Various ways to take into account density change in solid–liquid phase change models: Formulation and consequences

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ABSTRACT

In this paper, a classification of different methods for accommodating volume variations during solid–liquid phase change is presented. The impact of each method is analyzed with the help of a scale analysis. Neglecting fluid velocity at the interface or allowing fluid to enter/exit the domain may result in either local (at the solid–liquid interface) or global (within the system) mass imbalance. This can lead to significant differences in the transient phase change process itself (e.g., 19% more time and 9% more energy to completely solidify a given mass of water with models for which the total mass of the system is conserved). This paper aims at addressing this issue by deriving two new models of thermo-mechanical coupling between the PCM and its container. The first model is that of a PCM bounded by an elastic wall, whereas the second model assumes that a compressible air gap is adjacent to the PCM, which allows the PCM to expand more easily. Analytical expressions are developed for both models and can be used to predict important quantities at equilibrium, such as the position of the solid–liquid interface and the pressure rise within the system. Finally, the two thermo-mechanical coupling models are implemented numerically with a finite volume moving mesh method. Numerical simulations are performed to show the limits of the two models. It is observed that volume variations during phase change can have significant impacts on the evolution of the process.

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1. Introduction

Solidification and melting are complex processes in which the state of a substance changes, and as a result, so do its heat transfer properties. Significant differences in terms of thermal conductivity and specific heat are typically observed between the solid and liquid phases of a substance. Similarly, because molecules organize differently in solids or liquids, the density of a substance also changes with its phase. Phase change materials (PCM) either shrink or expand during phase change which can cause a significant impact in terms of deformations and mechanical constraints in the system, as well as on the heat transfer mechanisms themselves.

When developing an analytical or a numerical model, it can be quite a challenge to fully take into account the change of density in solid–liquid phase change processes. The presence of a net mass flux at the solid–liquid interface changes the overall volume of the PCM domain. Solutions to classical problems, such as the Stefan problem, have been developed by assuming a constant density (see, for example, Chapter 11 in [1]), i.e. without considering density change. In fact, in order to simplify the problem, the majority

of analytical or numerical studies on the modeling of melting or solidification assume that the PCM density is the same for both phases, while some studies neglect the net mass flux at the interface (which results in the destruction or generation of mass within the domain over time), see for example [2].

In experimental setups studying phase change, volume change of the PCM during solidification or melting needs to be accounted for even when it is not the main focus of a given study. For example, in their study on the effect of solid subcooling on natural convection melting of pure gallium in a rectangular enclosure [3], Beckermann and Viskanta accommodated volume change during phase change (gallium contracts by about 3% when melting) by allowing liquid gallium to enter the test cell through a small hole in the top wall of the enclosure. This strategy allowed the enclosure to remain completely filled with gallium throughout the experiments, thus minimizing the impact of volume change on the natural convection flow pattern in the enclosure. Braga and Viskanta later performed experiments on the effect of the density extremum on the solidification of water on a vertical wall of a rectangular cavity [4], where the expansion of water upon solidification was accommodated by leaving a small (~3 mm) gap at the top of the cavity to allow water to expand without pushing against the inner walls of the cavity. This strategy was also used in

Nomenclature

c_p	heat capacity [J kg^{-1} K^{-1}]
E	Young's modulus [N m^{-2}]
f	liquid fraction [–]
g	gravitational acceleration vector [m^2 s^{-1}]
h_{sl}	latent heat of fusion [J kg^{-1}]
H	height of the one-dimensional slab [m]
k	thermal conductivity [W m^{-1} K^{-1}]
L	length [m]
m''	total mass of the system per unit area [kg m^{-2}]
$\dot{m}''$	liquid mass flux at the solid–liquid interface [kg m^{-2} s^{-1}]
p	pressure [N m^{-2}]
Q''	latent heat flux [W m^{-2}]
q''	heat flux [W m^{-2}]
Ste	Stefan number [–]
t	time [s]
T	temperature [K]
T_C	cold-side temperature [K]
T_H	hot-side temperature [K]
T_m	solidification (or melting) temperature [K]
v	vertical component of the velocity in the liquid phase [m s^{-1}]

v_l	liquid velocity normal to the solid–liquid interface [m s^{-1}]
x, y, z	Cartesian coordinates [m]

