore diameter) (Nield and Bejan, 2006). Considering that the velocity in the mushy zone will be near zero near the solid (low values of $\varepsilon$) Reynolds number in this region should be very small.

Thus, the equation finally used in our computations is:

$$\rho\left[\frac{\partial \vec{u}}{\partial t} + \nabla\cdot\left(\frac{\vec{u}\vec{u}^*}{\varepsilon}\right)\right] = -\nabla(P_d) + \mu\nabla^2\vec{u} - \rho\varepsilon\vec{g}\beta(T-T_0) - \frac{150\mu(1-\varepsilon)^2\vec{u}}{d_p^2\varepsilon^2} \qquad \text{(Eq. 6)}$$

where $P_d = \varepsilon p_d$.

## 1.1 *Enthalpy – temperature function*

In order to solve equations 1 to 3, a function that relates the enthalpy $h$ and the temperature $T$ is needed. In this work, two approaches are adopted, one for the case of a pure substance, where the phase change temperature ($T_{sl}$) is well defined, and another for materials composed of more than one substance, where the phase change is produced in a temperature range.

- Fixed phase change temperature:

$$h = C_{ps}T, \quad T < T_{sl} \tag{Eq. 7}$$

$$h = C_{ps}T + \varepsilon L \text{ with } \varepsilon = \frac{h - h_s}{L}; \quad h_s < h < h_l, \quad T = T_{sl} \tag{Eq. 8}$$

$$h = C_{pl}\left(T - T_{sl}\right) + C_{ps}T_{sl} + L, \quad T > T_{sl} \tag{Eq. 9}$$

where $T_{sl}$ indicates the phase change temperature.

- Variable phase change temperature:

$$h = C_{ps}T \qquad\qquad\qquad T < T_s \tag{Eq. 10}$$

$$h = C_{ps}T + \varepsilon L \qquad\qquad \text{with} \quad \varepsilon = \frac{T - T_s}{T_l - T_s}; \quad T_s \leq T < T_{sl} \tag{Eq. 11}$$

$$h = C_{pl}\left(T - T_{sl}\right) + C_{ps}T_{sl} + \varepsilon L \qquad \text{with} \quad \varepsilon = \frac{T - T_s}{T_l - T_s}; \quad T_{sl} \leq T < T_l \tag{Eq. 12}$$

$$h = C_{pl}\left(T - T_{sl}\right) + C_{ps}T_{sl} + L \qquad\qquad T \geq T_l \tag{Eq. 13}$$

where $T_{sl}$ indicates the temperature in the phase change range ($T_s < T_{sl} < T_l$) beyond which the material has a mostly liquid behavior, and below which it behaves mostly as solid.

## 1.2 Discretization and implementation

Model 1 (using eq. 2 as the momentum equation) has been implemented in an in-house 2D structured grid CFD code and also in TermoFluids. It has been verified and validated using some benchmark problems of phase change with a fixed temperature (Galione et al., 2011) and has been used to simulate melting and solidification of PCM in a spherical capsule.

Model 2 (using eq. 6 as the momentum equation) has been implemented in the in-house 2D structured grid CFD code and is presently also being implemented in TermoFluids.

These equations are discretized using an explicit Finite Volume Method. The velocity–pressure coupling is resolved by adopting a Fractional Step Method.

As in this approach an explicit time scheme is used, the momentum source term intended to model the presence of solid is only needed in the control volumes that contain solid and liquid, not in the pure solid containing volumes, as in these a zero velocity can be imposed explicitly.

## 1.3 Case studies

Both models have been used to simulate solid-liquid phase change in a standard test case (tin melting in a square cavity) and their results compared.

This benchmark is based on the experimental work of Wolff and Viskanta (1987). A square cavity is filled with tin, initially at solid state at the phase change temperature. Suddenly, the left wall is heated to a uniform higher temperature and the tin starts to melt from the left to the right

walls. Top and bottom walls are adiabatic, while the right wall stays at the phase change temperature.

As the solid temperature cannot rise above the phase change temperature and the right wall is maintained constant, the solid is isothermal at every moment. Taking advantage of this fact, the simulations are run only over a portion of the whole cavity, since the objective is not to simulate the entire melting process but only the first 1000 – 2000 seconds.

The parameters of the problem – taken from Hannoun et al. (2003) – are the following:

- Aspect ratio $A_r = 1$, $H$ (height) = 0.1m;

- $\rho$ (density) = 7500 kg m$^{-3}$, $k$ (conductivity) = 60 W m$^{-1}$K$^{-1}$,

    $C_p$ (specific heat) = 200 J kg$^{-1}$K$^{-1}$;

- $Ra$ (Rayleigh) = 2.25E5, $Pr$ (Prandtl) = 0.04, $Ste$ (Stefan) = 0.01;

- Initial temperature of 505K, hot wall temperature of 508K and phase change temperature of 505K.

