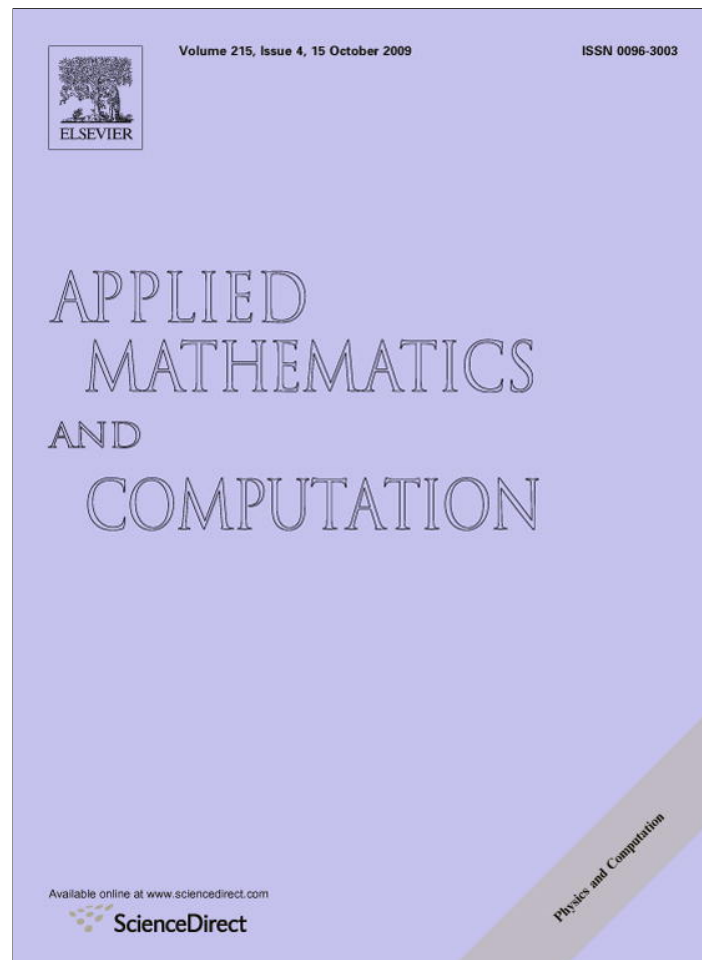


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# Finite-difference methods with increased accuracy and correct initialization for one-dimensional Stefan problems

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## ABSTRACT

Although the numerical solution of one-dimensional phase-change, or Stefan, problems is well documented, a review of the most recent literature indicates that there are still unresolved issues regarding the start-up of a computation for a region that initially has zero thickness, as well as how to determine the location of the moving boundary thereafter. This paper considers the so-called boundary immobilization method for four benchmark melting problems, in tandem with three finite-difference discretization schemes. We demonstrate a combined analytical and numerical approach that eliminates completely the *ad hoc* treatment of the starting solution that is often used, and is numerically second-order accurate in both time and space, a point that has been consistently overlooked for this type of moving-boundary problem.

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## 1. Introduction

Phase-change, or Stefan, problems in which a material melts or solidifies occur in a wide variety of natural and industrial processes. 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. Although a few analytic solutions to such problems are known, it is more common to have to apply numerical methods [1]; amongst these are the enthalpy method [2,3], the boundary immobilization method [4–8], the variable space grid method [2,7], the finite element numerical method [9], the nodal integral method [10] and the heat balance integral method [3,11–19].

In the numerical solution of many phase-change problems, a key issue is how to initiate a computation for a region which initially has zero thickness. A common approach has been to determine a starting solution analytically and then to input this as an initial condition into a numerical scheme at some arbitrarily small-time after phase-change has actually started. For one-dimensional Stefan problems, the boundary immobilization method [4–7] appears to have the merit that the computational domain will initially be of finite non-zero thickness, although it has been said that the method has a disadvantage, in that a singularity is introduced into the governing equations at the instant when phase-change begins [5]. One of the goals of this paper, however, is to demonstrate that this is actually not the case, and that a self-similar solution to the governing equations can be found, which can then be used as the initial condition for the temperature in the newly-formed phase; furthermore, this will resolve many of the issues concerning starting solutions for the boundary immobilization method, not only for the planar geometry considered here, but also for cylindrical and spherical geometries [5]. Another issue that will be addressed in detail is the order of accuracy of existing numerical implementations, and how this can be improved on using methods from more conventional fixed-boundary value problems.

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In Section 2, we formulate four benchmark one-dimensional melting problems that differ in the nature of the heating boundary condition. In Section 3, we perform an analysis of these problems in the small-time limit, which is necessary for the later numerical solutions. Section 4 explains how the resulting equations are implemented numerically by describing three different discretization schemes: semi-implicit, Keller box and Crank–Nicolson. The results are then presented and discussed in Section 5; for three of the problems, comparison can be made with available exact solutions, whereas for the fourth, which contains a time-dependent periodic boundary condition and does not have an analytical solution [6,20], we demonstrate that our approach has distinct advantages over earlier numerical methods [6]. Among the main conclusions, given in Section 6, is the fact that the small-time analysis developed here, coupled with the use of numerical schemes that are second-order accurate in both time and space, constitutes a significant improvement in the implementation of the boundary immobilization method for moving-boundary problems, as compared with earlier work; the use of these ideas in melting and solidification problems in higher dimensions is also discussed.

## 2. Mathematical model

Consider the melting of a certain material, occupying the half-plane  $x > 0$ , that is initially at its freezing temperature and which is heated at  $x = 0$  for time  $t > 0$ . The governing heat equation for the variable,  $T$ , which can be thought as the dimensionless temperature, can be written in non-dimensional form as

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2}, \quad 0 < x < s(t), \quad t > 0, \tag{1}$$

subject to the initial conditions

$$s(0) = 0, \tag{2}$$

$$T(x, 0) = 0, \tag{3}$$

and boundary conditions at  $x = 0$  and at the solid–liquid interface,  $x = s(t)$ . For the latter, we have

$$T(s(t), t) = 0, \tag{4}$$

$$\beta \frac{ds}{dt} = -\frac{\partial T}{\partial x} \Big|_{x=s(t)}, \tag{5}$$

where  $\beta$  is a strictly positive constant that corresponds to the reciprocal of the Stefan number. For the former, we will consider four different boundary conditions at  $x = 0$ :

$$(i) T = 1, \quad (ii) T = e^t - 1, \quad (iii) \frac{\partial T}{\partial x} = -e^t, \quad (iv) T = 1 - \epsilon \sin(\omega t), \tag{6}$$

where the parameters  $\epsilon$  and  $\omega$  in (iv) represent the amplitude and frequency of thermal oscillation, respectively. The solutions to problems involving boundary conditions (i)–(iii) are exact and have been given in earlier work [1,7]:

- the problem consisting of Eqs. (1)–(5) and (6i) has the solution

$$T(x, t) = 1 - \frac{\operatorname{erf}[x/(2\sqrt{t})]}{\operatorname{erf}(\alpha)}, \quad s(t) = 2\alpha\sqrt{t}, \tag{7}$$

where  $\alpha$  satisfies the transcendental equation

$$\sqrt{\pi} \beta \alpha \operatorname{erf}(\alpha) e^{\alpha^2} = 1; \tag{8}$$

- the problems consisting of Eqs. (1)–(5) and either (6ii) or (6iii) have the same solution (provided  $\beta = 1$ ),

$$T(x, t) = e^{t-x} - 1, \quad s(t) = t. \tag{9}$$

In the analysis described below, we keep  $\beta$  in the equations, but only consider  $\beta = 1$  in the results Section 5, to enable comparison of our numerical solutions with the exact solution (9).

On the other hand, numerical solutions to the problem involving (iv), which does not have an exact solution, have been considered previously by [6,20].

