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The extinction problem for three-dimensional inward solidification

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Abstract. The one-phase Stefan problem for the inward solidification of a three-dimensional body of liquid that is initially at its fusion temperature is considered. In particular, the shape and speed of the solid-melt interface is described at times just before complete freezing takes place, as is the temperature field in the vicinity of the extinction point. This is accomplished for general Stefan numbers by employing the Baiocchi transform. Other previous results for this problem are confirmed, for example the asymptotic analysis reveals the interface ultimately approaches an ellipsoid in shape, and furthermore, the accuracy of these results is improved. The results are arbitrary up to constants of integration that depend physically on both the Stefan number and the shape of the fixed boundary of the liquid region. In general it is not possible to determine this dependence analytically; however, the limiting case of large Stefan number provides an exception. For this limit a rather complete asymptotic picture is presented, and a recipe for the time it takes for complete freezing to occur is derived. The results presented here for fully three-dimensional domains complement and extend those given by McCue *et al.* [*Proc. R. Soc. London* A 459 (2003) 977], which are for two dimensions only, and for which a significantly different time dependence occurs.

Key words: extinction problem, inward solidification, matched asymptotic expansions, Stefan problem

1. Introduction

This paper is concerned with the inward solidification of a region of liquid which is initially at its fusion temperature. On assuming the physical properties of the liquid remain constant throughout the freezing process, and that heat flows through conduction only, we formulate a classical one-phase Stefan problem for the temperature in the *a priori* unknown solid phase. The interface between the solid and liquid phases is a moving boundary and, provided the initial liquid geometry satisfies some restrictions, the liquid phase contracts continuously to a point, which we refer to as the extinction point, in a finite time, which we refer to as the extinction time. The only parameter involved (apart from those which describe the initial geometry of the liquid region) is the Stefan number, which is a ratio of latent to sensible heat.

Inward solidification problems are well known to be difficult to treat analytically; as well as displaying the inherent complexities of a moving-boundary problem, they exhibit an intricate structure in the neighbourhood of the extinction point at times just before complete freezing. Accordingly, much interest has been devoted to numerical studies of inward solidification problems, such as those of Allen and Severn [1], Lazaridis [2], Crank and Gupta [3] and Crowley [4]. There has also been considerable progress made by the use of asymptotic methods, and this is the approach adopted in the present study. We therefore restrict ourselves to discussions on this topic.

For the case where the fixed boundary is spherical (or circular), one can develop perturbation solutions for the inward solidification problem in the limit of large Stefan number (see Pedroso and Domoto [5] and Riley *et al.* [6]). Under this assumption, the leading-order problem becomes quasi-steady, as the solid-liquid interface moves very slowly, and the time derivative of the temperature can be ignored. Such solutions, however, are singular at times close to extinction. Riley *et al.* [6] use the method of matched asymptotic expansions to deal with this singularity by considering a second time-scale in which it is no longer appropriate to neglect the time derivative. It happens that this solution in turn becomes singular, and further analysis in a third, exponentially short time-scale has been undertaken by both Stewartson and Waechter [7] and Soward [8] to complete the asymptotic description.

The question naturally arises as to what happens if the geometry lacks radial symmetry. In two dimensions, analyses of this problem were presented in Andreucci *et al.* [9] and McCue *et al.* [10]. Here, the solid-melt interface becomes elliptic in shape as the extinction time is approached, regardless of the initial geometry and the Stefan number. For the special limiting case of large Stefan number, McCue *et al.* [10] were able to give a rather complete asymptotic analysis of the problem by matching back onto earlier time-scales. They determined how the aspect ratio of the shrinking ellipse depends on the Stefan number and the initial geometry, and also were able to formulate recipes for the extinction time and the location of the extinction point. A related problem is the contraction of bubbles in Hele-Shaw cells, which has been studied by Entov and Etingof [11] and McCue *et al.* [12]. Here the bubble also becomes elliptic in shape just before extinction, regardless of the initial domain.

The present study is concerned with the more physically relevant situation in which the geometry is truly three-dimensional. That is, we extend the large-Stefan-number analyses of Stewartson and Waechter [7] and Soward [8] for the radially symmetric case to allow the initial region of liquid to have a general three-dimensional shape. All results presented here are analogous to those given in McCue *et al.* [10] (for example, in three dimensions we have shrinking ellipsoids), and the studies complement each other. We note that in three dimensions, the leading-order equations on the first time-scale are the same as those that describe contracting bubbles in porous media. This problem was analysed in McCue *et al.* [12], and we draw upon many of the results presented there.

It should be noted that the analysis presented for the third time-scale in [8] (where the solidification of a sphere was studied) is a generic extinction analysis, in the sense that it is in fact applicable for all values of the Stefan number. Such generic extinction behaviour was subsequently considered by Herrero and Velázquez [13], and this work was generalised to include fully three-dimensional domains by Andreucci *et al.* [9], who show that the vanishing region of liquid is ellipsoidal in shape. They also derive the rate at which the liquid region vanishes. We also present a generic extinction analysis, as it is needed to complete the asymptotic picture in the case of large Stefan number. In doing so, we are able to derive results not presented in Andreucci *et al.* [9] and to improve upon the accuracy of the asymptotic description for the rate at which the liquid region disappears. In fact, the asymptotic results given here are derived to as many orders as those of Soward [8] for the radially symmetric case.

The format of the paper is as follows. In the following section we derive the governing equations for our inward-solidification problem, and then reformulate them in terms of a Baiocchi transform. In Section 3, we summarise the generic extinction analysis, and improve on the results of Andreucci *et al.* [9]. The analysis for large Stefan number is presented in Section 4, and the paper is closed in Section 5 with a discussion.

2. Heat-conduction equations

We consider the solidification of a (convex) region of liquid that is initially at its fusion temperature u_F^*. The process begins at $t=0$ by fixing the temperature at the boundary of the liquid to be $u_W^* < u_F^*$. The result is that the liquid solidifies from the boundary inwards as the interface between the solid and the liquid regions propagates away from the fixed boundary into the fluid.

It is assumed that heat is transferred by conduction alone, and that the thermal diffusivity κ and the specific heat at constant pressure c_p are constant. Furthermore, it is supposed the density takes the same value in both the liquid and solid phases. We scale all lengths with respect to some representative length scale l, temporal scales with respect to l^2/κ, and we measure temperature relative to u_F^* in units of $u_F^* - u_W^*$. It follows that the governing equations in nondimensional variables are the heat equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \tag{1}$$

throughout the solid region, subject to the boundary conditions

$$u = -1 \quad \text{on } \partial B, \tag{2}$$

$$u = 0, \quad \beta = \nabla u \cdot \nabla \omega \quad \text{on } t = \omega(x, y, z). \tag{3}$$

Here the initial region of liquid is denoted by B, and its boundary by ∂B. The free boundary between the liquid and solid phases is denoted by $t = \omega(x, y, z)$. The one dimensionless group associated with the problem is the Stefan number β, which is defined by

$$\beta = \frac{L}{c_p(u_F^* - u_W^*)},$$

where L is the latent heat of fusion per unit mass of the fluid.

For the analysis presented in this paper, it is assumed that the free boundary $t = \omega(x, y, z)$ contracts continuously from ∂B at $t = 0$ to some point, (x_f, y_f, z_f) say, at some finite time, t_f say. We refer to (x_f, y_f, z_f) and t_f as being the extinction point and extinction time, respectively. (In reality, for a non-concave boundary ∂B, it may be the case that there is more than one extinction point; we discuss this topic briefly in Section 5.) It will prove useful to introduce the temporal variable τ, defined by $\tau = t_f - t$, so that the limit in which extinction occurs is both $t \to t_f^-$ and $\tau \to 0^+$. The goal is therefore to acquire information on the extinction time t_f, the location of the extinction point (x_f, y_f, z_f), the temperature field as $t \to t_f^-$, and the shape and speed of the free boundary $t = \omega(x, y, z)$ as $t \to t_f^-$. Furthermore, we wish to determine, where possible, how all these quantities depend on both the Stefan number β and the initial geometry B.

To achieve this end we reformulate the governing equations (1–3) with the use of the Baiocchi transform

$$w(x, y, z, t) = -\int_{\omega(x,y,z)}^{t} u(x, y, z, t')\,\mathrm{d}t'.$$

The governing equations are now

$$\frac{\partial w}{\partial t} = \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} - \beta \tag{4}$$

with the boundary conditions

$$w = \frac{\partial w}{\partial n} = 0 \quad \text{on } t = \omega(x, y, z), \tag{5}$$

$$w = t \quad \text{on } \partial B. \tag{6}$$

Given a solution w, the temperature u can be recovered via either $u = -\partial w/\partial t$ or $u = -\nabla^2 w + \beta$.

3. Generic extinction analysis

3.1. Introduction

This section is dedicated to the asymptotic solution to (4–6) in the limit $t \to t_\mathrm{f}^-$ for arbitrary Stefan number β. Results equivalent to those of this section have previously been derived by Andreucci *et al.* [9]. However, we include this analysis here for a number of reasons. By sacrificing rigour, we believe the current approach to gain in transparency. In addition, the analysis is required to describe the third and final (exponentially short) time-scale for the case in which the Stefan number $\beta \gg 1$. By matching back onto the second time-scale described later, we shall be able to complete the determination of the dependence of the aspect ratio of the evolving free boundary just before extinction on both the Stefan number β and the initial geometry B. We require this analysis to determine the final temperature distribution near the extinction point and the rate at which the free boundary contracts, the former becoming singular on the second time-scale. With these quantities determined, it becomes clear when and where the description for the second time-scale becomes invalid. Finally, we are able to derive results for the moving boundary and the final temperature distribution to a higher order than those presented by Andreucci *et al.* [9].

At this stage it is convenient to assume that the extinction point is located at the origin. In fact, for the generic extinction analysis we are unable to extract any information regarding the location of the extinction point. It will, however, prove possible in the limit $\beta \gg 1$; discussions on this topic are deferred until Section 4. For analysis in the limit $x, y, z, \tau \to 0$, we use the similarity variables

$$\xi = \frac{x}{\tau^{1/2}}, \quad \eta = \frac{y}{\tau^{1/2}}, \quad \zeta = \frac{z}{\tau^{1/2}}, \quad \rho = \frac{r}{\tau^{1/2}}, \tag{7}$$

$$T = -\log\tau, \quad w(x, y, z, \tau) = \tau\beta\, W(\xi, \eta, \zeta, T), \tag{8}$$

so that (4) and (5) become

$$\frac{\partial^2 W}{\partial \xi^2} + \frac{\partial^2 W}{\partial \eta^2} + \frac{\partial^2 W}{\partial \zeta^2} - \frac{1}{2}\left(\xi\frac{\partial W}{\partial \xi} + \eta\frac{\partial W}{\partial \eta} + \zeta\frac{\partial W}{\partial \zeta}\right) + W = \frac{\partial W}{\partial T} + 1, \tag{9}$$

$$W = \frac{\partial W}{\partial \nu} = 0 \text{ on the free boundary,} \tag{10}$$

where $\partial/\partial\nu$ denotes the derivative in the normal direction. The generic analysis involves three spatial regions, inner, intermediate and outer.

3.2. Inner region, $\rho = (\xi^2 + \eta^2 + \zeta^2)^{\frac{1}{2}} = O(\sigma)$

We introduce the quantity $\sigma(T)$, which measures the distance between the boundary of the shrinking liquid core and the origin. To be precise, we define σ by forcing the volume enclosed by the free boundary to be $4\pi\tau^{3/2}\sigma^3/3$.

The inner region has $\rho = O(\sigma)$, where $\sigma \ll 1$. The function $\sigma(T)$ is to be determined by the solution process. We introduce the variables

$$\hat{\xi} = \frac{\xi}{\sigma}, \quad \hat{\eta} = \frac{\eta}{\sigma}, \quad \hat{\zeta} = \frac{\zeta}{\sigma}, \quad \hat{\rho} = \frac{\rho}{\sigma},$$

and write

$$W \sim \sigma^2 \Phi_0(\hat{\xi}, \hat{\eta}, \hat{\zeta}) + O(\sigma^4) \quad \text{as } T \to \infty, \tag{11}$$

so that to leading order (9–10) give

$$\frac{\partial^2 \Phi_0}{\partial \hat{\xi}^2} + \frac{\partial^2 \Phi_0}{\partial \hat{\eta}^2} + \frac{\partial^2 \Phi_0}{\partial \hat{\zeta}^2} = 1, \quad \Phi_0 = \frac{\partial \Phi_0}{\partial \hat{\nu}} = 0 \text{ on the free boundary.} \tag{12}$$

In order to match with the intermediate region described below, the far-field condition must be of the form

$$\Phi_0 \sim \bar{a}\hat{\xi}^2 + \bar{b}\hat{\eta}^2 + (\tfrac{1}{2} - \bar{a} - \bar{b})\hat{\zeta}^2 - \delta + \frac{1}{3\hat{\rho}} + O(\hat{\rho}^{-3}) \tag{13}$$

as $\hat{\rho} \to \infty$. In general, Equation (13) will contain a linear combination of the quadratic terms $\hat{\xi}\hat{\eta}$, $\hat{\xi}\hat{\zeta}$ and $\hat{\eta}\hat{\zeta}$; however, we may orient the coordinate axes so that these terms vanish. In (13), $\bar{a}, \bar{b} > 0$ are important free constants which, without loss of generality, we restrict to satisfy $\bar{a} + \bar{b} < \frac{1}{2}$, $\frac{1}{4}(1 - 2\bar{a}) \le \bar{b} \le \bar{a}$. For $\beta \gg 1$ we shall determine $\bar{a}$ and $\bar{b}$ by matching back onto earlier time-scales; however, for general β this is not possible. The constant δ in (13) is found as a function of $\bar{a}$ and $\bar{b}$ as part of the solution to (12–13), by a process which we describe below. Finally, we mention the constant $1/3$ in front of the term $1/\rho$ in (13) is required for the volume enclosed by the free boundary to be consistent with our definition of σ. This may be shown by applying the divergence theorem to (12a) in an infinitely large volume excluding the region enclosed by the free boundary.

A short discussion on the boundary-value problem (12–13) is given in Appendix A. For our purposes it is sufficient to know that for the strict inequality $\frac{1}{4}(1 - 2\bar{a}) < \bar{b} < \bar{a}$, the solution for the constant δ is

$$\delta = F(\bar{\varphi}_0, \bar{q}/\bar{p})/2\bar{p}, \tag{14}$$

where $\bar{\varphi}_0 = \arcsin(\bar{p}/\bar{\lambda}_0)$ and $\bar{\lambda}_0$, $\bar{p}$ and $\bar{q}$ are constants given implicitly in terms of $\bar{a}$ and $\bar{b}$ by the relations

$$\bar{a} = \frac{\bar{\lambda}_0^2 - \bar{q}^2}{2(\bar{p}^2 - \bar{q}^2)} - \frac{E(\bar{\varphi}_0, \bar{q}/\bar{p})}{2\bar{p}(\bar{p}^2 - \bar{q}^2)}, \quad \bar{b} = -\frac{\bar{\lambda}_0^2 - \bar{p}^2}{2(\bar{p}^2 - \bar{q}^2)} - \frac{F(\bar{\varphi}_0, \bar{q}/\bar{p})}{2\bar{p}\bar{q}^2} + \frac{\bar{p}E(\bar{\varphi}_0, \bar{q}/\bar{p})}{2\bar{q}^2(\bar{p}^2 - \bar{q}^2)}, \tag{15}$$

$$\bar{\lambda}_0 \sqrt{(\bar{\lambda}_0^2 - \bar{p}^2)(\bar{\lambda}_0^2 - \bar{q}^2)} = 1. \tag{16}$$

Here $F(\varphi, k)$ and $E(\varphi, k)$ are elliptic integrals defined by (A.7). The free boundary is ellipsoidal in shape, and is given in original variables by

$$\frac{x^2}{\bar{\lambda}_0^2 - \bar{p}^2} + \frac{y^2}{\bar{\lambda}_0^2 - \bar{q}^2} + \frac{z^2}{\bar{\lambda}_0^2} = \tau\sigma^2.$$

If $\frac{1}{4}(1 - 2\bar{a}) = \bar{b} < \bar{a}$ or $\frac{1}{4}(1 - 2\bar{a}) < \bar{b} = \bar{a}$, then the free boundary is the shape of an oblate spheroid or a prolate spheroid, respectively. In these cases we may derive a result for δ by taking appropriate limits in (14–16) (see Appendix A for details). If $\bar{a}=\bar{b}=\frac{1}{6}$ then the free boundary is a sphere, and in this case $\delta=\frac{1}{2}$.

As noted above, we have chosen a coordinate system so that the principal axes of this ellipsoid coincide with the coordinate directions. We emphasise that this is done for convenience, and that we are unable to determine the orientation of this coordinate system within this generic extinction analysis (this is to be contrasted with the limit $\beta \gg 1$, described in Section 4, for which we relate the direction of the shrinking ellipsoid's principal axes to the initial geometry B).

3.3. Intermediate region, $\rho = O(1)$

In view of (9), for the intermediate region we write

$$W \sim \bar{a}\xi^2+\bar{b}\eta^2+(\tfrac{1}{2}-\bar{a}-\bar{b})\zeta^2+A(T)W_1(\rho,\theta,\phi)+\dot{A}(T)W_2(\rho,\theta,\phi)+\ddot{A}(T)W_3(\rho,\theta,\phi) \tag{17}$$

as $T\to\infty$, where (ρ,θ,ϕ) are spherical coordinates. Here the dots denote derivatives with respect to T, and it is assumed that $|\ddot{A}(T)| \ll |\dot{A}(T)| \ll |A(T)|$ as $T\to\infty$ (we may verify these assumptions *a posteriori*). The elliptic form of the first set of terms in (17) relates to established results for Darcy flow (see [12] and references therein) and its validity will be confirmed by matching; the subsequent expansion is familiar in problems in which the solution is almost, but not quite, of the self-similar form implied by the scaling properties of the partial differential equation and its self-consistency is again confirmed in the usual way via the subsequent matching arguments. Such quasi-self-similar behaviour is very familiar in blow-up problems for semilinear heat equations (see for example the review [14]), with which the current analysis has a number of aspects in common (including the key role played by polynomial solutions to the heat equation). It follows from (13) that matching conditions of the form

$$W_i \sim k_{i1}\frac{1}{\rho}+k_{i2} \quad \text{as } \rho\to 0 \tag{18}$$

must hold for $i=1,2,3$. The function $A(T)$ and the constants k_{i1} are found as part of the solution process, but to specify $A(T)$ uniquely we impose the conditions

$$k_{12}=1, \quad k_{i2}=0, \quad i\geq 2. \tag{19}$$

It is noted the behaviour of the higher-order terms in (11) as $\hat{\rho}\to\infty$ is consistent with (18).

Upon substituting (17) in (9) we find that the W_i satisfy the partial differential equations

$$\frac{\partial^2 W_i}{\partial\rho^2}+\left(\frac{2}{\rho}-\frac{1}{2}\rho\right)\frac{\partial W_i}{\partial\rho}+\frac{1}{\rho^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial W_i}{\partial\theta}\right)+\frac{1}{\rho^2\sin^2\theta}\frac{\partial^2 W_i}{\partial\phi^2}+W_i=W_{i-1}, \tag{20}$$

for $i=1,2,3$, with $W_0=0$. By separating variables, it is shown in Appendix B that the conditions (18) and (19) are consistent only with functions W_i (that do not grow exponentially as $\rho\to\infty$) which are independent of θ and ϕ. We are thus left with ordinary differential equations, with solutions of the form

$$W_1=L(\rho), \qquad W_2=(1-\gamma)L(\rho)+N(\rho), \qquad W_3=\bar{k}L(\rho)+(1-\gamma)N(\rho)+M(\rho), \tag{21}$$

where the functions $L(\rho)$, $N(\rho)$ and $M(\rho)$ are also given in Appendix B (namely by (B.1–B.2)), γ is Euler's constant, and the constants k_{i1} are

$$k_{11}=0, \qquad k_{21}=\frac{4\sqrt{\pi}}{3}, \qquad k_{31}=\frac{4\sqrt{\pi}}{9}(5-6\log 2).$$

The constant $\bar{k}$ in (21) can be determined by analysing the next order term W_4, but we shall not need to do so here. Matching with (13) thus implies that

$$A \sim -\delta\sigma^2 + O(\sigma^4), \qquad \dot{A} + \frac{5 - 6\log 2}{3}\ddot{A} + O(\dddot{A}) \sim \frac{1}{4\sqrt{\pi}}\sigma^3 + O(\sigma^5), \tag{22}$$

where δ is given by (14). Note that a different choice of the constant 1/3 in (13) would alter the definition of $\sigma(T)$, and the second equation in (22) would reflect that change in having a coefficient different from the $1/4\sqrt{\pi}$. We solve the two equations (22) asymptotically, the result being

$$A \sim -\frac{64\pi\delta^3}{(T+T_s)^2}\left[1 + \frac{2(-5+6\log 2)\log[(T+T_s)/(8\sqrt{\pi}\delta)]}{T+T_s} + O\left(\frac{\log(T+T_s)}{(T+T_s)^2}\right)\right], \tag{23}$$

$$\sigma \sim \frac{8\sqrt{\pi}\delta}{T+T_s}\left[1 + \frac{(-5+6\log 2)\log[(T+T_s)/(8\sqrt{\pi}\delta)]}{T+T_s} + O\left(\frac{\log(T+T_s)}{(T+T_s)^2}\right)\right] \tag{24}$$

as $T \to \infty$, where T_s is a free constant (reflecting the invariance of (22) under translations in T) which depends on the evolution over earlier times. We keep T_s here because for large Stefan number we find $T_s \gg 1$ and the above results are then valid for $T = O(T_s) \gg 1$; we note that T_s corresponds to a shift in T and hence, via (8), to a rescaling in the spatial and temporal variables. We also note that the correction terms in (11) contribute only $O(\sigma^4)$ terms in (22), and hence are negligible when matching with the intermediate region.

By using (21) and (B.3–B.4), the asymptotic behaviour

$$W_1 = -\tfrac{1}{6}\rho^2 + 1, \qquad W_2 \sim \tfrac{1}{3}\rho^2\log\rho - \tfrac{1}{6}(1-\gamma)\rho^2 - 2\log\rho + 1 - \gamma + O(\rho^{-4}), \tag{25}$$

$$W_3 \sim -\tfrac{1}{3}\rho^2\log^2\rho + \tfrac{1}{3}(1-\gamma)\rho^2\log\rho - \tfrac{1}{6}\bar{k}\rho^2 + 2\log^2\rho - 2(1-\gamma)\log\rho + O(1) \tag{26}$$

as $\rho \to \infty$ is determined, and this is used to formulate matching conditions for the outer region considered below. We introduce the variable R, defined by

$$R = -\log r = \tfrac{1}{2}T - \log\rho,$$

and note that $R = \frac{1}{2}T + O(1)$ in the intermediate region. Taylor expansions for $A(T)$ and its derivatives can now be used (along with (17), (25), (26)) to give the matching condition

$$\begin{aligned} W \sim\ & \bar{a}\xi^2 + \bar{b}\eta^2 + (\tfrac{1}{2} - \bar{a} - \bar{b})\zeta^2 - \tfrac{1}{6}\rho^2[A(2R) + (1-\gamma)\dot{A}(2R) + \bar{k}\ddot{A}(2R) + \cdots] \\ & + [A(2R) + (1-\gamma)\dot{A}(2R) + \bar{k}\ddot{A}(2R) + \cdots] + O(\rho^{-2}) \text{ as } \rho \to \infty, \end{aligned} \tag{27}$$

where here the ellipses denote terms of order $\dddot{A}(2R)$ as $R \to \infty$.

3.4. Outer region, $r = O(1)$

We denote w and u at $t = t_f$ by $w_f(x, y, z)$ and $u_f(x, y, z)$, respectively, and, recalling that $u = \partial w/\partial\tau$, write

$$w \sim w_f + \tau u_f + O(\tau^2) \text{ as } \tau \to 0$$

in the outer region, for which $r = O(1)$. The final temperature distribution u_f is determined by evolution over earlier time-scales, while w_f is given in terms of u_f by the linear boundary-value problem

$$\nabla^2 w_f = -u_f + \beta \quad \text{in } B, \quad w_f = t_f \text{ on } \partial B,$$

since $u_f = -1$ on ∂B.

In order to match with the intermediate region we require that

$$w_{\mathrm{f}} \sim \beta[\bar{a}x^2 + \bar{b}y^2 + (\tfrac{1}{2} - \bar{a} - \bar{b})z^2] - \tfrac{1}{6}\beta r^2[A(2R) + (1-\gamma)\dot{A}(2R) + \cdots] \qquad \text{as} \quad r \to 0,$$
$$u_{\mathrm{f}} \sim \beta[A(2R) + (1-\gamma)\dot{A}(2R) + \cdots] \qquad \text{as} \quad r \to 0$$

(see Equation (27)). It follows from (23) that for $r \ll \mathrm{e}^{-T_{\mathrm{s}}/2}$ the behaviour of w and u at extinction is given by

$$w_{\mathrm{f}} \sim \beta[\bar{a}x^2 + \bar{b}y^2 + (\tfrac{1}{2} - \bar{a} - \bar{b})z^2] + \frac{8\pi\delta^3\beta r^2}{3(-\log r + T_{\mathrm{s}}/2)^2} \times \left[1 + \frac{(-5 + 6\log 2)\log[(-\log r + T_{\mathrm{s}}/2)/(4\sqrt{\pi}\delta)] + \gamma - 1}{-\log r + T_{\mathrm{s}}/2}\right], \tag{28}$$

$$u_{\mathrm{f}} \sim \frac{-16\pi\delta^3\beta}{(-\log r + T_{\mathrm{s}}/2)^2}\left[1 + \frac{(-5 + 6\log 2)\log[(-\log r + T_{\mathrm{s}}/2)/(4\sqrt{\pi}\delta)] + \gamma - 1}{-\log r + T_{\mathrm{s}}/2}\right] \tag{29}$$

(recalling that $T_{\mathrm{s}} \gg 1$ for $\beta \gg 1$; for $T_{\mathrm{s}} \gg 1$ Equations (28–29) apply for $-\log r = O(T_{\mathrm{s}})$ with $-\log r + T_{\mathrm{s}}/2 > 0$). An interesting point to note is that, while the free boundary becomes ellipsoidal in shape as $t \to t_{\mathrm{f}}^-$, the final temperature distribution u_{f} is radially symmetric for small r.

We remark the results (24), (28) and (29) obtained here are more precise than those derived by Andreucci *et al.* [9], who only present results to leading order. That is, they do not compute the terms of order $\log(T + T_{\mathrm{s}})/(T + T_{\mathrm{s}})^2$ in (24), nor the second terms in the square brackets in each of (28) and (29).

Finally, it is worth mentioning that, for the corresponding problem in two dimensions, the time-dependence is slightly more complicated. In that case we have

$$\sigma(T) \sim E_\sigma\, \mathrm{e}^{-(T+T_{\mathrm{c}})^{1/2}/\sqrt{2}} \qquad \text{as } T \to \infty,$$

where T_{c} is a free constant (analogous to T_{s} in the three-dimensional case), and E_σ is a constant which is found to depend on the initial geometry B. At extinction we have

$$u_{\mathrm{f}} \sim E_u\, \beta(-\log r + \tfrac{1}{2}T_{\mathrm{c}})^{1/2}\mathrm{e}^{-2(-\log r + T_{\mathrm{c}}/2)^{1/2}} \qquad \text{as } r \to 0,$$

where again the constant E_u depends on the initial geometry. For details see [9] and [10].

3.5. Special case $\bar{a} = \bar{b} = 1/6$

For the special case in which the geometry B is a sphere, $\bar{a} = \bar{b} = 1/6$ and $\delta = 1/2$. In this case the free boundary is also spherical, and is described by $r = \tau^{1/2}\sigma(T)$. By substituting these values of $\bar{a}$, $\bar{b}$ and δ in (24) and (29) we find our results confirm those derived by Soward [8].

We mention that $\bar{a} = \bar{b} = 1/6$ holds for other geometries B apart from spheres. In particular, these values arise for any geometry which has sufficient symmetry, the cube being the most obvious example.

4. Large-Stefan-number asymptotics

4.1. Introduction

We have just presented an analysis describing the extinction behaviour of the Stefan problem (4–6) for general Stefan number β. Within this analysis we are able to derive results for the final temperature field, the shape of the shrinking solid-melt interface, and the rate at which the interface contracts, all up to the values of the free constants $\bar{a}$, $\bar{b}$ and T_s (recall the constant δ depends on $\bar{a}$ and $\bar{b}$ through (14)). In this section we consider the special case $\beta \gg 1$. This asymptotic limit is worthwhile because by considering early time-scales we are able to determine the relationship between the constants $\bar{a}$, $\bar{b}$ and T_s and the geometry B and the Stefan number β (through (57) and (58) with δ given by (14)), and because it is of wide practical relevance (see the data in [6], for example). The analysis of this limit will lead us to recipes for both the extinction point (x_f, y_f, z_f) and the extinction time t_f, results which cannot be obtained for general β. We note that this section is an extension of the work presented by Riley *et al.* [6], Stewartson and Waechter [7] and Soward [8] for spherical B to general three-dimensional domains.

4.2. Time-scale 1, $t = O(\beta)$

4.2.1. *Leading-order formulation*

The first time-scale has $t = O(\beta)$ and thus we scale time as $\hat{t} = t/\beta$. It is appropriate to write

$$w \sim \beta w_0(x, y, z, \hat{t}), \qquad \omega \sim \beta \hat{\omega}_0(x, y, z) \quad \text{as } \beta \to \infty,$$

so that the leading-order problem is to solve

$$\frac{\partial^2 w_0}{\partial x^2} + \frac{\partial^2 w_0}{\partial y^2} + \frac{\partial^2 w_0}{\partial z^2} = 1, \tag{30}$$

with

$$w_0 = \frac{\partial w_0}{\partial n} = 0 \quad \text{on } \hat{t} = \hat{\omega}_0(x, y, z), \tag{31}$$

$$w_0 = \hat{t} \quad \text{on } \partial B. \tag{32}$$

This formulation is typical for one-phase Stefan problems with $\beta \gg 1$. To leading order, the problem has become quasi-steady, since the free boundary moves very slowly in this limit. Equations (30–31) also describe flow of viscous fluid through porous media, with $\hat{t} = \hat{\omega}_0$ representing the free boundary between wet and dry regions (in two dimensions, the equations also describe flow in Hele-Shaw cells). In that context, the free boundary $\hat{t} = \hat{\omega}_0$ encloses a bubble or air, and Equations (30–32) lead to a non-trivial extinction problem in their own right. This problem was analysed by McCue *et al.* [12], and so here we only present the relevant results.

We let the extinction time for the bubble problem (30–32) be $\hat{t}_e$, denote the point to which the bubble contracts at $\hat{t}_e$ by (x_e, y_e, z_e) and set $w_e(x, y, z) = w_0(x, y, z, \hat{t}_e)$. Not surprisingly, we cannot in general solve the nonlinear free-boundary problem (30–32) for all time $\hat{t}$. At the extinction time $\hat{t} = \hat{t}_e$, however, it reduces to a linear boundary-value problem, since the free boundary shrinks to a point. We set $w_e = W_e(x, y, z) + \hat{t}_e$, so that W_e satisfies

$$\frac{\partial^2 W_e}{\partial x^2} + \frac{\partial^2 W_e}{\partial y^2} + \frac{\partial^2 W_e}{\partial z^2} = 1 \text{ in } B \text{ with } W_e = 0 \text{ on } \partial B. \tag{33}$$

The point (x_e, y_e, z_e) is where W_e achieves a global minimum (for simplicity we assume there to be only one such point) and the extinction time $\hat{t}_e$ is found from $\hat{t}_e = -W_e(x_e, y_e, z_e)$. This process is possible because time $\hat{t}$ appears in (30–32) as a parameter only, thus we may solve for w_0 at any time $\hat{t}$ without knowledge of the solution at previous times. Herein lies one of the main advantages of the Baiocchi transform formulation.

The linear boundary-value problem (33) provides a recipe for obtaining the extinction time $\hat{t}_e$ and extinction point (x_e, y_e, z_e). From here on, without loss of generality, we suppose that (x_e, y_e, z_e) coincides with the origin, and that the function w_e has the behaviour

$$w_e(x, y, z) \sim ax^2 + by^2 + (\tfrac{1}{2} - a - b)z^2 \quad \text{as } (x, y, z) \to (0, 0, 0). \tag{34}$$

(In general, the Cartesian coordinate system will have to be rotated for (34) to hold; we refer the reader to [12] for a discussion on this point.) Here, a and b are important constants that characterise the domain B. For definiteness, we assume $a, b > 0$, $a + b < 1/2$, $(1 - 2a)/4 \le b \le a$, so the coefficients of the x^2, y^2 and z^2 terms in (34) are of equal or decreasing size. Again, the solution of the linear problem (33) provides the values of a and b, and this can be done numerically if necessary.

4.2.2. *Main results*

In the limit $\hat{t} \to \hat{t}_e^-$ the analysis for the leading-order problem (30–32) breaks into two length scales. In the outer region, valid for $r = O(1)$, we have

$$w_0 \sim w_e(x, y, z) - (\hat{t}_e - \hat{t}) + \frac{4\pi}{3}\bar{T}(\hat{t}_e - \hat{t})^3 G(x, y, z) \quad \text{as } \hat{t} \to \hat{t}_e^-, \tag{35}$$

where G is the Green function, which satisfies

$$-\left(\frac{\partial^2 G}{\partial x^2} + \frac{\partial^2 G}{\partial y^2} + \frac{\partial^2 G}{\partial z^2}\right) = \delta(x)\delta(y)\delta(z) \text{ in } B \text{ with } G = 0 \text{ on } \partial B, \tag{36}$$

and has the local behaviour

$$G \sim \frac{1}{4\pi}\left(\frac{1}{r} - K_B\right) \quad \text{as } r \to 0 \tag{37}$$

for some positive constant K_B which depends on the geometry B and is determined as part of the solution to the linear problem (36). The function $\bar{T}(\hat{t}_e - \hat{t})$ in (35) is defined so that the volume enclosed by the free boundary $\hat{t} = \hat{\omega}_0$ is $4\pi\bar{T}^3/3$, and by matching with the inner region (which has $r = O(\bar{T})$), it is found that

$$\hat{t} = \hat{t}_e - d\bar{T}^2 + \tfrac{1}{3}K_B\bar{T}^3 + O(\bar{T}^5) \quad \text{as } \bar{T} \to 0. \tag{38}$$

Equivalently, we may write

$$\bar{T} = \frac{1}{\sqrt{d}}(\hat{t}_e - \hat{t})^{1/2} + \frac{K_B}{6d^2}(\hat{t}_e - \hat{t}) + O((\hat{t}_e - \hat{t})^{3/2}) \quad \text{as } \hat{t} \to \hat{t}_e^-. \tag{39}$$

The quantity d in (38) and (39) is a constant determined by considering the inner region. It turns out we must solve the boundary-value problem (A.1–A.3), and so for the strict inequality $(1 - 2a)/4 < b < a$, the constant d is given implicitly by the relations (A.5–A.6), where a and b are defined by (34). We find the free boundary on this time scale approaches the ellipsoid

$$\frac{x^2}{\lambda_0^2 - p^2} + \frac{y^2}{\lambda_0^2 - q^2} + \frac{z^2}{\lambda_0^2} = \bar{T}^2$$

as $\hat{t} \to \hat{t}_e^-$. If $(1 - 2a)/4 < b$ and $b = a$, the free boundary approaches a prolate spheroid as $\hat{t} \to \hat{t}_e^-$, with d given implicitly by (A.8–A.9), while if $(1 - 2a)/4 = b$, $b < a$, the free boundary approaches an oblate spheroid, with d given by (A.10–A.11). Finally, if $a = b = 1/6$, the free boundary approaches a sphere as $\hat{t} \to \hat{t}_e^-$, with $d = 1/2$.

4.3. Time-scale 2, $t_f - t = O(1)$

4.3.1. *Introduction*

At times just before extinction the solid-melt interface no longer moves slowly, and the equations governing the heat conduction are no longer quasi-steady. This new structure arises on a time-scale in which $\tau = t_f - t = O(1)$. From (39) we find the free boundary is a distance of order $\beta^{-1/2}$ away from the origin on this time-scale. There are two length scales to consider; the first is near the free boundary $r = O(\beta^{-1/2})$, while the other is for $r = O(1)$.

It proves useful to expand the extinction time as

$$t_f = \beta\tau_a + \tau_b + \frac{\tau_c}{\beta^{1/2}} + O(\beta^{-1}), \tag{40}$$

where the τ_j, $j = a, b, c$ are as yet unknown constants which depend on the Stefan number β and the geometry B. In addition, we define a function $\Omega(x, y, z) = t_f - \omega(x, y, z)$, so that an alternative description for the free boundary $t = \omega(x, y, z)$ is $\tau = \Omega(x, y, z)$.

4.3.2. *Region I* (*inner*), $x, y, z = O(\beta^{-1/2})$

For region I we use the scaled variables

$$\bar{x} = \beta^{1/2}x, \qquad \bar{y} = \beta^{1/2}y, \qquad \bar{z} = \beta^{1/2}z, \qquad \bar{r} = \beta^{1/2}r,$$

and write

$$w \sim \bar{W}(\bar{x}, \bar{y}, \bar{z}, \tau) + O(\beta^{-1/2}), \qquad \Omega \sim \Omega_0(\bar{x}, \bar{y}, \bar{z}) + O(\beta^{-1/2}) \quad \text{as } \beta \to \infty.$$

The leading-order problem is then to solve the free-boundary problem

$$\frac{\partial^2 \bar{W}}{\partial \bar{x}^2} + \frac{\partial^2 \bar{W}}{\partial \bar{y}^2} + \frac{\partial^2 \bar{W}}{\partial \bar{z}^2} = 1 \text{ outside } \tau = \Omega_0(\bar{x}, \bar{y}, \bar{z}), \tag{41}$$

$$\bar{W} = \frac{\partial \bar{W}}{\partial \bar{n}} = 0 \quad \text{on } \tau = \Omega_0(\bar{x}, \bar{y}, \bar{z}), \tag{42}$$

$$\bar{W} \sim a\bar{x}^2 + b\bar{y}^2 + \left(\tfrac{1}{2} - a - b\right)\bar{z}^2 + f_1(\tau) + h_1(\tau)\frac{1}{\bar{r}} \quad \text{as } \bar{r} \to \infty, \tag{43}$$

where the function h_1 is found as part of the solution process (it is given by (51) below) and f_1 is determined below by matching with the outer region.

4.3.3. *Region II* (*outer*), $r = O(1)$

For region II we require the form

$$w \sim \beta w_a(x, y, z) - \tau + w_b(x, y, z) + \frac{1}{\beta^{1/2}}\tilde{W}(x, y, z, \tau) + O(\beta^{-1}) \quad \text{as } \beta \to 0, \tag{44}$$

so that immediately we find, by matching with region I, that $f_1(\tau) = -\tau$. The functions w_a and w_b satisfy identical boundary-value problems

$$\frac{\partial^2 w_j}{\partial x^2} + \frac{\partial^2 w_j}{\partial y^2} + \frac{\partial^2 w_j}{\partial z^2} = 1 \quad \text{in } B, \qquad w_j = \tau_j \quad \text{on } \partial B, \tag{45}$$

$$w_j = \frac{\partial w_j}{\partial x} = \frac{\partial w_j}{\partial y} = \frac{\partial w_j}{\partial z} = 0 \quad \text{at } (x, y, z) = (0, 0, 0), \tag{46}$$

for $j=a,b$, while $\tilde{W}$ satisfies the initial-boundary-value problem

$$\frac{\partial^2 \tilde{W}}{\partial x^2}+\frac{\partial^2 \tilde{W}}{\partial y^2}+\frac{\partial^2 \tilde{W}}{\partial z^2}=-\frac{\partial \tilde{W}}{\partial \tau} \quad \text{in } B\setminus(0,0,0) \tag{47}$$

$$\tilde{W}=\tau_{\rm c}, \quad \text{on } \partial B, \tag{48}$$

$$\tilde{W}\sim h_1(\tau)\frac{1}{r}+f_2(\tau) \quad \text{as } r\to 0, \tag{49}$$

$$\tilde{W}\sim \frac{4\pi}{3d}G(x,y,z)\tau^{3/2}+O(\tau^{1/2}) \quad \text{as } \tau\to+\infty, \tag{50}$$

where $G(x,y)$ is the Green function defined by (36), h_1 is determined by the solution of (41)–(43), and the constant $\tau_{\rm c}$ (defined in (40)) and the function f_2 are to be found as part of the solution process. The last condition (50) is found by matching back onto the first time-scale (see (35) and (39)).

4.3.4. *Analysis of (I)BVPs for* $\bar{W}$, w_j *and* $\tilde{W}$

BVP for $\bar{W}$: To solve the boundary-value problem (41–43) for $\bar{W}$ we set

$$\bar{W}=(3h_1(\tau))^{2/3}\Phi(X,Y,Z),$$

where

$$X=\frac{\bar{x}}{(3h_1(\tau))^{1/3}}, \quad Y=\frac{\bar{y}}{(3h_1(\tau))^{1/3}}, \quad Z=\frac{\bar{z}}{(3h_1(\tau))^{1/3}},$$

so that Φ satisfies (A.1–A.2) with

$$\Phi\sim aX^2+bY^2+(\tfrac{1}{2}-a-b)Z^2-\frac{\tau}{(3h_1(\tau))^{2/3}}+\frac{1}{3R} \quad \text{as } R\to\infty,$$

where $R^2=X^2+Y^2+Z^2$ (recalling that f_1 in (43) is found to be $-\tau$ by matching between regions I and II). This is again the free-boundary problem considered in Appendix A, and thus the function h_1 must be

$$h_1(\tau)=\frac{\tau^{3/2}}{3d^{3/2}}. \tag{51}$$

Here d is the constant related to a and b by (A.5–A.6), as explained in Appendix A. The free boundary $\tau=\Omega_0$ is the ellipsoid

$$\frac{\bar{x}^2}{\lambda_0^2-p^2}+\frac{\bar{y}^2}{\lambda_0^2-q^2}+\frac{\bar{z}^2}{\lambda_0^2}=\frac{\tau}{d},$$

where, again, the constants λ_0, p and q are related to a and b by (A.5–A.6).

BVPs for w_a *and* w_b: The boundary-value problems for w_j, $j=a,b$ are identical to the problem for $w_{\rm e}$, as described in Section 4.2.1. It follows that $w_a=w_b=w_{\rm e}$ and $\tau_a=\tau_b=\hat{t}_{\rm e}$, so that

$$w_a(x,y,z)=w_b(x,y,z)\sim ax^2+by^2+(\tfrac{1}{2}-a-b)z^2 \quad \text{as } (x,y,z)\to(0,0,0),$$

$$t_{\rm f}=(\beta+1)\hat{t}_{\rm e}+\frac{1}{\beta^{1/2}}\tau_{\rm c}+O(\beta^{-1}),$$

$$w = (\beta+1)w_{\mathrm{e}}(x, y, z) - \tau + \frac{1}{\beta^{1/2}}\tilde{W}(x, y, z, \tau) + O(\beta^{-1}), \tag{52}$$

$$u = -1 + \frac{1}{\beta^{1/2}}\frac{\partial \tilde{W}}{\partial \tau} + O(\beta^{-1}), \tag{53}$$

as $\beta \to \infty$. The $(\beta+1)w_{\mathrm{e}}$ term in (52) can be interpreted in the following way. The β corresponds to the amount of latent heat released at the interface by freezing a unit volume, while the 1 corresponds to the amount of sensible heat lost in reducing the temperature of the volume from $u=0$ initially to the boundary value $u=-1$. From (53) we see that for these purposes the leading-order temperature at extinction is -1 everywhere within the solid.

IBVP for $\tilde{W}$: In general, it is not possible to solve the linear initial-boundary-value problem for $\tilde{W}$ analytically for all time (domains B in which the Helmholtz equation is separable provide exceptions), however we can determine some valuable information by considering the governing equations (47–50) in limit $\tau \to 0$. In this limit, the initial-boundary-value problem for $\tilde{W}$ has two length scales.

The inner region for the problem (47–50) is for $r = O(\tau^{1/2})$, with $\tau \ll 1$. We write

$$\tilde{W} = \tau \tilde{w}(\xi, \eta, \zeta, T),$$

where the independent variables are defined in (7–8), so that $\tilde{w}$ satisfies

$$\frac{\partial^2 \tilde{w}}{\partial \xi^2} + \frac{\partial^2 \tilde{w}}{\partial \eta^2} + \frac{\partial^2 \tilde{w}}{\partial \zeta^2} - \frac{1}{2}\left(\xi\frac{\partial \tilde{w}}{\partial \xi} + \eta\frac{\partial \tilde{w}}{\partial \eta} + \zeta\frac{\partial \tilde{w}}{\partial \zeta}\right) + \tilde{w} = \frac{\partial \tilde{w}}{\partial T}.$$

We treat this partial differential equation in the limit $T \to \infty$ ($\tau \to 0$) by writing

$$\tilde{w} \sim \tilde{w}_1(\rho, \theta, \phi)T + \tilde{w}_2(\rho, \theta, \phi),$$

where (ρ, θ, ϕ) are the appropriate polar coordinates. The result is that $\tilde{w}_1$ and $\tilde{w}_2$ satisfy the equations

$$\frac{\partial^2 \tilde{w}_i}{\partial \rho^2} + \left(\frac{2}{\rho} - \frac{1}{2}\rho\right)\frac{\partial \tilde{w}_i}{\partial \rho} + \frac{1}{\rho^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial \tilde{w}_i}{\partial \theta}\right) + \frac{1}{\rho^2 \sin^2\theta}\frac{\partial^2 \tilde{w}_i}{\partial \phi^2} + \tilde{w}_i = \tilde{w}_{i-1} \tag{54}$$

for $i = 1, 2$ with $\tilde{w}_0 = 0$. For boundary conditions, we exclude exponential growth as $\rho \to \infty$, and combine (49) and (51) to give

$$\tilde{w}_1 \sim O(1), \qquad \tilde{w}_2 \sim \frac{1}{3d^{3/2}}\frac{1}{\rho} + O(1) \quad \text{as } \rho \to 0.$$

Partial differential equations identical to (54) with boundary conditions of this form are discussed in detail in Appendix B. Using (almost) identical arguments, we deduce the solutions

$$\tilde{w}_1 = \frac{1}{4\sqrt{\pi} d^{3/2}} L(\rho),$$

$$\tilde{w}_2 = a_{0,0}L(\rho) + \rho^2 \sum_{m=0}^{2}(a_{m,2}\cos m\phi + b_{m,2}\sin m\phi)\, P_2^m(\cos\theta) + \frac{1}{4\sqrt{\pi} d^{3/2}}N(\rho),$$

where the relevant functions are defined in Appendix B, and $a_{0,0}$, $a_{m,2}$ and $b_{m,2}$ are constants which cannot be determined without the explicit behaviour of $\tilde{W}$ to $O(r^2)$ as $r \to 0$, which can only be found with knowledge of $\tilde{W}$ for all time τ. We note that as $\rho \to \infty$,

$$\tilde{w}_2 = \frac{1}{12\sqrt{\pi}d^{3/2}}\rho^2 \log\rho - \frac{1}{6}a_{0,0}\rho^2 + \rho^2 \sum_{m=0}^{2}(a_{m,2}\cos m\phi + b_{m,2}\sin m\phi)\, P_2^m(\cos\theta) - \frac{1}{2\sqrt{\pi}d^{3/2}}\log\rho + O(1).$$

This information is used below when matching with the outer region.

The outer region for the problem (47–50) is for $r = O(1)$. Here it is appropriate to write

$$\tilde{W} = w_c(x, y, z) + \tau u_c(x, y, z) + O(\tau^2)$$

for $\tau \ll 1$, where (in the absence of a solution to (47–50) for all time) w_c and u_c are unknown functions. By matching with the inner region we find as $r \to 0$ that

$$w_c \sim \frac{1}{12\sqrt{\pi}d^{3/2}}r^2 \log r - \frac{1}{6}a_{0,0}r^2 + r^2 \sum_{m=0}^{2}(a_{m,2}\cos m\phi + b_{m,2}\sin m\phi)\, P_2^m(\cos\theta),$$
$$u_c \sim -\frac{1}{2\sqrt{\pi}d^{3/2}}\log r.$$

Note that with this analysis we are unable to determine the contribution τ_c to the extinction time t_f, since τ_c is in effect determined by the condition $w_c = \tau_c$ on ∂B, and here we only derive the behaviour of w_c as $r \to 0$. To determine the value of τ_c (as well as the function $f_2(\tau)$), we must solve the entire linear initial-boundary-value problem (47–50) for all time. As mentioned above, this more complicated task is only possible analytically for certain domains B.

4.3.5. *Summary*

To summarise, at extinction we have

$$u_f \sim -1 + \frac{1}{\beta^{1/2}}\left[-\frac{1}{2\sqrt{\pi}d^{3/2}}\log r + \cdots\right], \tag{55}$$

$$w_f \sim (\beta+1)[ax^2 + by^2 + (\tfrac{1}{2} - a - b)z^2] + \frac{1}{\beta^{1/2}}\left[\frac{r^2\log r}{12\sqrt{\pi}d^{3/2}} - \frac{1}{6}a_{0,0}r^2 + r^2\sum_{m=0}^{2}(a_{m,2}\cos m\phi + b_{m,2}\sin m\phi)\, P_2^m(\cos\theta)\right], \tag{56}$$

with $r = O(\beta^{-1/2})$ and $\beta \to \infty$, where the ellipsis denotes terms of order one as $r \to 0$. Given that $u_f(0, 0, 0) = 0$, the apparent singularity in (55) occurs because the limits $r \to 0$ and $\beta \to \infty$ do not commute, and as such we need to consider a further time-scale.

We make the point that on the second time-scale we have had to treat an initial-boundary-value problem in the outer region, which is in contrast to the first time-scale, where the governing equations are quasi-steady (see [12]). The inner problems for each time-scale, however, have the same time-dependence, so that to leading order the evolution of the free boundary is the same. In the third (and final) time-scale this time-dependence does change, and the analysis for this behaviour is described below.

4.4. Time-scale 3, $\tau = O(\mathrm{e}^{-T_s})$

The third (and final) time-scale is for $\tau = O(\mathrm{e}^{-T_s})$, where the constant T_s introduced in Section 3.3 is determined below by matching back onto the second time-scale. The analysis for this time-scale is presented in Section 3, which we recall is valid for all Stefan numbers. For

$\beta \gg 1$, in order to make a match between the leading-order terms in (28) with those in (56), it is immediately clear that $\bar{a}=a+O(\beta^{-1})$, $\bar{b}=b+O(\beta^{-1})$ and $T_s=O(\beta^{1/2})$. By considering further terms it follows that for $\beta \gg 1$ we require

$$T_s = 8\sqrt{\pi}\delta^{3/2}\beta^{1/2} + \tfrac{1}{2}(-5+6\log 2)\log\beta + O(1), \tag{57}$$

$$\bar{a} = a + \frac{1}{\beta}(a-\tfrac{1}{6}) + O(\beta^{-3/2}), \qquad \bar{b} = b + \frac{1}{\beta}(b-\tfrac{1}{6}) + O(\beta^{-3/2}), \tag{58}$$

where δ is computed by (14) with $\bar{a}$ and $\bar{b}$ given by (58).

We can now rewrite (28) and (29) in a way which is valid for all $r \ll 1$, namely

$$\begin{aligned} w_f \sim & (\beta+1)[ax^2+by^2+(\tfrac{1}{2}-a-b)z^2] - \tfrac{1}{6}r^2 \\ & + \frac{r^2}{6\psi(R)^2}\left[1+\frac{(-5+6\log 2)\log\psi(R)+O(1)}{4\sqrt{\pi}\delta^{3/2}\beta^{1/2}\psi(R)}\right], \end{aligned} \tag{59}$$

$$u_f \sim -\frac{1}{\psi(R)^2}\left[1+\frac{(-5+6\log 2)\log\psi(R)+O(1)}{4\sqrt{\pi}\delta^{3/2}\beta^{1/2}\psi(R)}\right] \quad \text{as } \beta\to\infty, \tag{60}$$

where the function ψ is defined by

$$\psi(R) = 1 + \frac{R}{4\sqrt{\pi}\delta^{3/2}\beta^{1/2}},$$

remembering that $R=-\log r$. So for $1 \ll R \ll \beta^{1/2}$, Equations (59) and (60) reduce to (55) and (56), while for $R \gg \beta^{1/2}$ we have (28) and (29) with (57) and (58). In the latter case we have, to leading order,

$$u_f \sim -\frac{16\pi\delta^3\beta}{R},$$

so that $u_f(0,0,0)=0$, as required. The volume enclosed by the solid-melt interface is given asymptotically for $T \gg 1$ by

$$\frac{4\pi}{3}\sigma^3\tau^{3/2} \sim \frac{4\pi\tau^{3/2}}{3\delta^{3/2}\beta^{3/2}\psi(\frac{1}{2}T)^3}\left[1+\frac{3(-5+6\log 2)\log\psi(\frac{1}{2}T)+O(1)}{8\sqrt{\pi}\delta^{3/2}\beta^{1/2}\psi(\frac{1}{2}T)}\right] \quad \text{as } \beta\to\infty,$$

which is valid for all $T=-\log\tau \gg 1$.

For $\beta \gg 1$ the third time-scale is evidently exponentially short ($-\log\tau = O(\beta^{1/2})$), and it thus does not contribute (significantly) to the extinction time expansion (40). However, the analysis is important because it removes the nonuniformity in the final temperature distribution on the second time-scale.

5. Discussion

We have studied the problem of freezing a general three-dimensional region of liquid, with emphasis on determining the behaviour of the temperature field and the solid-melt interface at times leading up to complete freezing. To simplify the analysis we have assumed a one-phase problem, with the liquid phase held at the fusion temperature.

There is a generic extinction analysis, initially presented by Andreucci *et al.* [9] and also given here, which shows that, regardless of both the Stefan number β and the initial geometry B, the solid-melt interface becomes ellipsoidal in shape as extinction is approached. The universality of this result is noteworthy, especially for the cases in which β is not large. Other results from this analysis include the time-dependence of the shrinking liquid region (24) and the behaviour of the temperature field near the extinction point at the extinction time (29). There is certain information about the freezing process which we are unable to obtain by considering the generic extinction analysis alone. This includes the location of the extinction point within the intial geometry and the time it takes for complete freezing. In addition, there are quantities in (24) and (29) that depend on the evolution of the temperature field over earlier times, namely the free constants $\bar{a}$, $\bar{b}$ (δ depends on $\bar{a}$ and $\bar{b}$) and T_s.

It happens that for large Stefan number $\beta \gg 1$ there are three distinct time-scales for the solidification problem, with the generic extinction analysis coinciding with the final (exponentially-short) time-scale. In this special case, we are able to determine the unknown quantities mentioned in the previous paragraph by matching back from this final time-scale onto the previous one. This analysis forms the main contribution of the study.

In presenting the analysis for $\beta \gg 1$ we have called upon many of the results of McCue *et al.* [12], where the analogous problem of shrinking bubbles in porous media is considered. These results are relevant for the first time-scale, where the problem becomes quasi-steady to leading order. Some specific examples of how the aspect ratios of the shrinking bubble (or in our case, the shrinking region of liquid) depend on the inital geometry are presented in [12].

As was the case in [12], we have assumed here that the initial geometry B is such that there is only one extinction point. For non-convex boundaries ∂B, there may be multiple extinction points, and in this case the function w_e introduced in Section 4.2.1 can have more than one local minimum (with each minimum corresponding to an extinction point). We do not consider necessary conditions for multiple extinction points here, but note that multiple minima of w_e are likely to be accompanied by a break-up of the liquid region, and ultimately the behaviour of the temperature field and the solid-melt interface in the neighbourhood of each extinction point should be qualitatively the same as that described above. While we believe the extinction behaviour we have described to be generic (non-generic (exceptional) extinction structures are also to be expected, for example in describing the borderline case for non-convex domains that separate a regime in which extinction occurs at two points from one in which it occurs at a single point), it is only neutrally stable in the sense that perturbing the initial data (such as the boundary shape ∂B) will also perturb the aspect ratios of the evolving free boundary just before extinction.

Finally, we note that it is possible to extend the Stefan problem (1–3) to include other physical effects, such as surface tension and kinetic undercooling, although particular care must be taken when deriving the correct equations in the one-phase limit (see [15] for details). A generic extinction analysis has been given by Herraiz *et al.* [16] for the case in which the problem is radially symmetric and surface-tension effects are included; however, the formulation differs slightly from that of Evans and King [15]. Herraiz *et al.* [16] show that the inclusion of surface tension leads to completely different scalings to the case in which these effects are ignored (the latter case covered by Herrero and Velázquez [13], Soward [8], and discussed in Section 3.5).

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Appendix A. The inner free-boundary problem

Here we present the solution to the free-boundary problem

$$\frac{\partial^2\Phi}{\partial X^2}+\frac{\partial^2\Phi}{\partial Y^2}+\frac{\partial^2\Phi}{\partial Z^2}=1 \text{ outside } \Omega_0 \tag{A.1}$$

with

$$\Phi=\frac{\partial\Phi}{\partial N}=0 \quad \text{on } \partial\Omega_0, \tag{A.2}$$

$$\Phi\sim aX^2+bY^2+(\tfrac{1}{2}-a-b)Z^2-d+\frac{1}{3R}+O(R^{-3}) \quad \text{as } R\to\infty, \tag{A.3}$$

where $R^2=X^2+Y^2+Z^2$ and $\partial/\partial N$ is used to denote the rescaled normal derivative. The location of the free boundary, as well as the constant d and the $O(R^{-3})$ terms in (A.3), are found as part of the solution process, and depend on the special constants a and b. The details of the solution process are described in [12], and we present only the most important aspects of the solution here.

For $a+b<1/2$, $(1-2a)/4<b<a$, we use ellipsoidal coordinates (λ,μ,ν), defined by

$$X=\left[\frac{(\lambda^2-p^2)(p^2-\mu^2)(p^2-\nu^2)}{p^2(p^2-q^2)}\right]^{\frac{1}{2}},\quad Y=\left[\frac{(\lambda^2-q^2)(\mu^2-q^2)(q^2-\nu^2)}{(p^2-q^2)q^2}\right]^{\frac{1}{2}},\quad Z=\frac{\lambda\mu\nu}{pq},$$

where p and q are constants which take values so that $0<\nu<q<\mu<p<\lambda<\infty$. Surfaces of constant λ are ellipsoids. We denote the free boundary Ω_0 by $\lambda=\lambda_0$, so it is given by

$$\frac{X^2}{\lambda_0^2-p^2}+\frac{Y^2}{\lambda_0^2-q^2}+\frac{Z^2}{\lambda_0^2}=1. \tag{A.4}$$

The solution for Φ is of the form

$$\Phi=g_1(\lambda)+g_2(\lambda)\mu^2\nu^2+g_3(\lambda)(\mu^2+\nu^2);$$

the functions g_i, for $i=1,2,3$ are derived by McCue *et al.* [12]. For our purposes, it is sufficient to know the solutions for the constants p, q, λ_0 and d in terms of a and b. These are given implicitly by the relations

$$a=\frac{\lambda_0^2-q^2}{2(p^2-q^2)}-\frac{E(\varphi_0,q/p)}{2p(p^2-q^2)},\qquad b=-\frac{\lambda_0^2-p^2}{2(p^2-q^2)}-\frac{F(\varphi_0,q/p)}{2pq^2}+\frac{pE(\varphi_0,q/p)}{2q^2(p^2-q^2)}, \tag{A.5}$$

$$\lambda_0\sqrt{(\lambda_0^2-p^2)(\lambda_0^2-q^2)}=1,\qquad d=F(\varphi_0,q/p)/2p, \tag{A.6}$$

where $\varphi_0=\arcsin(p/\lambda_0)$, and $F(\varphi,k)$ and $E(\varphi,k)$ are, respectively, elliptic integrals of the first and second kind, defined by

$$F(\varphi,k)=\int_0^{\sin\varphi}\frac{\mathrm{d}t}{\sqrt{(1-t^2)(1-k^2t^2)}} \quad\text{and}\quad E(\varphi,k)=\int_0^{\sin\varphi}\sqrt{\frac{1-k^2t^2}{1-t^2}}\,\mathrm{d}t. \tag{A.7}$$

For the case in which $b=a$, we have $q=p$ and the free boundary is a prolate spheroid with $\frac{1}{6}<a<\frac{1}{4}$. By taking the limit $q\to p$ in (A.5–A.6) we find

$$a=b=\frac{\lambda_0^3}{4(\lambda_0^3-1)}-\frac{\lambda_0^{3/2}}{8(\lambda_0^3-1)^{3/2}}\log\left[\frac{\lambda_0^{3/2}+(\lambda_0^3-1)^{1/2}}{\lambda_0^{3/2}-(\lambda_0^3-1)^{1/2}}\right], \tag{A.8}$$

$$p=q=\frac{(\lambda_0^3-1)^{1/2}}{\lambda_0^{1/2}},\qquad d=\frac{\lambda_0^{1/2}}{4(\lambda_0^3-1)^{1/2}}\log\left[\frac{\lambda_0^{3/2}+(\lambda_0^3-1)^{1/2}}{\lambda_0^{3/2}-(\lambda_0^3-1)^{1/2}}\right]. \tag{A.9}$$

Here, the free boundary is given by $\lambda_0(X^2+Y^2)+Z^2/\lambda_0^2=1$. Another limiting case is $b=\frac{1}{4}(1-2a)$, which implies $q=0$ and corresponds to the free boundary being the oblate spheroid $\lambda_0^4X^2+(Y^2+Z^2)/\lambda_0^2=1$. In this instance we find

$$a=\tfrac{1}{2}-2b=\frac{\lambda_0^6}{2(\lambda_0^6-1)}-\frac{\lambda_0^6}{2(\lambda_0^6-1)^{3/2}}\arctan(\lambda_0^6-1)^{1/2}, \tag{A.10}$$

$$p=\frac{(\lambda_0^6-1)^{1/2}}{\lambda_0^2},\qquad d=\frac{\lambda_0^2}{2(\lambda_0^6-1)^{1/2}}\arctan(\lambda_0^6-1)^{1/2}, \tag{A.11}$$

with $\frac{1}{6}<a<\frac{1}{4}$. Finally, for the special case $a=b=\frac{1}{6}$, the free boundary is just the sphere $X^2+Y^2+Z^2=1$, and the value of d is $d=\frac{1}{2}$.

Appendix B. Analysis of the partial differential equation (20)

In what follows we use the three functions

$$L(\rho)=1-\tfrac{1}{6}\rho^2,\ N(\rho)=-2\log\rho+\tfrac{1}{3}\rho^2\log\rho+2\rho^2\int_\rho^\infty\frac{I(t)}{t^3}\,\mathrm{d}t, \tag{B.1}$$

$$\begin{aligned}M(\rho)=&\,2\log^2\rho-\tfrac{1}{3}\rho^2\log^2\rho-4\rho^2\int_\rho^\infty\frac{I(t)\log t}{t^3}\,\mathrm{d}t\\&+2\rho^2\int_\rho^\infty\frac{J(t)}{t^3}\,\mathrm{d}t+4\rho^2\int_\rho^\infty\frac{1}{t}\int_t^\infty\frac{I(s)}{s^3}\,\mathrm{d}s\,\mathrm{d}t,\end{aligned} \tag{B.2}$$

where the integrals $I(\rho)$ and $J(\rho)$ are defined by

$$I(\rho)=2\sqrt{\pi}\int_\rho^\infty\frac{\mathrm{e}^{t^2/4}}{t^2}\mathrm{erfc}(\tfrac{1}{2}t)\,\mathrm{d}t=\int_0^\infty\frac{\sqrt{t+1}-1}{t}e^{-\rho^2t/4}\,\mathrm{d}t,$$

$$J(\rho)=-4\int_0^\infty\frac{1}{t}\left[\sqrt{1+t}\log\sqrt{1+t}-\tfrac{1}{2}(\sqrt{1+t}+1)\log(\tfrac{1}{2}(\sqrt{1+t}+1))\right]\mathrm{e}^{-\rho^2t/4}\,\mathrm{d}t,$$

and $\mathrm{erfc}(z)$ is the complementary error function, defined by

$$\mathrm{erfc}(z)=\frac{2}{\sqrt{\pi}}\int_z^\infty\mathrm{e}^{-t^2}\,\mathrm{d}t.$$

The integrals $I(\rho)$ and $J(\rho)$ are almost identical to ones arising in Soward [8]. We shall also require the asymptotic behaviours

$$N(\rho)=\frac{4\sqrt{\pi}}{3}\frac{1}{\rho}-1+\gamma+\sqrt{\pi}\rho+O(\rho^2\log\rho)\quad\text{as }\rho\to0,$$

$$M(\rho)=\frac{4\sqrt{\pi}}{9}(-6\log2+3\gamma+2)\frac{1}{\rho}+O(1)\quad\text{as }\rho\to0,$$

$$N(\rho)=\tfrac{1}{3}\rho^2\log\rho-2\log\rho+\frac{1}{2\rho^4}+O(\rho^{-6})\quad\text{as }\rho\to\infty, \tag{B.3}$$

$$M(\rho)=-\tfrac{1}{3}\rho^2\log^2\rho+2\log^2\rho-2(\log\rho+1)\frac{1}{\rho^2}+O(\rho^{-4})\quad\text{as }\rho\to\infty, \tag{B.4}$$

where γ is Euler's constant $\gamma = 0{\cdot}5772\ldots$. The technique used to evaluate the behaviour of $I(\rho)$ and $J(\rho)$ as $\rho \to 0$ involves dividing the range of integration into two parts, and is described in Soward [8].

With the use of the method of separation of variables, we find that the appropriate linearly independent homogeneous solutions W_{iH} to (20) with right-hand side replaced by zero are (as usual) of the form

$$R_n(\rho)(A^{(i)}_{m,n}\cos m\phi + B^{(i)}_{m,n}\sin m\phi)\, P^m_n(\cos\theta),$$

where here m and n are non-negative integers, $P^m_n(z)$ is the associated Legendre function of the first kind [17, p. 332], $A^{(i)}_{m,n}$ and $B^{(i)}_{m,n}$ are arbitrary constants (chosen to satisfy boundary conditions as $\rho \to 0$), and $R_n(\rho)$ satisfies

$$\frac{\mathrm{d}^2 R_n}{\mathrm{d}\rho^2} + \left(\frac{2}{\rho} - \frac{1}{2}\rho\right)\frac{\mathrm{d}R_n}{\mathrm{d}\rho} + \left(1 - \frac{n(n+1)}{\rho^2}\right) R_n = 0.$$

Linearly independent solutions to this ordinary differential equation which do not grow exponentially are

$$R_n = \frac{8\sqrt{2}}{\rho^{3/2}}\mathrm{e}^{\rho^2/8}\, W_{\frac{7}{4},\frac{1}{4}+\frac{1}{2}n}(\tfrac{1}{4}\rho^2),$$

where $W_{\kappa,\mu}(z)$ is Whittaker's function [17, p. 505]. For the particular values $n=0$ and $n=2$, these solutions reduce to

$$R_0 = \rho^2 - 6, \qquad R_2 = \rho^2.$$

Otherwise, these solutions behave like

$$R_n \sim \frac{2^{n+3}\Gamma(n+\frac{1}{2})}{\Gamma(\frac{1}{2}n-1)}\frac{1}{\rho^{n+1}} \qquad \text{as } \rho \to 0\,(n=1, \;\; n \geq 3), \tag{B.5}$$

where $\Gamma(z)$ denotes the usual Gamma function [17, p. 255].

Now consider the partial differential equation (20) with $i=1$. This equation is homogeneous, with (given the required periodicity in θ and ϕ) general solution

$$W_1 = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} R_n(\rho)(A^{(1)}_{m,n}\cos m\phi + B^{(1)}_{m,n}\sin m\phi)\, P^m_n(\cos\theta).$$

The condition (18) as $\rho \to 0$ implies that

$$A^{(1)}_{m,n} = B^{(1)}_{m,n} = 0 \qquad \text{for } n=1, \quad n \geq 3,$$

since the algebraic singularities given by (B.5) as $\rho \to 0$ are not allowed. We are left with

$$\begin{aligned} W_1 &= A^{(1)}_{0,0}(\rho^2-6) + \rho^2 \sum_{m=0}^{2}(A^{(1)}_{m,2}\cos m\phi + B^{(1)}_{m,2}\sin m\phi)\, P^m_2(\cos\theta) \\ &= A^{(1)}_{0,0}(\rho^2-6) + \rho^2[\tfrac{1}{4}A^{(1)}_{0,2}(3\cos 2\theta + 1) \\ &\quad - \tfrac{3}{2}(A^{(1)}_{1,2}\cos\phi + B^{(1)}_{1,2}\sin\phi)\sin 2\theta + \tfrac{3}{2}(A^{(1)}_{2,2}\cos 2\phi + B^{(1)}_{2,2}\sin 2\phi)(1-\cos 2\theta)], \end{aligned}$$

where the constants are yet to be determined.

To solve (20) with $i=2$ we first write $W_2 = W_{2H} + W_{2P}$, where W_{2P} is a particular solution, which we choose to be

$$W_{2P} = -6A_{0,0}^{(1)} N(\rho) + \left(\frac{30}{\rho^2} + 10 - 2\rho^2 \log\rho + 120\sqrt{\pi}\rho^2 \int_\rho^\infty \frac{e^{t/4}}{t^6} \operatorname{erfc}(\tfrac{1}{2}t)\, \mathrm{d}t \right) \times \sum_{m=0}^{2} (A_{m,2}^{(1)} \cos m\phi + B_{m,2}^{(1)} \sin m\phi)\, P_2^m(\cos\theta),$$

where $N(\rho)$ is given by (B.1). This function has the behaviour

$$W_{2P} = A_{0,0}^{(1)} \left(-8\sqrt{\pi}\frac{1}{\rho} + 6(1-\gamma) + O(\rho) \right) + \left(24\sqrt{\pi}\frac{1}{\rho^3} + 10\sqrt{\pi}\frac{1}{\rho} + O(\rho) \right) \sum_{m=0}^{2} (A_{m,2}^{(1)} \cos m\phi + B_{m,2}^{(1)} \sin m\phi)\, P_2^m(\cos\theta)$$

as $\rho \to 0$. We find that no choice of the constants $A_{m,n}^{(2)}$ and $B_{m,n}^{(2)}$ in the homogeneous part W_{2H} can eliminate the singularity of order ρ^{-3} (forbidden by (18)) in W_{2P}, and as such, we must set $A_{m,2}^{(1)} = B_{m,2}^{(1)} = 0$, $m = 0, 1, 2$. Furthermore, (18) implies we must also have $A_{m,n}^{(2)} = B_{m,n}^{(2)} = 0$ for $n = 1$, $n \geq 3$, so we are left with

$$W_1 = A_{0,0}^{(1)}(\rho^2 - 6),$$

$$W_2 = A_{0,0}^{(2)}(\rho^2 - 6) - 6A_{0,0}^{(1)} N(\rho) + \rho^2 \sum_{m=0}^{2} (A_{m,2}^{(2)} \cos m\phi + B_{m,2}^{(2)} \sin m\phi)\, P_2^m(\cos\theta).$$

It is clear that a similar argument for W_{i+1} will eliminate the constants $A_{m,n}^{(i)}$ and $B_{m,n}^{(i)}$ for $m, n \geq 1$ and $i \geq 1$, and that the solutions to (20) which satisfy the boundary conditions (18) as $\rho \to 0$ must be radially symmetric. The constants $A_{0,0}^{(i)}$ are determined by (19).

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