To simulate cases were a mushy zone is developed a phase change temperature range has been artificially defined as:

- $T_s$ (solid) = 505.0K, $T_l$ (liquid) = 505.5K

In order to use model 2, the value of $d_p$ (pore diameter) is needed. This value will evidently not be constant in the whole mushy zone, as it is likely to be higher where the liquid fraction is higher. Therefore, an expression for $d_p$, probably depending on $\varepsilon$, should be determined in order to accurately simulate the phase change of the material involved. As such a correlation is not available – and as our main goal is to develop a simulation tool for phase change phenomena in a temperature range – some arbitrary values will be adopted, and the results obtained compared.

Source term $\dfrac{150\mu(1-\varepsilon)^2 \vec{u}}{d_p^{\,2}\varepsilon^2}$ , in a non-dimensional form can be written as $\dfrac{150c\,\mathrm{Pr}(1-\varepsilon)^2 \vec{u}}{\varepsilon^2}$

where $c$ depends on the value of $d_p$ and $\vec{u}$ in the last expression corresponds to the non-dimensional velocity. In this work, two values of $c$ are adopted in order to simulate two hypothetical situations: one where the resistance to the flow of the fluid through the solid pores is higher and another where it is lower. Thus,

- Case 1: $c = 10000$ (higher resistance)

- Case 2: $c = 100$ (lower resistance)

Structured grids of 60x100 and 120x200 have been used for the reduced domain (of 0.06 x 0.1 m).

Firstly, simulations using a fixed temperature for the phase change have been carried out in order to verify and validate the code. Results have been compared against previous numerical and experimental results (Hannoun et al., 2003; Wolff and Viskanta, 1987) and will presented elsewhere.

Secondly, the change of phase has been assumed to occur under a temperature range (indicated above) with the consequence of the formation of a mushy zone, in which models 1 and 2 have been used for the momentum balance. Results are presented in the next section.

## 3. Results and Discussion

### 3.1 Melting of pure tin

Results of the simulations of the melting of pure tin (with a fixed phase change temperature) will be presented in a future paper (currently in process) and are not included in this work. However, it can be said that they are close to at least some of the obtained by Hannoun et al. (2003). In general, it could be said that they are most comparable to the presented by Hannoun et al. (2003) using an upwind scheme with a mesh of 400x400.

As stated in Hannoun et al. (2003), numerical solutions deviate considerably from experimental results obtained by Wolff and Viskanta (1987), as in the latter there is no apparent multi-cellular behaviour like the obtained in the numerical simulations. They also observe that the results obtained with coarser grids are closer to experimental than the grid-converged simulations, which is also observed in our results.

### 3.2 Melting of tin with a modified phase change temperature

Figs. 2 to 9 show some simulation results of the melting of tin (modified by the assumption that it changes of phase under a range of temperatures) at 200 and 1000s. These results have been obtained with the 60x100 grid. However, some of these cases have been run with a 120x200 grid, showing almost no differences with the presented here.

It can be observed that for Case 1, there are no significant differences between the results obtained using either model. This is due to the fact that the resulting velocities of the flow in the mushy region are negligible with respect to the velocities in the liquid region, and therefore, the changes to the momentum equation – which act only in the mushy zone – have negligible effects on the melting configuration.

However, in figs. 6 to 9 corresponding to Case 2, some differences can indeed be observed in the configuration of the fluid flow and the shape of the mushy zone. In this case, the velocities of the flow in the mushy zone are not negligible (where the liquid fraction is higher), and some of the streamlines penetrate this region. These differences are not very pronounced, though. However, for materials with a lower resistance to the flow in its mushy zone and in cases where this region is broader, the differences between simulation results are expected to be more important.

Although the simulations performed in this work are not validated experimentally, it can be concluded that the two different formulations tested in this work for the momentum equations in the mushy zone of a changing phase material, return different flow configurations and therefore, different evolutions of the melting process are obtained. From the fact that the approach developed by Voller and Prakash (1987) was based on the assumption that the mushy zone could be treated as a porous material, it is concluded that a more accurate approach for the flow in a porous medium (as Hsu and Cheng's formulation) should be more adequate.

