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A comprehensive benchmark of fixed-grid methods for the modeling of melting

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ABSTRACT

Numerical simulation of melting processes is known to be tricky yet due to new application fields they raise again the attention of both, researchers and engineers. Several approaches were developed to solve this moving boundary problem, fixed grid methods being the most widespread ones. However, up to now no holistic and quantitative comparison, even of the most common enthalpy methods (some of these being included in famous commercial software), exists. Therefore, within this work, an exhaustive study is performed to evaluate the corresponding accuracy of the five most used macroscopic energy formulations with a strong coupling between temperature and enthalpy. In addition to pure conductive cases with analytical solution, an experimental test including natural convection is considered. Thus, the influence of the time step, of the grid and of the tolerance within the energy equation are investigated. In the same way several thermodynamical modelings are considered: either isothermal or non-isothermal phase change, several temperature ranges being used in this later case. From the more than 2500 simulations obtained, painstaking quantitative error analysis are conducted and quality thresholds are defined. Generally, approaches formulated in terms of enthalpy appear to be more robust than the ones using temperature formulations instead. The popular effective heat capacity method (with iterative correction) leads to the largest errors when considering the complete enthalpy in the convection term.

1. Introduction

Solid-liquid phase-change is known to be overspread in the nature or in human activities, *e.g.* casting and welding, production of high quality metals or alloys, energy storage. However, it is also known to be a tough problem since it rises both fundamental and numerical issues, as for example when one seeks to write the modeling equations governing such a situation or, for a given set of partial differential equations, when one tries to solve them. For these two main reasons, this topic has motivated numerous studies, be it experimental, theoretical or numerical ones. Indeed, for a good control of the processes, it is often mandatory to have some knowledge about the composition of either the liquid or the solid phase (concentrations of various species) and their behavior (conduction or convection regime, dendrites structures …), about the interface position (and sometimes of the associated morphology), about the temperature field and the corresponding heat fluxes (mainly at the boundaries), *etc.*

From a mathematical point of view, the solid-liquid transition is referred as a moving boundary problem and due to this interface movement, it is non linear. Indeed, the position and velocity of the solid-liquid interface cannot be calculated analytically because it depends on the time but also since there is a strong coupling between the velocity and the temperature fields. Moreover, the equation of state linking the enthalpy to the temperature is rather complicated, especially when a discontinuity is present (this will be further discussed later), and the associated equations are difficult to handle. Since the study of the crust formation of Earth by Lamé and Clapeyron [1],[1] or the ice formation problem of Stefan [4], some solutions have been proved to exist in the limiting cases of constant properties and conduction in the liquid phase only [4] or conduction in both the liquid and solid phases [5]. Although a similarity solution seemed to have been proposed by Neumann in some of its lectures, the first proof of existence and uniqueness of the solution for the one-dimensional Stefan problem seems to be due to

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[1] which, by the way, was approximated as a 1D infinite problem [2,3].

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Rubinstein [6] and then it has been shown that a general solution exists for non-constant properties [7], and its uniqueness was proven [8]. Some other fundamental aspects have been discussed for the multi-dimensional case [9–15]. Lastly, an exact solution for non-isothermal transitions has been proposed [16]. For a more general overview of the historical state of progress, one may have a look at Rubenstein [[17], pp 1–15 of the Introduction] concerning the mathematical considerations and at Crank [[18], section 1.3, pp 1–29] for the various Stefan-type problems and at Crank [[18], p2] to have an overview of literature surveys concerning the Stefan problem. For a more specific historical review, see Yao and Prusa [[19], section II. A, pp 4–5] for a description of the seminal studies and also for the progressive incorporation of convection in phase-change problems [[19], section III.A.1, pp 44–49], and [20] for a complete biography of Jožef Stefan and historical roots of its nine problems. Finally, an exhaustive synthesis of analytical and approximated solutions for such problems is given by Tarzia [21].

Concerning the physical and numerical modelings, many possibilities are available, with their own advantages and disadvantages. To give a brief summary, one can rely on pure fluid equations or on a multiphase approach. Thus, when one turns to the numerical solving of a solid-liquid phase-change problem, it is common to divide the schemes into two main families: the multi-domain or 2-domain, or variable domain methods, and the one-domain, or fixed-grid methods (FGM) or P (physical)-grid methods (PGM). It is also worth mentioning that two other classes of methods exist, that cannot fit perfectly this taxonomy, namely the meshfree or meshless methods and the lattice Boltzmann methods. The present paper will restrict to FGM since it is clearly the most used approach, and because of the huge numerical issues already involved with such a “basic” model.