Greek symbols

α	thermal diffusivity [m^2 s^{-1}]
δ	position of the solid–liquid interface [m]
η	effective compressibility of the PCM [m^2 N^{-1}]
κ''	effective spring constant [Pa m^{-1}]
v	Poisson coefficient [–]
ρ	density [kg m^{-3}]
τ_{diff}	diffusion time scale [s]
τ_m	solidification/melting time scale [s]

Subscripts

f	final value
g	gas property
i	initial value
l	liquid phase property
s	solid phase property
w	elastic wall property

Refs. [5,6] in the design of experimental apparatus in order to accommodate the expansion of the PCM during phase change.

Volume changes during phase change are also of significant importance in thermal energy storage applications that use PCMs (e.g. encapsulated PCMs). For example, Lopez et al. [7] developed one-dimensional models (assuming spherical symmetry) to understand salt melting within graphite matrices. The thermo-mechanical models developed by the authors are based on mass and energy conservation equations (enthalpy formulation with variable melting temperature and latent heat of fusion), pressure-dependent liquid–crystal equilibriums, isotropic and linear elasticity laws and Poiseuille-like flows. The model explains some of the main observations for the melting of salts within spherical shells made of graphite (e.g. melting within a wide range of temperatures, incomplete melting and loss of heat storage capacity). The models developed in [7] were then extended by Pitié et al. [8] to represent the confined melting of PCMs coated by silicon carbide. Models from [7,8] were specifically developed to study the thermo-mechanical behavior of encapsulated PCMs in thermal energy storage systems.

In their study on the planar solidification of a finite slab, Conti [9] and Conti et al. [10] developed a thermo-mechanical model which was used to determine the effects of pressure on the solidification process as the PCM expanded while constrained by an elastic wall. However, as will be explained in more details below, some assumptions made while developing their model made it valid only under a restrictive set of conditions. In addition, the authors assumed the PCM to be compressible, but used a constant density for each phase, which resulted in a non-conservation of the total mass of the system.

More recently, an experimental and numerical study on melting in a spherical shell al has been performed by Assis et al. [11]. A constant density was used for each phase, and it was assumed that the density varied linearly between the solid and liquid density within the mushy region. A large air cavity was modeled at the top of the PCM to allow the latter to expand during melting. Since both the PCM and the air are assumed to be incompressible, an additional small opening was modeled at the top of the air cavity to allow it to leave the computational domain as the PCM expands. In order

to represent the moving interface between the PCM and the air cavity, a volume-of-fluid model was used. The same approach has been adopted by Shmueli et al. [12] for an experimental and numerical study on melting in a vertical cylinder tube. Even though the numerical results from both works are in good agreement with the experiments performed by the authors, they do not address the thermo-mechanical coupling between the PCM and its boundaries, i.e. there is no pressure rise within the system caused by the expansion of the PCM, which could influence the melting properties.

Similarly, an experimental and numerical study on the melting process of PCMs in a rectangular enclosure was recently performed by Ho et al. [13]. In their work, the expansion of the PCM during melting is addressed by allowing the top boundary to move freely while maintaining the two vertical walls and the bottom wall stationary. The authors present experimental and numerical results for a wide range of subcooling, Stefan, and Rayleigh numbers. The numerical predictions are in good agreement with the experimental results. However, the experiments and numerical simulations performed in their work do not include thermo-mechanical coupling between the PCM and the cavity boundaries.

Kowalczyk et al. [14] studied solid–liquid phase change at high pressure. Recognizing that melting point and latent heat can be influenced by pressure, they proposed a model with pressure-dependant properties. Nevertheless, density was assumed constant in their model and their experimental set-up had a volume adaptation approach in order to control the pressure level due to expansion of water during phase change.

Bilir and Ilken [15] studied numerically the solidification time of PCM in enclosures. Despite the fact that the PCM is physically bounded by the walls of the container, the density was assumed to be the same for both phases in such a way that no pressure build up due to the PCM expansion was accounted for in the heat transfer process. Similarly, the solid–liquid phase change numerical model developed in Wang et al. [16] also assumes that both phases have the same density.

In their review, Sharma et al. [17] describe the typical numerical model used in literature. Their presentation is based on the assumption of a constant density. Nevertheless, they mention in