A common feature of all four formulations is that there is a degeneracy associated with Eq. (3), since the melt region initially has zero thickness, in view of Eq. (2); one of the goals of this paper is to show how an appropriate coordinate transformation, when used with the boundary immobilization method, both addresses and resolves this degeneracy. At the heart of this is the initialization of the numerical scheme, as there appears to be some ambiguity in the literature [1,7] as regards the initial condition for the actual physical problem and the condition that is used for initialization; another of the goals here is to demonstrate that our approach handles all cases, irrespective of the boundary condition at  $x = 0$  or whether the

equation system has an exact solution or not. We also point out how cases (i)–(iv) complement each other to give an overall understanding:

- cases (i)–(iii) have exact analytical solutions, which we will later use to test the accuracy of our numerical method, whereas case (iv) does not;
- cases (ii) and (iii) have the same solution, even though they have different types of boundary condition, Dirichlet and Neumann respectively, at  $x = 0$ ;
- cases (i) and (iv) use the same transformation for initialization, even though they do not have the same solution;
- case (ii) uses a different transformation for initialization to that for (i) and (iv), even though all contain a Dirichlet condition at  $x = 0$ ;
- the method used for establishing the order of accuracy of the numerical scheme for case (iv), which does not have an analytical solution, can be tested for consistency on cases (i)–(iii).

### 3. Analysis as $t \rightarrow 0$

Since the melt region is initially of zero thickness, it is advantageous to work in transformed coordinates whose form is suggested by the exact solutions (7) and (9), but which will also be valid for more general problems in which there is no simple closed-form solution. For the most general case, we set

$$\xi = \frac{x}{s(t)}, \quad T = h(t)F(\xi, t), \tag{10}$$

so that Eqs. (1), (4)–(6) become

$$h \frac{\partial^2 F}{\partial \xi^2} = s \left[ s \frac{dh}{dt} F + sh \frac{\partial F}{\partial t} - \xi \frac{ds}{dt} h \frac{\partial F}{\partial \xi} \right], \tag{11}$$

$$F = 0, \quad \text{at } \xi = 1, \tag{12}$$

$$\beta s \frac{ds}{dt} = -h \frac{\partial F}{\partial \xi}, \quad \text{at } \xi = 1, \tag{13}$$

$$(i) F = \frac{1}{h}, \quad (ii) F = \frac{e^t - 1}{h}, \quad (iii) h \frac{\partial F}{\partial \xi} = -se^t, \quad (iv) F = \frac{1 - \epsilon \sin(\omega t)}{h}, \quad \text{at } \xi = 0. \tag{14}$$

Eq. (2) remains unchanged, but the interpretation of Eq. (3) in terms of  $F$  must be treated on a case-by-case basis. In addition, we need to choose  $h(t)$  in such a way as to ensure that a self-consistent boundary-value problem is obtained in the limit as  $t \rightarrow 0$ , in the sense that the problem remains well-posed. Ultimately, this analysis will constitute the basis of the numerical scheme, since it dictates the transformation used for the governing equations.

- (i) For boundary condition (14i), the choice  $h(t) = 1$  ensures that  $F(0, t)$  is independent of time as  $t \rightarrow 0$ . Also, setting  $s(t) = 2\alpha\sqrt{t}$ , the system (11)–(14) reduces to

$$\frac{\partial^2 F}{\partial \xi^2} = -2\alpha^2 \xi \frac{\partial F}{\partial \xi}, \tag{15}$$

subject to

$$F(1) = 0, \quad F(0) = 1, \quad 2\alpha^2 \beta = - \left. \frac{\partial F}{\partial \xi} \right|_{\xi=1}, \tag{16}$$

in the limit as  $t \rightarrow 0$ . This has solution

$$F(\xi) = 1 - \frac{\text{erf}(\alpha\xi)}{\text{erf} \alpha}, \tag{17}$$

where  $\alpha$  again satisfies (8); moreover, this solution is consistent with initial condition (3). Note that since  $\xi = \frac{x}{s} = \frac{x}{2\alpha\sqrt{t}}$ , the self-similarity solution is actually the exact solution (7) for all time. Although this model problem is studied extensively in the literature, it turns out from our results in Section 5 below that this is a misleading test case for comparing the order of accuracy of various numerical methods, apparently because the solution is independent of  $t$  once the coordinate transformation is applied. A more representative problem is the one using time-dependent condition (ii), which we consider next.

- (ii) In the case of boundary condition (14ii), the expansion

$$e^t - 1 \sim t \left( 1 + \frac{1}{2}t + \dots \right),$$

for small  $t$  indicates that we should take  $h(t) = t$ . Then, from examining the Stefan condition (13), we must have  $s \frac{ds}{dt} = \mathcal{O}(t)$ , which implies that  $s(t) \sim \lambda t$  for some strictly positive constant  $\lambda$ . The system (11)–(13), (14i) becomes, in the limit as  $t \rightarrow 0$ ,

$$\frac{\partial^2 F}{\partial \xi^2} = 0, \tag{18}$$

subject to

$$F(1) = 0, \quad F(0) = 1, \quad \beta\lambda^2 = -\frac{\partial F}{\partial \xi}\Big|_{\xi=1}. \tag{19}$$

This has solution

$$F(\xi) = 1 - \xi, \quad \lambda = \frac{1}{\sqrt{\beta}}, \tag{20}$$

where we take the positive root for  $\lambda$ , and once again consistency with initial condition (3) is maintained.

(iii) For boundary condition (14iii), it is clear that we should choose  $h(t) = s(t)$  which gives  $\frac{\partial F}{\partial \xi}\Big|_{\xi=0} \rightarrow -1$  as  $t \rightarrow 0$ . The Stefan condition (12) shows that  $\frac{ds}{dt} = \mathcal{O}(1)$  and so again a self-consistent boundary-value problem is obtained as  $t \rightarrow 0$  if  $s(t) \sim \lambda t$ . Then the system (11)–(13), (14i) again reduces to Eq. (18) subject to

$$F(1) = 0, \quad \frac{\partial F}{\partial \xi}\Big|_{\xi=0} = -1, \quad \beta\lambda = -\frac{\partial F}{\partial \xi}\Big|_{\xi=1}, \tag{21}$$

in the limit as  $t \rightarrow 0$ . This also has solution  $F(\xi) = 1 - \xi$ , but now  $\lambda = \frac{1}{\beta}$ .

(iv) Finally, it is clear that the boundary condition (14iv) requires the same choice  $h(t) = 1$  as for boundary condition (14i). The boundary condition at  $\xi = 0$  also reduces to  $F(0) = 1$  in the limit  $t \rightarrow 0$  and so we again solve (15,16) to give solution (17).

In summary, we have found that for both temperature and heat-flux conditions at  $x = 0$  it is possible to find appropriate coordinate transformations which ensure that the original problem can be recast into a self-consistent and self-similar problem as  $t \rightarrow 0$ , and then leads to the appropriate initial condition for the full PDE, without the need for any additional assumptions. Although the self-similarity solution happens to be the exact solution for all time in one of the cases we have looked at here, and there is an analytical solution for two of the other cases, we have shown that the idea can be extended to cases where the solution cannot be found in closed form.

Before describing the numerical schemes, we briefly highlight other examples without an exact solution. Consider the following two cases, similar to boundary conditions (ii) and (iii),

$$(ii') \quad T \sim t^\alpha, \quad (iii') \quad \frac{\partial T}{\partial x} \sim -t^\alpha, \quad \text{at } x = 0 \text{ as } t \rightarrow 0, \tag{22}$$

where  $\alpha > 0$ , which lead to the following development:

(ii') Here we set

$$h(t) = t^\alpha,$$

with  $s(t) \sim \lambda t^{\frac{\alpha+1}{2}}$  initially. In the limit as  $t \rightarrow 0$ , the PDE (11) reduces to (18) subject to

$$F(1) = 0, \quad F(0) = 1, \quad \frac{\beta\lambda^2(\alpha+1)}{2} = -\frac{\partial F}{\partial \xi}\Big|_{\xi=1}.$$

As before, this gives the solution  $F(\xi) = 1 - \xi$ , with  $\lambda = \sqrt{\frac{2}{\beta(\alpha+1)}}$ .