The *multi-domain methods* belong to the sharp interface methods family and can therefore be separated into the moving grid methods (MGM) and into Eulerian methods. With MGM, or r-methods (for relocation-method), the mesh is deformed so as to follow the interface during its displacement, the corresponding velocity used to move the grid may be that of the fluid (Lagrangian methods) or an arbitrary one (Arbitrary-Lagrangian-Eulerian -ALE-methods[2]). With Eulerian methods, a fixed grid is used jointly with a method to either follow or reconstruct the interface. In the first case, the front tracking methods (FTM), the interface is explicitly followed and consequently liquid and solid phases are clearly separated, the interface movement being governed by the energy balance which corresponds to a boundary condition for the two phases. This interface tracking may be based either on a surface tracking or on a volume tracking. In the second case, the front capturing methods (FCM), the interface is now implicitly followed thanks to a new equation which permits to reconstruct its position. These methods being closed to or having been used jointly with FGM, a brief description is proposed. In summary, there are two main ideas underlying these approaches. Firstly, the interface is now diffuse, because of the modeling or due to numerical smearing. Secondly, this thick front is used to propose a macroscopic description of the interface including microscopic phenomenon. In phase field methods (PFM) [22], a continuous and fast variation of properties is supposed across the interface, *i.e.* from the two bulk values for the solid and liquid phases. Then, the interface is identified through a phase-field variable, usually called ϕ, which obeys a new PDE, not necessarily based on or respecting physical principles (especially thermodynamical ones) even if it would be preferable. Generally, ϕ is involved in a free energy equation which is minimized. To have a more complete overview, one may have a look at [[23], chap.11, pp.366–378] or [24],[3] or even to [25–28] to find a review of various PFM and enlightening explanations and examples. In volume-of-fluid (VOF) methods [29] and level-set methods (LSM) [30–32], the function used to position the interface is not unavoidably a physical variable but a numerical one, the color or distance function. These methods being clearly more used for liquid/gas change of phase, they are not detailed any further. In the third case, the mapping methods (MM) or T-grid methods, for transformed-grid methods (TGM), a new function is used to transform the curved domain containing the interface into a domain with a regular shape. This permits to immobilize the moving boundary on a uniform and fixed grid. In the last case (less common), the front-fixing methods (FFM), the idea is to have an adaptable space step or time step so as to have the interface always lying on a mesh point or line or to have it moving completely across a cell during one temporal iteration. For more precise information or descriptions of the previous methods, and a thorough analysis of their advantages and drawbacks, one can have a look at the corresponding literature [26,33–62].

The *one-domain methods* aim at solving a complete and unique system of partial differential equations on the entire domain. This set of equations may be based on a multi-phase approach (two-fluid models), with some non-equilibrium or equilibrium assumptions, or on a one-phase approach (one-fluid models) corresponding to an homogeneous equivalent fluid, each one being more appropriate to deal with a certain feature of the solid-liquid transition and requiring more or less human and computational efforts. Since the PDE are valid in the whole domain, special treatment will be needed to cancel the velocity in the solid state, the various available techniques being presented in section 2. Concerning the interface, it is not necessary anymore to track it, neither explicitly nor implicitly, and no remeshing is required. Moreover, these methods are simpler to implement and rely on less human and computational efforts. Eventually, they can deal relatively easily with complex multi-dimensional problems and with the dynamic appearance/disappearance of multiple interfaces. A complete presentation and description of the non-equilibrium models is out of scope of the present article and consequently the interested reader will be referred to some fundamental references [46,54,57,63–81]. Concerning the corresponding disadvantages, they will be presented later, when describing the various classes of FGM for one-fluid models in section 2. Indeed, these can be subdivided into the enthalpy-based formulations or temperature-based formulations.[4] The first one contains the enthalpy method which corresponds to the usual energy equation and the total enthalpy method which uses a transformation to write the Fourier's law in function of the enthalpy. The second one contains the source based method (or fictitious heat flow), where the latent heat is incorporated thanks to a source term in the right-hand side (RHS) of the energy equation, and the apparent or effective heat capacity methods, where the latent part of the energy is included in a revised form of the heat capacity. Some more complete analysis and descriptions

[2] *n.b.*: then an other important step is required so as to remap the domain: the rezone phase, which can be based on a p-, h- or r-adaptation (the most common).

[3] In spite of the solidification-oriented titles, interesting informations are available here.

[4] *n.b.*: The heat balance integral method (HBIM) [82–84], which consists in using polynomials to fit the temperature fields in the solid and liquid phases so as to permit an integration of the PDE to obtain ordinary differential equations (ODE) easier to solve, and the freezing index method [85–87], which consists in transforming the variable so as to have a continuously differentiable function together with an homographic approximation, and the discontinuous integration method [88–90], which consists in separating the integration of the enthalpy together with adding a supplementary degree of freedom to account for the interface location inside an element, will not be discussed since they are not used anymore nowadays.