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On the accurate numerical solution of a two-phase Stefan problem with phase formation and depletion

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ABSTRACT

In this paper, the Keller box finite-difference scheme is employed in tandem with the so-called boundary immobilization method for the purposes of solving a two-phase Stefan problem that has both phase formation and phase depletion. An important component of the work is the use of variable transformations that must be built into the numerical algorithm in order to resolve the boundary-condition discontinuities that are associated with the onset of phase formation and depletion. In particular, this allows the depletion time to be determined, and the solution to be computed after depletion. The method gives second-order accuracy in both time and space for all variables throughout the entire computation.

1. Introduction

Phase-change, or Stefan, problems in which a material melts or solidifies occur in a wide variety of natural and industrial processes, e.g. the evaporation of fuel droplets [1], the melting or freezing of spheres [2–10], the solidification of metal in continuous casting processes [11–14]. Mathematically, these are special cases of moving-boundary problems, in which the location of the front between the solid and liquid is not known beforehand, but must be determined as part of the solution. Analytical solutions are available in only a very limited number of cases and in general numerical methods are necessary. Furthermore, numerical methods are most often applied to only the part of the problem during which the moving boundary exists. However, it is desirable to have a method which is able to give a solution for the entire problem, i.e. before phase change starts, whilst it proceeds and after it finishes. Although the first and third stages simply constitute fixed-boundary problems, and are therefore numerically less challenging than the second stage, an important issue is whether the accuracy of any given numerical scheme is still preserved as we transfer from one stage to the next. Limiting the discussion to the use of the formally second-order accurate Keller box scheme, which we have recently applied to a number of phase-change problems [15–21], it is evident that accuracy is not preserved without specific precautions, since the onset of phase formation or subsequent depletion will result in discontinuities in the boundary conditions.

In our earlier work [17], we considered the case of a one-dimensional non-classical two-phase Stefan problem in the context of cooling heat transfer and solidification, posed on a semi-infinite spatial domain, in which the solid phase first appears only after a finite delay time; this can occur if the phase change is caused by a heat-flux boundary condition,

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rather than the classical isothermal cooling boundary condition. A natural extension of this, which is more relevant to actual applications, is a two-phase Stefan problem that is posed on a finite spatial domain; in this case, the liquid phase that was initially present will deplete after a finite time, at the expense of the solid phase that was not initially present at all. Although the earlier paper demonstrated how the accuracy of the applied numerical scheme could be preserved in spite of the boundary-condition discontinuity at the onset of phase change, the situation now proposed leads to two new complications:

- how to handle numerically the depleting phase;
- how to continue the integration after phase depletion.

We have considered the first issue on a number of occasions in the context of one-phase Stefan problems [18–20], for which there is a finite extinction time for the whole problem; now, however, the situation is slightly different again, since the other phase still remains and we will need to continue the numerical integration for that phase. As regards the second issue, we have previously considered the case of boundary-condition discontinuities [21], but only when the initial condition was analytically prescribed; here, however, we effectively will need to compute the initial-like condition for the subsequent post-depletion regime, and it is clear that any loss of accuracy in the pre-depletion computation is likely to propagate into the post-depletion regime. The purpose of this paper is therefore to resolve these issues, in tandem with the use of the Keller box scheme. An additional distinction to [17] is that here we consider a fixed boundary condition, rather than a heat-flux condition, which causes the solid phase to appear immediately.

The layout of the paper is as follows. In Section 2, we formulate and nondimensionalize a one-dimensional problem for the solidification, due to a constant cooling temperature, of material of finite extent that is initially above its melting temperature. In Section 3, we explain how the Keller box scheme, in tandem with the boundary immobilization method, is applied to this particular problem. The results are then presented and discussed in Section 5, and conclusions are drawn in Section 6.

2. Mathematical formulation

Consider the cooling of a liquid, occupying the region $0 < y < Y$, that is initially at a temperature, T_{hot}, which is greater than its melting temperature, T_{melt}, and is cooled at $y = 0$ for time $t > 0$ by prescribing a fixed temperature T_{cold}, where $T_{cold} < T_{melt} < T_{hot}$. Solidification begins immediately with solid occupying the region $0 \leq y \leq y_m(t)$ and the remaining liquid occupying $y_m(t) < y < Y$, where $y_m(t)$ denotes the location of the solidification front.

Assuming the material properties of the solid and liquid phases to be constant, the equations governing the subsequent heat transfer are as follows. In the solid, we have

$$\rho_s c_{ps} \frac{\partial T_s}{\partial t} = k_s \frac{\partial^2 T_s}{\partial y^2}, \quad 0 < y < y_m, \tag{1}$$

where T_s is the solid temperature, k_s is the thermal conductivity of the solid, c_{ps} is its specific heat capacity and ρ_s its density. Also, the governing equation in the liquid is

$$\rho_l c_{pl} \frac{\partial T_l}{\partial t} = k_l \frac{\partial^2 T_l}{\partial y^2}, \quad y_m < y < Y, \tag{2}$$

where T_l is the liquid temperature, k_l is the thermal conductivity of the liquid, c_{pl} is its specific heat capacity and ρ_l its density. We assume henceforth for simplicity that $\rho_l = \rho_s = \rho$.

For boundary conditions, we have, at $y = 0$,

$$T_s = T_{cold}. \tag{3}$$

Next, provided that $y_m < Y$, we have, at $y = y_m$,

$$T_s = T_l = T_{melt}, \tag{4}$$

and the Stefan condition

$$\rho \Delta H_f \frac{\mathrm{d}y_m}{\mathrm{d}t} = k_s \frac{\partial T_s}{\partial y} - k_l \frac{\partial T_l}{\partial y}, \tag{5}$$

where ΔH_f is the latent heat of fusion. In addition, at $y = Y$, we have

$$\frac{\partial T_l}{\partial y} = 0. \tag{6}$$

However, once y_m reaches Y, Eqs. (4)–(6) will be replaced by just

$$\frac{\partial T_s}{\partial y} = 0 \quad \text{at } y = Y. \tag{7}$$