(iii') For this condition we set

$$h(t) = t^{2\alpha+1},$$

with  $s(t) \sim \lambda t^{\alpha+1}$  initially. In the limit as  $t \rightarrow 0$ , we therefore solve (18) subject to

$$F(1) = 0, \quad \frac{\partial F}{\partial \xi}\Big|_{\xi=0} = -\lambda, \quad \beta\lambda^2(\alpha+1) = -\frac{\partial F}{\partial \xi}\Big|_{\xi=1}.$$

The solution here is  $F(\xi) = \lambda(1 - \xi)$ , with  $\lambda = \frac{1}{\beta(\alpha+1)}$ .

Furthermore, this type of analysis is also applicable to problems with the Robin condition specified at  $x = 0$ , which in canonical form is given by

$$\frac{\partial T}{\partial x} = T - 1.$$

Applying the change of variables in (10) shows that  $h = s$  and so this case can be solved in the same way as boundary condition (iii) in the limit  $t \rightarrow 0$ .

#### 4. Numerical schemes

In this section, three finite-difference schemes are described to solve the system (11)–(14). These are applied in the transformed coordinates  $(\xi, t)$  which allows the use of (17) and (20) to initialize each numerical scheme. In all cases, we assume a uniform discretization for  $\xi$  and  $t$ .

##### 4.1. A semi-implicit finite-difference scheme

Suppose we apply a semi-implicit discretization, based on that in [1], to (11)–(13), (14i) Since  $h(t) = 1$  here, it is convenient to define  $z = s^2$  which avoids a singularity in the Stefan condition at  $t = 0$ . This change of variable is also used in [7], although the reason given there is algebraic simplicity, rather than the realization that it helps to remove the singularity. In other work, for example [1,2,4,6], this transformation is not used at all and the singularity at  $t = 0$  is avoided only by solving in the region  $t > t^* > 0$ , where  $t^*$  is arbitrary, and taking the exact solution as the initial condition; using the correct initialization as described above, however, will enable us to solve the system from  $t = 0$ . Then, (11)–(13), (14i) reduce to

$$\frac{\partial^2 F}{\partial \xi^2} = z \frac{\partial F}{\partial t} - \frac{\xi}{2} \frac{dz}{dt} \frac{\partial F}{\partial \xi}, \tag{23}$$

$$F = 0, \quad \text{at } \xi = 1, \tag{24}$$

$$\frac{\beta}{2} \frac{dz}{dt} = -\frac{\partial F}{\partial \xi}, \quad \text{at } \xi = 1, \tag{25}$$

$$F = 1, \quad \text{at } \xi = 0, \tag{26}$$

with  $z(0) = 0$ . We discretize implicitly for  $F$  and explicitly for  $z$  and obtain

$$\left[ r + \frac{v}{4} \xi_i \left( \frac{dz}{dt} \right)^n \right] F_{i+1}^{n+1} - \{2r + z^n\} F_i^{n+1} + \left[ r - \frac{v}{4} \xi_i \left( \frac{dz}{dt} \right)^n \right] F_{i-1}^{n+1} = -z^n F_i^n, \tag{27}$$

which holds for  $i = 1, \dots, I - 1$  and  $n = 0, 1, 2, \dots$ , with  $r = \Delta t / (\Delta \xi)^2$  and  $v = \Delta t / \Delta \xi$ , where  $\Delta t$  and  $\Delta \xi (= 1/I)$  denote the sizes of the temporal and spatial steps, respectively. The Stefan condition in (25) becomes

$$\left( \frac{dz}{dt} \right)^n = -\frac{2(3F_i^n - 4F_{i-1}^n + F_{i-2}^n)}{2\beta \Delta \xi}. \tag{28}$$

In addition, the boundary conditions (24) and (26) are  $F_I^{n+1} = 0$  and  $F_0^{n+1} = 1$  respectively, and  $z$  is updated using the equation

$$z^{n+1} = z^n + \Delta t \left( \frac{dz}{dt} \right)^n. \tag{29}$$

Also, using the initial condition (17), we arrive at

$$F_i^0 = 1 - \frac{\text{erf}(\alpha \xi_i)}{\text{erf} \alpha}, \quad i = 0, 1, \dots, I. \tag{30}$$

The system (11)–(14iv) is identical except that  $F_0^{n+1} = 1$  is replaced by  $F_0^{n+1} = 1 - \epsilon \sin(\omega t^{n+1})$ . Note that the same is true for both the Keller box scheme and Crank–Nicolson schemes described in Sections 4.2 and 4.3 respectively, and so we do not repeat this below.

For boundary condition (ii), we solve the system (11)–(13), (14i) with  $h(t) = t$  and starting solution (20). Discretizing again implicitly for  $F$  and explicitly for  $s$ , (11) becomes

$$\left[ r + \frac{v}{2} \xi_i s^n \left( \frac{ds}{dt} \right)^n \right] F_{i+1}^{n+1} - \left[ 2r + (s^n)^2 + \Delta t \frac{(s^n)^2}{t^n} \right] F_i^{n+1} + \left[ r - \frac{v}{2} \xi_i s^n \left( \frac{ds}{dt} \right)^n \right] F_{i-1}^{n+1} = -(s^n)^2 F_i^n. \tag{31}$$

The Stefan condition in (13) is now

$$\left( \frac{ds}{dt} \right)^n = -\frac{t^n (3F_i^n - 4F_{i-1}^n + F_{i-2}^n)}{2\beta s^n \Delta \xi}. \tag{32}$$

We use  $F_I^{n+1} = 0$  for the boundary condition (12) and  $s$  update  $s$  using the equivalent form of (29). The boundary condition (14ii) is written as  $F_0^{n+1} = (e^{t^{n+1}} - 1) / t^{n+1}$  which is taken at  $n + 1$  to be consistent with the fact that we are discretizing  $F$  implicitly. When  $n = 0$  we use the initial condition (20) to deduce that  $F_0^0 = 1$ ; note also that, in equation Eq. (32), we set  $t^0 / s^0 = 1$ , since  $s \sim t$  as  $t \rightarrow 0$ . The initial condition is given here by

$$F_i^0 = 1 - \xi_i, \quad i = 0, 1, \dots, I. \tag{33}$$

In the case of boundary condition (iii), we solve the system (11)–(13), (14i) with  $h(t) = s(t)$  and starting solution (20). Similar to (31), this is discretized as

$$\left[ r + \frac{\nu}{2} \xi_i s^n \left( \frac{ds}{dt} \right)^n \right] F_{i+1}^{n+1} - \left[ 2r + (s^n)^2 + \Delta t s^n \left( \frac{ds}{dt} \right)^n \right] F_i^{n+1} \left[ r - \frac{\nu}{2} \xi_i s^n \left( \frac{ds}{dt} \right)^n \right] F_{i-1}^{n+1} = -(s^n)^2 F_i^n. \tag{34}$$

The Stefan condition here is simply

$$\left( \frac{ds}{dt} \right)^n = - \frac{3F_l^n - 4F_{l-1}^n + F_{l-2}^n}{2\beta \Delta \xi}, \tag{35}$$

and as usual  $F_l^{n+1} = 0$ . Finally we discretize (14iii) as

$$\frac{F_1^{n+1} - F_{-1}^{n+1}}{2\Delta \xi} = -e^{t^{n+1}}, \tag{36}$$

which is used to eliminate  $F_{-1}^{n+1}$  in (34). Thus the boundary condition at  $\xi = 0$  is

$$2rF_1^{n+1} - \left[ 2r + (s^n)^2 + \Delta t s^n \left( \frac{ds}{dt} \right)^n \right] F_0^{n+1} = -(s^n)^2 F_0^n - 2r\Delta \xi e^{t^{n+1}}. \tag{37}$$

For this case, the initial condition is as given in equation (33).

