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# An implicit algorithm for melting and settling of phase change material inside macrocapsules

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ABSTRACT

A new, implicit algorithm for melting and settling of macro-encapsulated phase change material (PCM) is presented. The fixed grid mathematical model is based on the enthalpy-porosity technique and the volume of fluid (VOF) method. An immersed boundary method is applied to calculate the solid settling velocity, which is then prescribed by an extended Darcy term. As a test case, unfixed melting in a quasi two-dimensional cubic capsule is chosen. The newly introduced implicit algorithm is compared to an existing explicit algorithm and it is shown that the implicit calculation greatly improves the stability of the model. Moreover, the numerical model is validated against experiments performed within this work, whereby for the first time the settling velocity of the solid PCM is measured directly. Good agreement is found between simulation and experiment. The abilities of the new algorithm are demonstrated by multiple calculations with varying wall temperatures. Thereby, it is found that the solid settling velocity is at a quasi steady state only for a certain time. This time span reduces for higher wall temperatures.


## 1. Introduction

Due to a wide variety of application fields the scientific interest in melting processes has never diminished. Although research has been conducted for over 100 years, analytical solutions for melting problems still only exist for strongly simplified cases, e.g. simple geometries or the assumption of diffusive dominated phase change. In the absence of analytical solutions numerical methods are of great interest for various applications such as latent thermal heat storage [1,2] and metal processing [3].

The main difficulty in solving liquid-solid phase change problems lies in the moving boundary condition, which for melting problems is called the Stefan condition [4]. The numerical treatment of the moving boundary condition can be used to classify numerical methods for melting problems into deforming and fixed grid schemes [5,6]. In deforming grid schemes the position of the interface is determined by rearranging the mesh, whereas in fixed grid schemes the phase boundary is not explicitly tracked. Instead, an additional variable - the phase fraction - is introduced. It is expressed as a function of the temperature or the enthalpy and determines the position of the phase boundary. Although the Stefan condition is implicitly fulfilled in fixed grid schemes, two difficulties arise. First, the energy equation becomes non-linear due to the evolution of latent heat at the phase boundary. This led to the development of different methods to solve the non-linear energy equation on fixed grids: source based, apparent heat capacity and temperature transforming methods [7].

Second, the solid velocity must be set for convective phase change. In early fixed grid methods only diffusive phase change was considered [8,9]. Later, various authors described convective phase change on fixed grids by applying different approaches to set the solid velocity to zero. Morgan et al. [10] overwrote the velocity to zero in cells with a phase fraction under a threshold enthalpy value. Gartling [11] used a very high viscosity in the solid phase to suppress the solid velocity. Voller and Prakash [12] added a source term to the momentum equations to describe isothermal and non-isothermal phase change. Non-isothermal phase change occurs if mixtures are melted, which is the case for most industrial grade phase change material (PCM). Here the phase boundary is blurred and a two-phase melting area, called the mushy zone, develops. The source term, called Darcy term, sets the solid velocity to zero and describes the mushy zone as a porous media according to Darcy's law.

PCM generally have a very low thermal conductivity [13,14] and one way to enhance the heat transfer is through macro encapsulation. For macro encapsulated PCM, the solid phase is unfixed and is therefore allowed to move during the melting process. The most important mechanism for solid movement inside macro capsules is the density difference between liquid and solid phase. In the present study, the PCM consists of paraffins. For paraffins,