Finally, an experimental validation is needed in order to conclude the validity of either model. Nevertheless, the authors have not yet found in the literature experimental studies on the

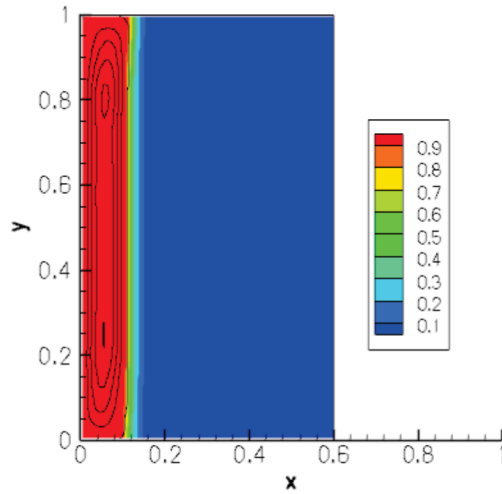melting of materials which undergo a phase change under a temperature range.



**Fig. 2: Tin melting at t = 200s. Phase change temperature range: 505 – 505.5 K. Using Voller approach. Case 1 ($c$ = 10000). Mesh: 60x100. Colour map indicate values of ε. In the liquid region, flow streamlines are presented.**
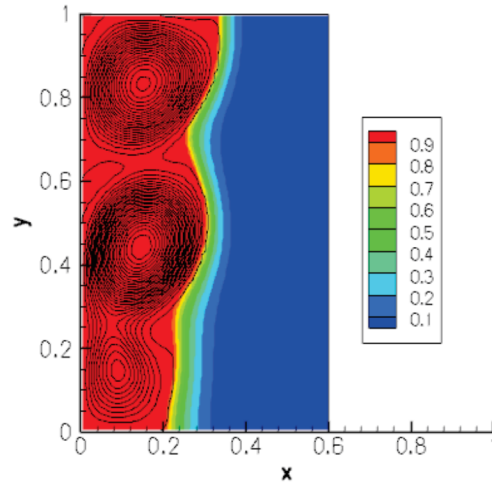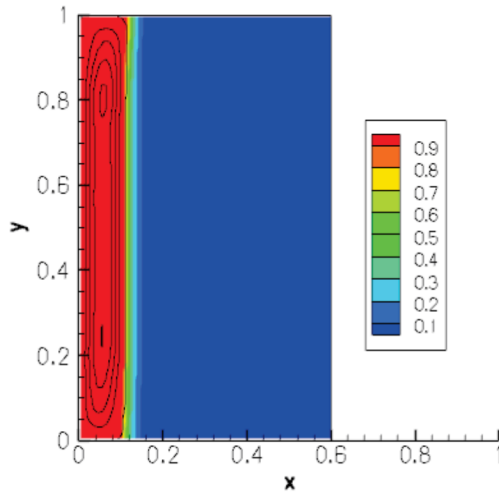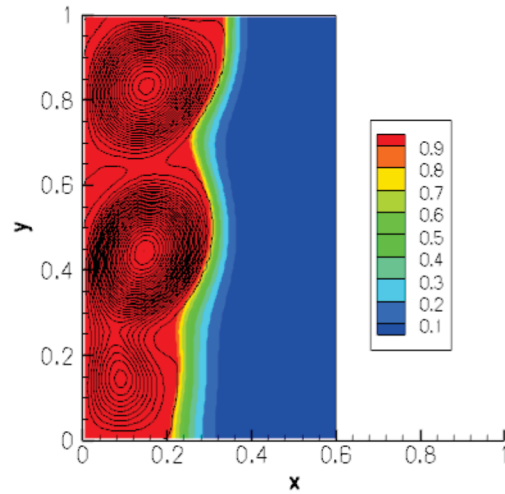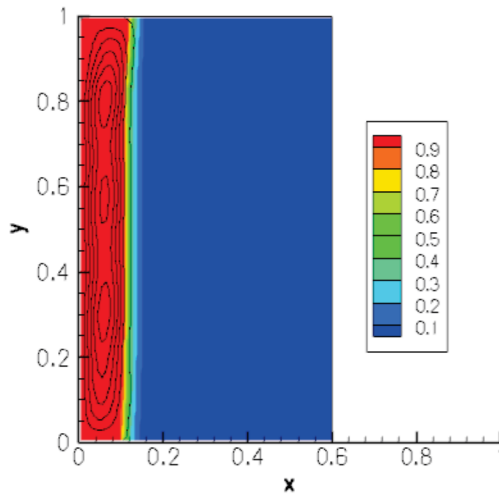


**Fig. 3: Tin melting at t = 1000s. Phase change temperature range: 505 – 505.5 K. Using Voller approach. Case 1 ($c$ = 10000). Mesh: 60x100. Colour map indicate values of ε. In the liquid region, flow streamlines are presented.**

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**Fig. 4: Tin melting at t = 200s. Phase change temperature range: 505 – 505.5 K. Using new approach. Case 1 ($c$ = 10000). Mesh: 60x100. Colour map indicate values of ε. In the liquid region, flow streamlines are presented.**



**Fig. 5: Tin melting at t = 1000s. Phase change temperature range: 505 – 505.5 K. Using new approach. Case 1 ($c$ = 10000). Mesh: 60x100. Colour map indicate values of ε. In the liquid region, flow streamlines are presented.**
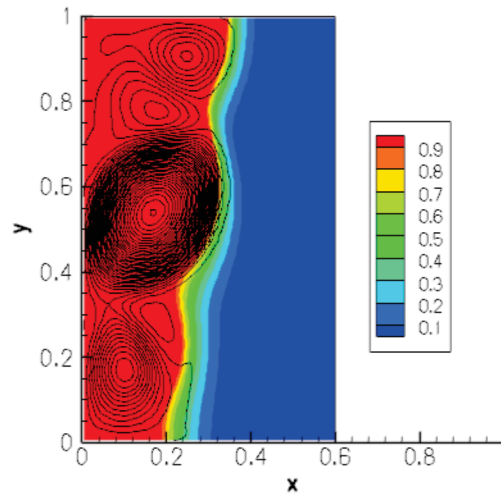
**Fig. 6:** Tin melting at t = 200s. Phase change temperature range: 505 – 505.5 K. Using Voller approach. Case 2 (*c* = 100). Mesh: 60x100. Colour map indicate values of ε. In the liquid region, flow streamlines are presented.
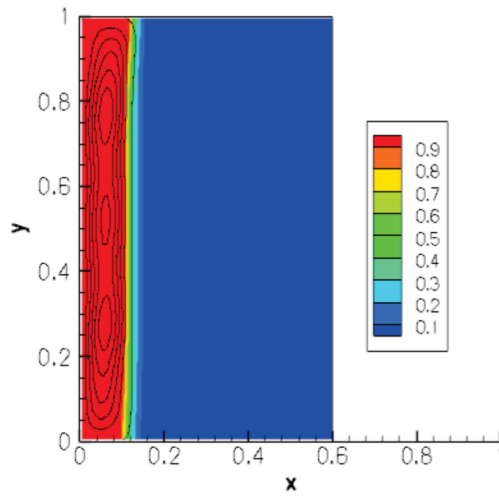


**Fig. 7:** Tin melting at t = 200s. Phase change temperature range: 505 – 505.5 K. Using Voller approach. Case 2 (*c* = 100). Mesh: 60x100. Colour map indicate values of ε. In the liquid region, flow streamlines are presented.



**Fig. 8:** Tin melting at t = 200s. Phase change temperature range: 505 – 505.5 K. Using new approach. Case 2 (*c* = 100). Mesh: 60x100. Colour map indicate values of ε. In the liquid region, flow streamlines are presented.
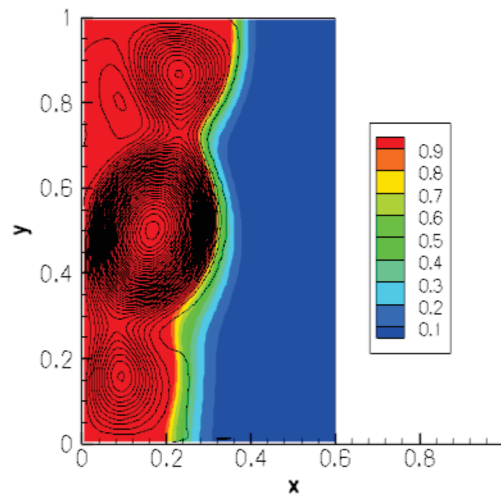


**Fig. 9:** Tin melting at t = 1000s. Phase change temperature range: 505 – 505.5 K. Using new approach. Case 2 (*c* = 100). Mesh: 60x100. Colour map indicate values of ε. In the liquid region, flow streamlines are presented.

## 4. Conclusions

Simulations of the melting of a PCM with a change of phase occurring under a temperature range have been performed.

Two different formulations for the momentum equation in the mushy zone have been used and its results compared. It is shown that when the resistance to the fluid flow inside the mushy zone is not very high, the change of formulation has an effect on the resulting flow configuration and on the shape of the mushy zone.

The approach developed by Voller and Prakash (1987) was based on the assumption that the mushy zone could be treated as a porous material, therefore, it is concluded that a more accurate approach for the flow in a porous medium (as Hsu and Cheng's formulation) should be more adequate.

Numerical simulations need further experimental validation in order to assess on the validity of the presented formulations.

The inclusion of "mushy zone" formulation in TermoFluids will allow simulating the change of phase of materials which undergo a temperature variation in the phase change process, in a variety of 3D configurations using efficient parallel algorithms and unstructured meshes.

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## 6. Acknowledgements