#### 4.2. The Keller box scheme

As discussed in Section 4.1 above, when applying finite-difference schemes to moving-boundary problems it is common [1,7] to use either a fully explicit scheme, or a semi-implicit scheme which treats  $F$  implicitly and  $s$  explicitly. The resulting discretized system is then linear and therefore straightforward to solve. However, a major difficulty with the fully explicit scheme is that it imposes a severe restriction on the size of timestep that can be used in order that stability is maintained [7]. The semi-implicit scheme, on the other hand, does not suffer from this constraint, but it is formally only first-order accurate due to the explicit discretization for  $s$  and the fully implicit discretization of the heat equation. An improvement in accuracy can come through implicit discretization about  $(n + \frac{1}{2})$ , rather than  $n + 1$ , since this will lead to a stable, second-order accurate scheme; as an alternative which has these properties, we propose first the very compact Keller box scheme [8,21,22], which uses four neighboring values of the unknowns and is fully *implicit*, as it involves two points at the new time level. Whilst this method has been used previously for moving-boundary problems [8], the novelty here is a different, and arguably simpler, iteration strategy for solving for  $F$  and  $s$ , as well as the natural incorporation of the small-time analysis to start the solution procedure.

Following [22], we begin by defining the following finite difference operators for a variable,  $U$ :

$$\mu_\xi U_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{2} (U_{j+1}^{n+\frac{1}{2}} + U_j^{n+\frac{1}{2}}), \quad \delta_\xi U_{j+\frac{1}{2}}^{n+\frac{1}{2}} = U_{j+1}^{n+\frac{1}{2}} - U_j^{n+\frac{1}{2}}, \tag{38}$$

$$\mu_t U_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{2} (U_{j+\frac{1}{2}}^{n+1} + U_{j+\frac{1}{2}}^n), \quad \delta_t U_{j+\frac{1}{2}}^{n+\frac{1}{2}} = U_{j+\frac{1}{2}}^{n+1} - U_{j+\frac{1}{2}}^n; \tag{39}$$

however, each of the cases (i)–(iii) needs to be considered separately. For boundary condition (i), we found earlier that  $h(t) = 1$  and so Eqs. (23)–(26) can be used directly. It is first convenient, as described in [8], to re-write them as a first-order system by setting  $V = \frac{\partial F}{\partial \xi}$ , which gives

$$\frac{\partial F}{\partial \xi} = V, \quad \frac{\partial V}{\partial \xi} = z \frac{\partial F}{\partial t} - \frac{\xi}{2} \frac{dz}{dt} V, \tag{40}$$

$$F = 0, \quad \text{at } \xi = 1, \tag{41}$$

$$\frac{\beta}{2} \frac{dz}{dt} = -V, \quad \text{at } \xi = 1, \tag{42}$$

$$F = 1, \quad \text{at } \xi = 0. \tag{43}$$

Then the box scheme applied to the PDEs in (40) can be written as

$$\frac{\delta_\xi F_{i+\frac{1}{2}}^{n+1}}{\Delta \xi} = \mu_\xi V_{i+\frac{1}{2}}^{n+1}, \tag{44}$$

$$\frac{\mu_t \delta_\xi V_{i+\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta \xi} = \mu_t z^{n+\frac{1}{2}} \frac{\mu_\xi \delta_t F_{i+\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta t} - \frac{\xi_{i+\frac{1}{2}}}{2} \frac{\delta_t z^{n+\frac{1}{2}}}{\Delta t} \mu_\xi \mu_t V_{i+\frac{1}{2}}^{n+\frac{1}{2}}, \tag{45}$$

which holds for  $i = 0, \dots, l-1$  and  $n = 0, 1, 2, \dots$ . The box scheme discretization of the Stefan condition in (42) becomes

$$\frac{\beta}{2} \frac{\delta_t z^{n+\frac{1}{2}}}{\Delta t} = -\mu_t V_l^{n+\frac{1}{2}}, \tag{46}$$

with  $z^0 = 0$ . The boundary conditions are  $F_l^n = 0$  and  $F_0^n = 1$  for  $n = 0, 1, 2, \dots$ . Using the initial condition (17), we deduce that

$$F_i^0 = 1 - \frac{\operatorname{erf}(\alpha \xi_i)}{\operatorname{erf} \alpha}, \quad V_i^0 = -\frac{2\alpha e^{-\alpha^2 \xi_i^2}}{\sqrt{\pi} \operatorname{erf} \alpha}, \quad \text{for } i = 0, \dots, I, \quad (47)$$

where  $V_i^0$  is found from differentiating  $F$  in (17) with respect to  $\xi$ .

In the case of boundary condition (ii), we consider (11)–(13), (14ii) with  $h(t) = t$ . The box scheme can be written as

$$\frac{\delta_\xi F_{i+\frac{1}{2}}^{n+1}}{\Delta \xi} = \mu_\xi V_{i+\frac{1}{2}}^{n+1}, \quad (48)$$

$$t^{n+\frac{1}{2}} \frac{\mu_t \delta_\xi V_{i+\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta \xi} = \left(\mu_t S^{n+\frac{1}{2}}\right)^2 \mu_\xi \mu_t F_{i+\frac{1}{2}}^{n+\frac{1}{2}} + t^{n+\frac{1}{2}} \left(\mu_t S^{n+\frac{1}{2}}\right)^2 \frac{\mu_\xi \delta_t F_{i+\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta t} - t^{n+\frac{1}{2}} \xi_{i+\frac{1}{2}} \mu_t S^{n+\frac{1}{2}} \frac{\delta_t S^{n+\frac{1}{2}}}{\Delta t} \mu_\xi \mu_t V_{i+\frac{1}{2}}^{n+\frac{1}{2}}, \quad (49)$$

which holds for  $i = 0, \dots, I - 1$  and  $n = 0, 1, 2, \dots$ . The Stefan condition (13) becomes

$$\beta \mu_t S^{n+\frac{1}{2}} \frac{\delta_t S^{n+\frac{1}{2}}}{\Delta t} = -t^{n+\frac{1}{2}} \mu_t V_I^{n+\frac{1}{2}}, \quad (50)$$

with  $s^0 = 0$ , and the boundary conditions are  $F_I^n = 0$  and  $F_0^n = (e^{t^n} - 1)/t^n$  for  $n = 0, 1, 2, \dots$ . Using the initial condition (20) we deduce that

$$F_i^0 = 1 - \xi_i, \quad V_i^0 = -1, \quad \text{for } i = 0, \dots, I. \quad (51)$$

Finally, consider the system (11)–(13), (14iii) with  $h(t) = s(t)$ . Analogous to Eqs. (48) and (49), the box scheme here is given by

$$\frac{\delta_\xi F_{i+\frac{1}{2}}^{n+1}}{\Delta \xi} = \mu_\xi V_{i+\frac{1}{2}}^{n+1}, \quad (52)$$

$$\frac{\mu_t \delta_\xi V_{i+\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta \xi} = \mu_t S^{n+\frac{1}{2}} \frac{\delta_t S^{n+\frac{1}{2}}}{\Delta t} \mu_\xi \mu_t F_{i+\frac{1}{2}}^{n+\frac{1}{2}} + \left(\mu_t S^{n+\frac{1}{2}}\right)^2 \frac{\mu_\xi \delta_t F_{i+\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta t} - \xi_{i+\frac{1}{2}} \mu_t S^{n+\frac{1}{2}} \frac{\delta_t S^{n+\frac{1}{2}}}{\Delta t} \mu_\xi \mu_t V_{i+\frac{1}{2}}^{n+\frac{1}{2}}, \quad (53)$$

which holds for  $i = 0, \dots, I - 1$  and  $n = 0, 1, 2, \dots$ . The Stefan condition (13) is simply

$$\beta \frac{\delta_t S^{n+\frac{1}{2}}}{\Delta t} = -\mu_t V_I^{n+\frac{1}{2}}, \quad (54)$$

with  $s^0 = 0$ . The boundary conditions satisfy  $F_I^n = 0$  and  $V_0^n = -e^{t^n}$  for  $n = 0, 1, 2, \dots$ , and initial conditions are again as given by (51).

It should be noted that all three systems, (44) and (45), (48) and (49) and (52) and (53), involve  $z^{n+1}$  or  $s^{n+1}$  and so it is necessary to solve a nonlinear equation at each timestep. This is achieved by iterating on  $z$  or  $s$ , using their values at level  $n$  as a starting guess, and then updating using the Stefan condition (46), (50) or (54) until some desired tolerance,  $\varepsilon$ , is reached. Denoting by  $s_{(m)}^{n+1}$  and  $z_{(m)}^{n+1}$  the values for  $s^{n+1}$  and  $z^{n+1}$  after  $m$  iterations, the convergence criterion used is

$$\left| z_{(m+1)}^{n+1} - z_{(m)}^{n+1} \right| < \varepsilon, \quad (55)$$

for the problem with boundary condition (i), and

$$\left| s_{(m+1)}^{n+1} - s_{(m)}^{n+1} \right| < \varepsilon, \quad (56)$$

for the problems with boundary conditions (ii) and (iii).

### 4.3. The Crank–Nicolson scheme

We now consider the well-known Crank–Nicolson scheme which, like the Keller box scheme, is unconditionally stable and second-order accurate. The method involves using a central difference at time  $t^{n+\frac{1}{2}}$  and a second-order central difference for the space derivative at position  $\xi_i$ .

For boundary condition (i), we apply the Crank–Nicolson scheme to the system (23)–(26). The discretization of the PDE (23) is therefore

$$\frac{1}{2} \left( \frac{F_{i+1}^{n+1} - 2F_i^{n+1} + F_{i-1}^{n+1}}{\Delta \xi^2} \right) + \frac{1}{2} \left( \frac{F_{i+1}^n - 2F_i^n + F_{i-1}^n}{\Delta \xi^2} \right) = z^{n+\frac{1}{2}} \left[ \frac{F_i^{n+1} - F_i^n}{\Delta t} \right] - \frac{\xi_i}{2} \frac{z^{n+1} - z^n}{\Delta t} \left[ \frac{1}{2} \left( \frac{F_{i+1}^{n+1} - F_{i-1}^{n+1}}{2\Delta \xi} \right) + \frac{1}{2} \left( \frac{F_{i+1}^n - F_{i-1}^n}{2\Delta \xi} \right) \right], \quad (57)$$



which holds for  $i = 1, \dots, I - 1$  and  $n = 0, 1, 2, \dots$ . Note that  $z^{n+\frac{1}{2}} = \frac{1}{2}(z^n + z^{n+1})$ , and similarly for  $s^{n+\frac{1}{2}}$  in the equations given below. The boundary conditions become  $F_I^{n+1} = 0$  and  $F_0^{n+1} = 1$  and the Stefan condition (25) is approximated by

$$\frac{\beta}{2} \left( \frac{z^{n+1} - z^n}{\Delta t} \right) = -\frac{1}{2} \left( \frac{F_{I+1}^{n+1} - F_{I-1}^{n+1}}{2\Delta\xi} \right) - \frac{1}{2} \left( \frac{F_{I+1}^n - F_{I-1}^n}{2\Delta\xi} \right). \tag{58}$$

Eq. (58) involves the fictitious values  $F_{I+1}^{n+1}$  and  $F_{I+1}^n$ , but these can be eliminated using (57) evaluated at  $i = I$ . This leads to the following quadratic equation for  $z^{n+1}$ :

$$\frac{\beta\xi_I}{2\Delta t} (z^{n+1})^2 + \left[ -\frac{\beta\xi_I}{\Delta t} z^n + \frac{2\beta r}{v} + F_I^{n+1} - F_I^n \right] z^{n+1} + \frac{\beta\xi_I}{2\Delta t} (z^n)^2 - \frac{2\beta r}{v} z^n + (2r + z^n)F_I^{n+1} + (2r - z^n)F_I^n - 2r(F_{I-1}^{n+1} + F_{I-1}^n) = 0. \tag{59}$$

In the case of boundary condition (ii), we apply the Crank–Nicolson scheme to the system (11)–(13), (14i) with  $h(t) = t$ . Then

$$t^{n+\frac{1}{2}} \left[ \frac{1}{2} \left( \frac{F_{i+1}^{n+1} - 2F_i^{n+1} + F_{i-1}^{n+1}}{\Delta\xi^2} \right) + \frac{1}{2} \left( \frac{F_{i+1}^n - 2F_i^n + F_{i-1}^n}{\Delta\xi^2} \right) \right] = (s^{n+\frac{1}{2}})^2 \frac{1}{2} (F_i^{n+1} + F_i^n) + t^{n+\frac{1}{2}} (s^{n+\frac{1}{2}})^2 \frac{F_i^{n+1} - F_i^n}{\Delta t} - \xi_i t^{n+\frac{1}{2}} s^{n+\frac{1}{2}} \frac{s^{n+1} - s^n}{\Delta t} \left[ \frac{1}{2} \left( \frac{F_{i+1}^{n+1} - F_{i-1}^{n+1}}{2\Delta\xi} \right) + \frac{1}{2} \left( \frac{F_{i+1}^n - F_{i-1}^n}{2\Delta\xi} \right) \right]. \tag{60}$$

The boundary conditions are  $F_I^{n+1} = 0$  and

$$\frac{1}{2} (F_0^{n+1} + F_0^n) = \frac{1}{2} \left( \frac{e^{t^{n+1}} - 1}{t^{n+1}} + \frac{e^{t^n} - 1}{t^n} \right), \tag{61}$$

and the Stefan condition (13) is now

$$\beta s^{n+\frac{1}{2}} \left( \frac{s^{n+1} - s^n}{\Delta t} \right) = -\frac{1}{2} t^{n+\frac{1}{2}} \left( \frac{F_{I+1}^{n+1} - F_{I-1}^{n+1}}{2\Delta\xi} \right) - \frac{1}{2} t^{n+\frac{1}{2}} \left( \frac{F_{I+1}^n - F_{I-1}^n}{2\Delta\xi} \right). \tag{62}$$

Again we use (60) to eliminate  $F_{I+1}^{n+1}$  and  $F_{I+1}^n$  which gives a quartic expression to solve for  $s^{n+1}$ :

$$2r(t^{n+1} + t^n)(F_{I-1}^{n+1} + F_{I-1}^n) - \left[ 2r(t^{n+1} + t^n) + \frac{1}{2} \Delta t (s^{n+1} + s^n)^2 \right] (F_I^{n+1} + F_I^n) - \frac{4\beta}{v} \left[ r(t^{n+1} + t^n) + \frac{\xi_I}{4\Delta\xi} (t^{n+1} + t^n)((s^{n+1})^2 - (s^n)^2) \right] \frac{(s^{n+1})^2 - (s^n)^2}{t^{n+1} + t^n} - \frac{1}{2} (t^{n+1} + t^n)(s^{n+1} + s^n)^2 (F_I^{n+1} - F_I^n) = 0. \tag{63}$$

Finally, we consider boundary condition (iii) and therefore apply the Crank–Nicolson scheme to (11)–(13), (14i) with  $h(t) = s(t)$ . Then

$$\frac{1}{2} \left( \frac{F_{i+1}^{n+1} - 2F_i^{n+1} + F_{i-1}^{n+1}}{\Delta\xi^2} \right) + \frac{1}{2} \left( \frac{F_{i+1}^n - 2F_i^n + F_{i-1}^n}{\Delta\xi^2} \right) = s^{n+\frac{1}{2}} \frac{s^{n+1} - s^n}{\Delta t} \frac{1}{2} (F_i^{n+1} + F_i^n) + (s^{n+\frac{1}{2}})^2 \frac{F_i^{n+1} - F_i^n}{\Delta t} - \xi_i s^{n+\frac{1}{2}} \frac{s^{n+1} - s^n}{\Delta t} \left[ \frac{1}{2} \left( \frac{F_{i+1}^{n+1} - F_{i-1}^{n+1}}{2\Delta\xi} \right) + \frac{1}{2} \left( \frac{F_{i+1}^n - F_{i-1}^n}{2\Delta\xi} \right) \right]. \tag{64}$$

We again have  $F_I^{n+1} = 0$  and the boundary condition (14iii) is approximated as

$$\frac{1}{2} \left( \frac{F_1^{n+1} - F_{-1}^{n+1}}{2\Delta\xi} \right) + \frac{1}{2} \left( \frac{F_1^n - F_{-1}^n}{2\Delta\xi} \right) = \frac{1}{2} (e^{t^{n+1}} + e^{t^n}). \tag{65}$$

The fictitious values  $F_{-1}^{n+1}$  and  $F_{-1}^n$  are again eliminated using (64), which leads to the expression

$$2rF_1^{n+1} - \left[ 2r + \frac{1}{2} ((s^{n+1})^2 - (s^n)^2) + \frac{1}{2} (s^{n+1} + s^n)^2 \right] F_0^{n+1} = -2r\Delta\xi (e^{t^{n+1}} + e^{t^n}) - 2rF_1^n + \left[ 2r + \frac{1}{2} ((s^{n+1})^2 - (s^n)^2) - \frac{1}{2} (s^{n+1} + s^n)^2 \right] F_0^n. \tag{66}$$

The Stefan condition (13) is now

$$\beta \frac{s^{n+1} - s^n}{\Delta t} = -\frac{1}{2} \left( \frac{F_{I+1}^{n+1} - F_{I-1}^{n+1}}{2\Delta\xi} \right) - \frac{1}{2} \left( \frac{F_{I+1}^n - F_{I-1}^n}{2\Delta\xi} \right), \tag{67}$$

which, after using (64) to eliminate  $F_{I+1}^{n+1}$  and  $F_{I-1}^{n+1}$ , gives the following cubic polynomial for  $s^{n+1}$ :

$$2r(F_{I-1}^{n+1} + F_{I-1}^n) - \frac{4\beta}{v} \left[ r + \frac{\xi_I}{4\Delta\xi} ((s^{n+1})^2 - (s^n)^2) \right] (s^{n+1} - s^n) - \left[ 2r + \frac{1}{2} ((s^{n+1})^2 - (s^n)^2) \right] (F_I^{n+1} + F_I^n) - \frac{1}{2} (s^{n+1} + s^n)^2 (F_I^{n+1} - F_I^n) = 0. \tag{68}$$

As occurs for the box scheme, the Eqs. (57), (60) and (64) involve  $z$  or  $s$  at the new time level and so we iterate using their values at level  $n$  as starting guesses. We again update using the Stefan conditions or (58), (62), or (67) but for the time-dependent boundary conditions (ii) and (iii) these are cubic and quartic, respectively, and so require a further nonlinear solve at each timestep. Computationally, this is marginally more expensive than the box scheme and also gives rise to possible multiple roots for  $s$ , although since the solution for  $s$  at level  $n$  is used as the initial guess, this does not lead to any insurmountable difficulty. Here also, criteria (55) and (56) are used for determining convergence.

### 5. Results and discussion

In presenting the results, we consider first cases (i)–(iii) for which comparison with exact analytical solutions is possible; then, we consider case (iv), for which there is no analytical solution.

#### 5.1. Cases (i)–(iii)

In this section, results are given for boundary conditions (i)–(iii) obtained using the three numerical schemes described above in Section 4, by comparison with the exact solutions (7) and (9). Note that, in the results shown below,  $\beta = 1$  for boundary conditions (ii) and (iii). In all computations, we have taken  $\Delta t = \Delta\xi$ , so that  $v = 1$ . For  $\Delta\xi$ , we consider a sequence  $\Delta\xi_k$ , where

$$\Delta\xi_k = 2^{-k} \Delta\xi_0, \quad k = 1, 2, \dots,$$

and  $\Delta\xi_0 = 0.1$ ; in addition, we denote the meshes by

$$\xi_{i,k} = i \Delta\xi_k, \quad i = 0, 1, \dots, I_k, \quad k = 0, 1, 2, \dots,$$

where

$$I_k = 2^k I_0, \quad k = 1, 2, \dots,$$

with  $I_0 = 10$ . Also, for the computations using the Keller box and Crank–Nicolson schemes, which involve an iterative loop for  $s$ , we use  $\varepsilon = 10^{-13}$ ; this leads to an iteration count until convergence of between 10 and 20 on average, which can be reduced by taking  $\varepsilon$  larger, if necessary.

##### 5.1.1. Results for $s(t)$

We begin by presenting, in Fig. 1, the absolute error in  $s$  as a function of time, found from computing

$$|s(t^n) - s^n|,$$

with  $\Delta t = \Delta\xi = 0.1$ . Observe here that, whereas there are two orders of magnitude difference in the errors between the results of the semi-implicit and the other two schemes when using boundary conditions (ii) and (iii), there is nowhere near the same difference when using boundary condition (i). This result, along with those given for  $F$  in the next section, support our hypothesis that for this boundary condition the PDE is effectively an ODE, so that the only discretization errors arising are those due to the discretization in  $\xi$ .

##### 5.1.2. Results for $F$

Whereas most authors present only results for  $s(t)$  as evidence of the effectiveness of their numerical scheme, we demonstrate that it is just as important to investigate the numerical results for the temperature-related variable,  $F$ . To do this, we follow Strikwerda [23] and determine formally the order of accuracy of the three finite-difference schemes. Denoting the exact solution at  $\xi = \xi_i$  and  $t = t^n$  by  $F(\xi_i, t^n)$  and the numerical solution by  $F_i^n$ , the error at time  $t^n$  is given by

$$\text{Error}(t^n) = E^n = \left( \Delta\xi \sum_{i=0}^I (F(\xi_i, t^n) - F_i^n)^2 \right)^{1/2}. \tag{69}$$

The order of accuracy of the solution is defined to be the number  $p$ , if it exists, where

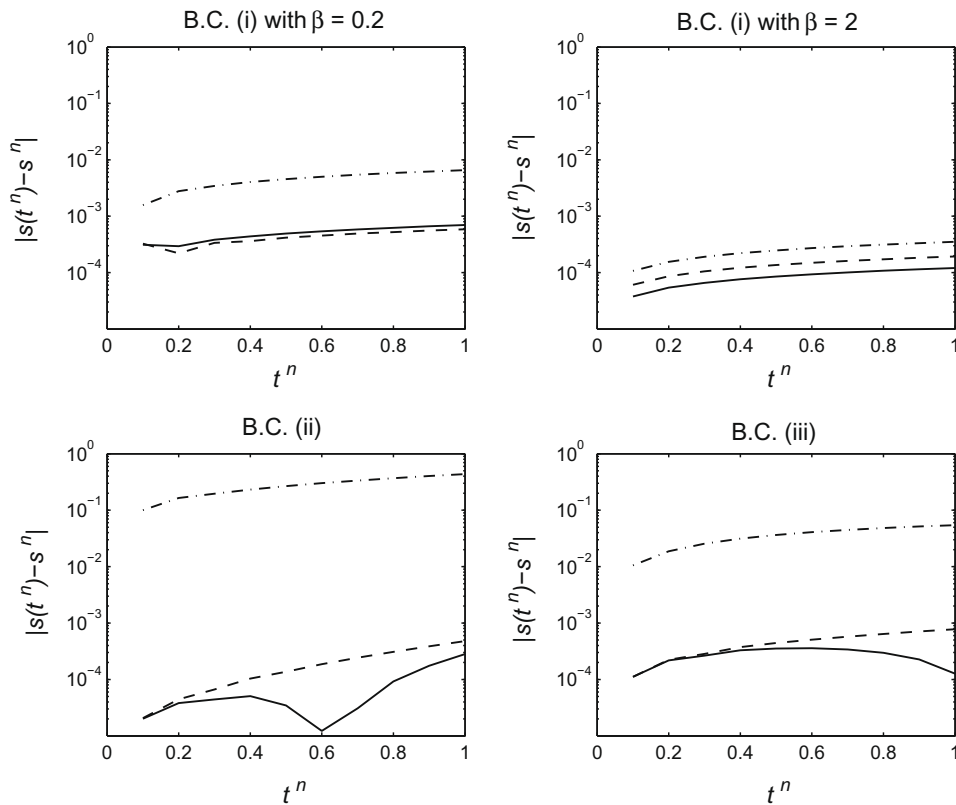


Fig. 1. Comparison of the absolute error in  $s$ , for  $0 \leq t \leq 1$  (where --- denotes semi-implicit, — denotes Keller box and - · - denotes Crank–Nicolson).

$$E^n = \mathcal{O}(\Delta \xi^p). \tag{70}$$

Defining the sequence

$$E_k^n := \left( \Delta \xi_k \sum_{i=0}^{I_0} (F(\xi_{i,0}, t^n) - F_{2^k i}^n)^2 \right)^{1/2}, \quad k = 0, 1, 2, \dots, \tag{71}$$

it follows that, if (70) holds,

$$p = \frac{\ln(E_k^n / E_{k+1}^n)}{\ln(\Delta \xi_k / \Delta \xi_{k+1})} = \frac{\ln(E_k^n / E_{k+1}^n)}{\ln 2}. \tag{72}$$

If the initial and boundary data are smooth, the order of accuracy of the solution is equal to the order of accuracy of the numerical scheme.

The errors in  $F$  are shown in Tables 1–4. As expected,  $p$  converges to 2 for the Keller box and Crank–Nicolson schemes in all cases and so they are second-order accurate. On the other hand, the semi-implicit scheme exhibits characteristics that are consistent with second-order accuracy in Tables 1 and 2, which show the results for boundary condition (i) for  $\beta = 0.2$  and  $\beta = 2$  respectively, although the convergence of  $p$  towards 2 is much slower than for the other two schemes. However,  $p$  tends towards 1 for this scheme in Tables 3 and 4, which show the results for boundary conditions (ii) and (iii), respectively. Thus, whilst the semi-implicit scheme is much simpler in its algebraic conception, it is considerably less accurate, for a given

Table 1

Comparison of the order of accuracy of the numerical solutions, using (72), for  $F$  at fixed  $t^n = 1$  for boundary condition (i),  $\beta = 0.2$ .

$\Delta \xi$	Semi-implicit		Keller box		Crank–Nicolson	
	$E^n$	Order, $p$	$E^n$	Order, $p$	$E^n$	Order, $p$
1/10	$2.50 \times 10^{-4}$		$2.47 \times 10^{-4}$		$3.31 \times 10^{-4}$	
1/20	$7.08 \times 10^{-5}$	1.81737	$6.16 \times 10^{-5}$	2.00331	$8.27 \times 10^{-5}$	2.00102
1/40	$1.86 \times 10^{-5}$	1.93151	$1.54 \times 10^{-5}$	2.00088	$2.07 \times 10^{-5}$	2.00029
1/80	$4.74 \times 10^{-6}$	1.97050	$3.85 \times 10^{-6}$	2.00022	$5.17 \times 10^{-6}$	2.00008
1/160	$1.20 \times 10^{-6}$	1.98634	$9.61 \times 10^{-7}$	2.00006	$1.30 \times 10^{-6}$	2.00002

**Table 2**

Comparison of the order of accuracy of the numerical solutions, using (72), for  $F$  at fixed  $t^n = 1$  for boundary condition (i),  $\beta = 2$ .

$\Delta \zeta$	Semi-implicit		Keller box		Crank–Nicolson	
	$E^n$	Order, $p$	$E^n$	Order, $p$	$E^n$	Order, $p$
1/10	$2.27 \times 10^{-5}$		$7.71 \times 10^{-6}$		$2.04 \times 10^{-7}$	
1/20	$5.43 \times 10^{-6}$	2.06463	$1.93 \times 10^{-6}$	1.99987	$5.40 \times 10^{-8}$	1.91905
1/40	$1.33 \times 10^{-6}$	2.03364	$4.82 \times 10^{-7}$	2.00015	$1.36 \times 10^{-8}$	1.98695
1/80	$3.28 \times 10^{-7}$	2.01716	$1.20 \times 10^{-7}$	2.00005	$3.41 \times 10^{-9}$	1.99703
1/160	$8.14 \times 10^{-8}$	2.00867	$3.01 \times 10^{-8}$	2.00002	$8.53 \times 10^{-10}$	1.99919

**Table 3**

Comparison of the order of accuracy of the numerical solutions, using (72), for  $F$  at fixed  $t^n = 1$  for boundary condition (ii),  $\beta = 1$ .

$\Delta \zeta$	Semi-implicit		Keller box		Crank–Nicolson	
	$E^n$	Order, $p$	$E^n$	Order, $p$	$E^n$	Order, $p$
1/10	$1.05 \times 10^{-2}$		$1.17 \times 10^{-4}$		$8.95 \times 10^{-5}$	
1/20	$5.16 \times 10^{-3}$	1.01803	$2.93 \times 10^{-5}$	1.99858	$2.25 \times 10^{-5}$	1.99203
1/40	$2.56 \times 10^{-3}$	1.01090	$7.34 \times 10^{-6}$	1.99950	$5.63 \times 10^{-6}$	1.99943
1/80	$1.28 \times 10^{-3}$	1.00589	$1.83 \times 10^{-6}$	1.99987	$1.41 \times 10^{-6}$	1.99991
1/160	$6.37 \times 10^{-4}$	1.00305	$4.59 \times 10^{-7}$	1.99997	$3.52 \times 10^{-7}$	1.99998

**Table 4**

Comparison of the order of accuracy of the numerical solutions, using (72), for  $F$  at fixed  $t^n = 1$  for boundary condition (iii),  $\beta = 1$ .

$\Delta \zeta$	Semi-implicit		Keller box		Crank–Nicolson	
	$E^n$	Order, $p$	$E^n$	Order, $p$	$E^n$	Order, $p$
1/10	$7.14 \times 10^{-2}$		$5.39 \times 10^{-4}$		$9.60 \times 10^{-5}$	
1/20	$3.38 \times 10^{-2}$	1.07993	$1.2 \times 10^{-4}$	2.09558	$2.20 \times 10^{-5}$	2.12541
1/40	$1.64 \times 10^{-2}$	1.03983	$3.05 \times 10^{-5}$	2.04974	$5.26 \times 10^{-6}$	2.06468
1/80	$8.10 \times 10^{-3}$	1.01996	$7.48 \times 10^{-6}$	2.02536	$1.29 \times 10^{-6}$	2.03128
1/160	$4.02 \times 10^{-3}$	1.01000	$1.85 \times 10^{-6}$	2.01280	$3.18 \times 10^{-7}$	2.01509

value of  $\Delta t$ , than the other two methods. Whilst this lower accuracy can be made up for, in some sense, simply by using smaller time steps of size  $(\Delta \zeta)^2$ , this will clearly increase the computational load required to obtain solutions of comparable accuracy.

5.2. Case (iv)

In this section, we apply the three numerical schemes to boundary condition (iv). For brevity, we only show results for the temperature-related variable,  $F$ . Although there is no exact solution for comparison with the numerical solution, we can estimate the order of accuracy  $p$  in a similar manner to that described above. The standard procedure is to define, instead of  $E_k^n$  in (71),

$$\bar{E}_k^n := \left( \sum_{i=0}^{I_0} (F_{2^{k+1}i}^n - F_{2^k i}^n)^2 \right)^{1/2}, \quad k = 0, 1, 2, \dots, \tag{73}$$

and then

$$p = \frac{\ln(\bar{E}_k^n / \bar{E}_{k+1}^n)}{\ln(\Delta \zeta_k / \Delta \zeta_{k+1})} = \frac{\ln(\bar{E}_k^n / \bar{E}_{k+1}^n)}{\ln 2}. \tag{74}$$

To show that this approach gives the correct order of accuracy, we apply it to one of the cases that has an exact solution, for which the formal order of convergence has already been calculated. The results are shown in Table 5 for case (ii) and we observe the same order of convergence as in Table 3; this case was chosen as it also describes a fixed time-dependent boundary condition at  $x = 0$ , although either case (i) or (iii) could equally have been used.

To highlight the advantages of our approach, we note the differences as compared with the solution of the problem by Savović and Caldwell [6]. They apply an explicit finite-difference method to the (23)–(26), but with  $F(0, t) = 1 - \epsilon \sin(\omega t)$  replacing (26) and without the transformation from  $s$  to  $z$ ; subsequently, they use a forward difference scheme for the time

**Table 5**

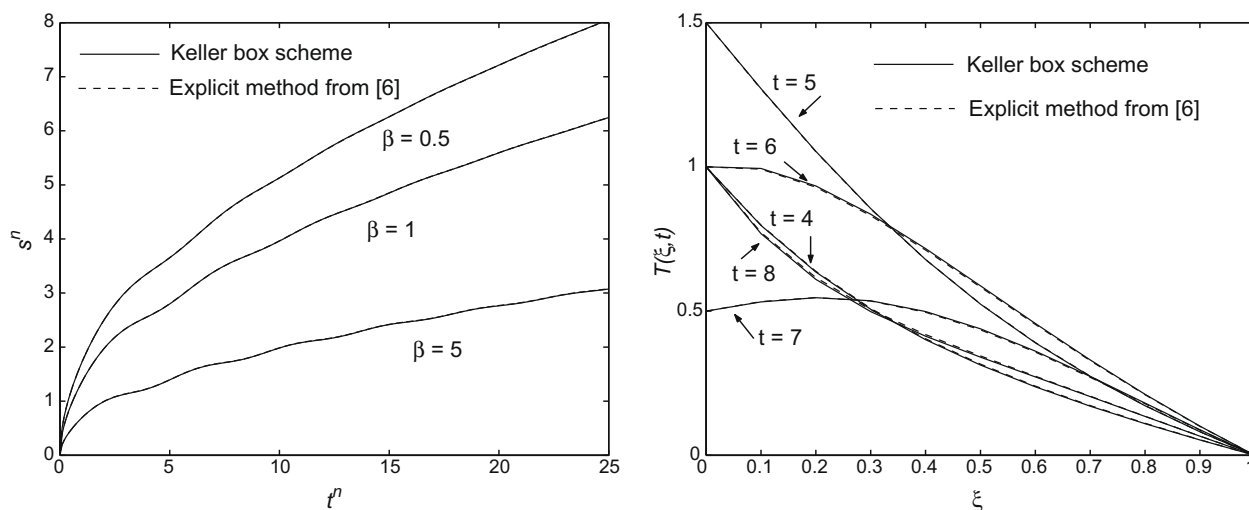
Comparison of the order of accuracy of the numerical solutions, using (74), for  $F$  at fixed  $t^n = 1$  for boundary condition (ii),  $\beta = 1$ .

$k$	Semi-implicit	Keller box	Crank–Nicolson
0	1.02528	1.99851	1.99050
1	1.01588	1.99934	1.99944
2	1.00871	1.99978	2.00001

**Table 6**

Comparison of the order of accuracy of the numerical solutions, using (74), for  $F$  at fixed  $t^n = 5$  for boundary condition (iv),  $\beta = 1, \epsilon = 0.5$  and  $\omega = \pi/2$ .

$k$	Semi-implicit	Keller box	Crank–Nicolson
0	1.04161	2.01142	1.96721
1	1.02070	2.00261	1.99186
2	1.01030	2.00064	1.99797



**Fig. 2.** Comparison of the Keller box scheme (—) and Savović and Caldwell's explicit scheme (---) with  $\epsilon = 0.5$  and  $\omega = \pi/2$ . Left: evolution of the moving boundary  $s$  for different values of  $\beta$ . Right: temperature distributions for  $\beta = 1$  at various times.

derivative and a central difference for the space derivative. Hence, not only does their method have severe stability restrictions, resulting from the use of an explicit formulation, but it also results in the appearance of  $s$  in the denominator of a term in the difference equations, leading to difficulties as  $t \rightarrow 0$ . To avoid these, the exact solution corresponding to the constant boundary condition  $F(0, t) = 1$  is used until a short time interval  $t_{in}$  after  $t = 0$ . Our analysis in §3, on the other hand, shows how to avoid this difficulty, so that we can solve the full problem from  $t = 0$ . It also explains why the same initialization procedure could be used by Savović and Caldwell [6] for case (iv) as by Rizwan-uddin [20] for the case of a ramped temperature boundary condition,  $T(x = 0, t) = 1 - 0.2t$ : in both cases,  $T(x = 0, t) \rightarrow 1$  as  $t \rightarrow 0$ . In addition, none of the finite-difference schemes presented here have stability restrictions.

In Table 6 we present the order of accuracy for the numerical solutions. Following [6], we use  $\beta = 1, \epsilon = 0.5$  and  $\omega = \pi/2$ , and as before set  $\Delta t = \Delta \xi$ , so that  $\nu = 1$ . Notice that we also obtain second-order accuracy in both time and space for this boundary condition.

The results shown in Table 6 are given at  $t = 5$  because [6] are interested in applying their numerical scheme for large times; their plots of the moving boundary are presented up until  $t = 25$ . In Fig. 2 we compare the Keller box scheme with the explicit scheme defined in [6]. The left plot shows  $s(t)$  against  $t$  for the same values of  $\beta (= 1/Ste)$ , i.e.  $\beta = 1, 0.5, 5$ . For the box scheme we choose  $\Delta \xi = \Delta t = 0.1$  for all values of  $\beta$ . For the explicit scheme we choose the largest values of  $\Delta \xi$  and  $\Delta t$  which guarantee stability, namely  $\Delta \xi = 0.1, \Delta t = 1 \times 10^{-4}$  for  $\beta = 0.5, 1$  and  $\Delta \xi = 0.2, \Delta t = 1 \times 10^{-4}$  for  $\beta = 5$ . We see excellent agreement between both schemes but the considerable advantage of the box scheme is the fact that the timestep is  $\mathcal{O}(10^3)$  larger. This also affects the CPU time: to produce the results in the left plot in Fig. 2 the box scheme discretization required three orders of magnitude less CPU time than the explicit scheme on the same computational architecture.

**6. Conclusions**

This paper has considered the so-called boundary immobilization method for four benchmark time-dependent Stefan problems involving melting, in tandem with three finite-difference discretization schemes. A combined analytical and

numerical approach eliminated completely the *ad hoc* treatment for the starting solution that is often used; a systematic treatment for this was applied to the four test problems. Most usefully, the analysis presented here shows how to obtain starting solutions for cases where there is no analytic solution. In addition, an often-used semi-implicit finite-difference discretization scheme for the governing heat equation was shown to be only first-order accurate, and therefore inferior to the second-order accurate Keller box and Crank–Nicolson schemes. Although there is little to distinguish between the efficiency of these two schemes, the handling of updates for the location of the moving boundary with the Keller box method was independent of the type of boundary condition used and was therefore marginally preferable. In general terms, however, the box scheme is preferred since the derivatives are computed naturally as part of the formulation, and can be shown to be significantly more accurate than the derivatives of the Crank–Nicolson scheme, with typically at least one order of magnitude difference in the errors. In addition, the box scheme is amenable to the use of non-uniform meshes.

Further extensions of this work include application to problems where the governing equation itself is nonlinear, i.e. where the specific heat capacity and the thermal conductivity are both functions of temperature, and where there is heat transfer in the unmelted phase, leading to a two-phase moving-boundary problem. Also, we note that although the analysis presented here was ostensibly for a one-dimensional time-dependent problem, it also applies in the case of 2D and cylindrically symmetric *steady-state* asymptotic models for solidification in industrial continuous casting [24–26], wherein the axis along the direction of casting acts as the time-like variable.

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