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**Nomenclature**

| | |
|---|---|
| $a$ | acceleration, m/s$^2$ |
| $c_p$ | heat capacity, kJ/(kg K) |
| $\hat{e}$ | unit vector |
| $\vec{f}, f$ | force balance, N |
| $h$ | enthalpy, kJ/kg |
| $\vec{g}, g$ | gravitational acceleration, m/s$^2$ |
| $l$ | length, m |
| $\vec{n}$ | normalized gradient |
| $p$ | pressure, Pa |
| $t$ | time, s |
| $\vec{u}$ | velocity vector, m/s |
| $v$ | velocity in $y$ direction, m/s |
| $x$ | coordinate, m |
| $y$ | coordinate, m |
| $\vec{A}$ | Darcy term, m/s$^2$ |
| $D$ | Darcy constant, kg/(m$^3$ s) |
| $\vec{D}$ | drag force, N |
| $\vec{F}, F$ | force, N |
| $\vec{G}$ | weight force, N |
| $\vec{I}$ | inertia force, N |
| $L$ | latent heat of fusion, kJ/kg |
| $\vec{P}$ | pressure force, N |
| $\vec{S}, S$ | surface, m$^2$ |
| $T$ | temperature, K |
| $V$ | volume, m$^3$ |
| $\alpha$ | phase fraction |
| $\beta$ | volumetric coefficient of thermal expansion, 1/K |
| $\delta$ | melt gap thickness, mm |
| $\epsilon$ | small numerical constant |
| $\zeta$ | discontinuous variable |
| $\lambda$ | thermal conductivity, W/(m K) |
| $\nu$ | kinematic viscosity, m$^2$/s |
| $\rho$ | density, kg/m$^3$ |
| $\tau$ | stress tensor, Pa |
| $\omega$ | under relaxation factor |
| $\Delta$ | difference |
| $b$ | bottom |
| $f$ | face |
| $g$ | global |
| $h$ | hot |
| $i$ | index |
| $in$ | inertial |
| $ini$ | initial |
| $k$ | index |
| $l$ | liquid |
| $m$ | index |
| $max$ | maximum |
| $o$ | other |
| $old$ | old time step |
| $ref$ | reference |
| $res$ | residuum |
| $s$ | solid |
| $set$ | settling |
| $t$ | threshold value |
| $y$ | y component |
| $L$ | liquidus |
| $S$ | solidus |

the solid density is higher than the liquid density and the solid moves downwards. This is the case for most PCM. Although the solid PCM moves downwards, melting at the bottom of the capsule assures that the solid PCM never reaches the bottom and a small melting gap remains. The whole phenomenon is called close-contact melting [15,16] and reduces the melting time drastically [17]. Interestingly, the solid can also settle without a density difference just due to natural convection, but in these cases the settling velocity is much smaller [18,19]. Close-contact melting has been studied extensively in the past using reduced forms of the Navier-Stokes equations originating from lubrication theory [20–23]. This approach allows analytical solutions but it relies on the assumption that the melting gap is always small. Moreover, it can neither describe the influence of the side walls nor natural convection in the melt.

Only a few authors have studied unfixed melting without any assumptions regarding the melt gap thickness. Still, multiple numerical approaches have been developed to couple melting and solid settling. Asako et al. [24] and Asako and Faghri [25] used a variable viscosity to allow settling of the solid. A disadvantage of this approach is the non-physical solid viscosity which can lead to deformations of the solid body [26]. Assis et al. [27] set the Darcy constant to an arbitrary low value to implement settling inside a spherical capsule. A low Darcy constant, however, leads to a different description of the mushy zone and therefore to an incorrect melting behavior. Nevertheless, multiple authors followed this approach [28,29]. A physically more useful implementation was done by Rösler [30] by means of an extended Darcy term and a force balance around the solid body. But the explicit calculation of the solid settling velocity gives rise to strong oscillations and therefore allows only small temperature gradients.

Recently, Kozak and Ziskind [31] proposed a new method for simultaneous melting and settling of PCM, which also relies on a force balance around the solid body but uses forcing functions instead of an extended Darcy term to prescribe the solid velocity. Their approach gives physically correct results but requires a time step which is orders of magnitude smaller than the one used in the present work.

In this paper, an improved numerical algorithm for melting and settling based on an extended Darcy term is proposed. The algorithm strongly reduces oscillations and is able to handle large temperature gradients. As a test case the melting and settling of unfixed PCM in a cubic enclosure is chosen. Experiments are performed for one wall temperature to validate the numerical results. Moreover, the effect of the wall temperature on solid settling velocity, melt gap, heat flux and global liquid fraction is studied numerically.

## 2. Mathematical model

### 2.1. Conservation equations

The flow is assumed to be Newtonian, laminar and incompressible. The density $\rho$ is constant except for the gravitational term, where the Boussinesq approximation is applied. Both phases are treated on one grid. To this end, the Volume of Fluid (VOF) approach is used. Pressure and viscous terms in the energy equation are not taken into account. The dynamic viscosity $\eta$ is modeled as a linear function of the temperature. The influence of the second viscosity term $\nabla \cdot (\nu \nabla (\vec{u})^T)$ was tested and found to be small. Therefore this term is neglected. Considering these assumptions the resulting mass, momentum and energy equations are: