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# SOME REMARKS ON THE REGULARIZATION OF SUPERCOOLED ONE-PHASE STEFAN PROBLEMS IN ONE DIMENSION

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**1. Introduction.** The classical one-dimensional Stefan problem has been widely studied since 1831 (see [1]); it models conductive heat transfer on either side of a phase boundary in pure material on the assumptions (i) that the temperature at the phase boundary is constant, say zero, (ii) that there is a release of latent heat at the phase boundary on solidification, and an uptake on melting, and (iii) that the material on the solid and liquid sides of the phase boundary has negative and positive temperature, respectively.

With these assumptions the problem admits a weak formulation in which the relevant unknown function is the enthalpy and a global solution is known to exist (see, e.g., the literature quoted in [2]). If the data are such that just one phase boundary exists the problem has also been shown to be well-posed in the classical sense [3,4].

On the other hand, if the initial and/or boundary data violate the sign requirement (iii), i.e., if the liquid is supercooled or the solid is superheated, a solution still may exist, at least formally, but the result is generally only local in time and finite time blow-up (preventing the continuation of the solution) can easily occur.

In this paper we will consider as a model problem the simplest case when the solid is at zero temperature and the liquid is supercooled throughout. The aim is twofold. First we seek more information on the possible behaviour of the solution, complementing the analysis performed in [5]; then we shall use the results obtained to suggest a regularization of the model which avoids blow-up and describes phase change to completion.

For simplicity we assume that the liquid is thermally insulated on one side. Thus the liquid temperature $u(x,t)$ and the phase boundary $x = s(t)$ satisfy the following

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system (all quantities are nondimensional and normalized)

$$u_t = uxx \quad \text{in } D_T = \{(x,t)\colon 0 < x < s(t),\ 0 < t < T\}, \tag{1.1}$$

$$s(0) = 1, \qquad u(x,0) = u_0(x), \qquad 0 < x < 1, \tag{1.2}$$

$$u_x(0,t) = 0, \qquad 0 < t < T, \tag{1.3}$$

$$u(s(t),t) = 0, \qquad 0 < t < T, \tag{1.4}$$

$$u_x(s(t),t) = -\dot{s}(t), \qquad 0 < t < T, \tag{1.5}$$

where $u_0(x) \le 0$ and $T \le +\infty$ is the maximal time for which (1.1)–(1.5) are satisfied in the classical sense.

Let

$$Q = \int_0^1 (u_0(x) + 1)\, dx. \tag{1.6}$$

In the special case in which the equation $u_0(x) = -1$ has no more than one root in [0,1] $Q < 0$ is necessary and sufficient for blow-up in the sense that $T = t^* < \infty$, $s(t^*) > 0$ and $\lim_{t \to t^{*-}} \dot{s}(t) = -\infty$; on the other hand $Q > 0$ and $Q = 0$ characterize global existence ($T = +\infty$) and finite time extinction ($s(t) = 0$), respectively [5]. In any event it is known [6] that if $Q < 0$ blow-up certainly occurs. The need thus arises for a regularization of the model if it is to describe the phase change to completion. In two or three space dimensions we could appeal, on physical grounds, either to surface energy effects [12] or to kinetic undercooling [13, 14, 26], but only the latter is available to us in one space dimension. Moreover, the effect of the change necessary in (1.4) to incorporate kinetic undercooling is usually very small except in extreme circumstances [25]. However, as discussed in [15], there is a possibility of a different kind of regularization of the model (1.1)–(1.5) based on the remarkable fact that (1.1), (1.4), (1.5) are, formally, the field equation and free boundary conditions for $\partial c/\partial t = u$, where $c$ satisfies the so-called Crank-Gupta or oxygen diffusion-consumption problem [18]. Under fairly general conditions, to be discussed more precisely in the next section, the solution to this problem *never* blows up in finite time provided that $c(x,t)$ satisfies the additional constraint

$$c \ge 0. \tag{1.7}$$

If this constraint is not imposed, the free boundary in the oxygen-consumption problem coincides with that of the problem (1.1)–(1.5) and both problems have finite time blow-up at the time at which the negativity set of $c$ reaches $x = s(t)$.

In this paper we address the possible mathematical and physical implications for (1.1)–(1.5) of the good behaviour resulting from the constraint (1.7), which is physically realistic when interpreted in terms of oxygen consumption.

However, before enumerating the possibilities and making some of the above statements more precise, we make two further remarks about this kind of regularization.

Firstly, it is in the same spirit as, although technically quite different from, the mathematical regularization of the two-phase volumetrically heated Stefan problem considered in [19]. There the "classical" solution with a single sharp boundary involves a region of superheated solid, but the weak solution of the enthalpy formulation avoids superheating at the expense of introducing a mushy zone. In turn, a classical reformulation of the problem including mushy zones can be shown to possess a smooth solution [20, 21]. In this paper it is the variational formulation in terms of the time integral of the temperature that suggests a regularized version of the problem. We could add that while the mushy region formulation is aimed at excluding the possibility of superheating or supercooling in the presence of heat sources or sinks, the regularization suggested here allows for supercooling but still provides a governing mechanism for the solidification process until its completion.

Secondly, we note that it may be possible to achieve a kind of regularization similar to the one considered here in higher space dimensions. However, in this case a further difficulty can arise because of the possible presence of cusps at the blow-up time [22]. This latter statement is certainly true in the Hele-Shaw special case in which $u_t$ is deleted from the two-dimensional version of (1.1)–(1.5) [22, 23] and for which cusp formation occurs when the negativity set of the relevant oxygen concentration reaches the free boundary. However, this Hele-Shaw problem does not have finite-time blow-up in one dimension, and will not be further considered here. Nor will two-dimensional problems generally, both because of their technical difficulty and because they are thought to be frequently regularized by surface energy effects [12, 22].

In the next section we will discuss the general relationship between the supercooled liquid problem and the oxygen diffusion-consumption problem, together with the basic ideas of the proposed regularization.

In Sec. 3 we will analyze the possible singularities which can arise in the unregularized supercooled liquid problem. In particular we will show that there are cases in which the solution exists for all times, but the free boundary has an isolated singular point (i.e., $\dot{s}(t)$ is not bounded).

Further consequences of the result obtained are illustrated in Sec. 4.

Finally the regularization procedure is discussed in Sec. 5.

**2. The supercooled Stefan problem and the oxygen diffusion-consumption problem.** Developing the ideas outlined in the introduction, the kind of regularization we will discuss is based on the fact that if $u$ solves (1.1)–(1.5) and if we define

$$c(x,t) = \int_{s(t)}^{X} d\xi \int_{s(t)}^{\xi} [u(\eta,t)+1] d\eta \tag{2.1}$$

then $c(x,t)$ solves the problem

$$c_t = c_{xx} - 1 \quad \text{in } D_T, \tag{2.2}$$

$$s(0) = 1, \qquad c(x,0) = c_0(x), \qquad 0 < x < 1, \tag{2.3}$$

$$c_x(0,t) = c_0'(0), \qquad 0 < t < T, \tag{2.4}$$

$$c(s(t),t) = 0, \qquad 0 < t < T, \tag{2.5}$$

$$c_x(s(t),t) = 0, \qquad 0 < t < T, \tag{2.6}$$

where

$$c_0(x) = \int_1^X d\xi \int_1^\xi (u_0(\eta)+1) d\eta. \tag{2.7}$$

Using (1.6) we have

$$c_0'(0) = -Q. \tag{2.8}$$

REMARK 2.1. The correspondence between $c_t$ and $u$ was noted in [16] for some special cases and discussed in a more general context in [17]. Of course if (1.3) is replaced by $u(0,t) = F(t)$ or by $u_x(0,t) = G(t)$, the fixed boundary condition (2.4) has to be replaced by

$$c(0,t) = c_0(0) + \int_0^t F(\tau)d\tau$$

or by

$$c_x(0,t) = c_0'(0) + \int_0^t G(\tau)d\tau,$$

respectively.

On the other hand, for any classical solution $(c,s)$ of (2.2)–(2.6) with conditions $c(0,t) = f(t)$ or $c_x(0,t) = g(t)$, the pair $(u,s)$ with $u = c_t$ solves a problem of Stefan type with data $u(x,0) = c_0''(x) - 1$ and $u(0,t) = \dot{f}(t)$ or $u_x(0,t) = \dot{g}(t)$, provided suitable compatibility conditions are satisfied at the corner points (0,0) and (1,0) (otherwise the fixed boundary conditions may have to be measures). □

Problem (2.2)–(2.6) is a typical example of a free boundary problem with Cauchy data prescribed on the free boundary and it is known as the oxygen diffusion-consumption model [18]. Other problems of the same kind are optimal stopping time problems, filtration in partially saturated porous media, etc.

If the quantity $c$ in (2.2)–(2.6) is to have a physical interpretation (e.g., oxygen concentration) it must be subjected to the constraint

$$c(x,t) \geq 0 \quad \text{in } D_T. \tag{2.9}$$

With such a constraint problem (2.2)–(2.6) can be interpreted as a parabolic obstacle problem and is amenable to a variational inequality (see [2, 7–11]). In this context one should remark that (2.1) is a Baiocchi-type transform on which the variational formulation of the Stefan problem can be based.

The obstacle problem never exhibits blow-up, in the sense that either

$$\text{(i)} \quad c(x,t) \geq 0, \qquad c(x,t) \not\equiv 0$$

for all $t > 0$, or

$$\text{(ii)} \quad c(x,t) \equiv 0$$

for $t$ greater than some finite $T$ (extinction time), while (i) holds for $0 < t < T$.

Returning to problem (2.2)–(2.6), with $c_0(x)$ given by (2.7), if (2.9) is not imposed we can still say that $u = c_t$ solves (1.1)–(1.5), but we are no longer in a position to rely on the global existence result for the obstacle problem. As a matter of fact we will see that if $c$ becomes negative at some point in $\overline{D}_T$, then the set $\{(x,\tau)\colon c(x,\tau) < 0,\ 0 < x < s(\tau),\ 0 < \tau < t\}$ expands as $t$ increases and it is bound to meet the free boundary in a finite time $t = t^*$, at which blow-up occurs.

The above facts suggest the idea of regularizing the supercooled Stefan problem by imposing the constraint (2.9) on the time integral $c$ of the solution $u$. Such a procedure will be developed in Sec. 4.

However, since blow-up of the solution is the phenomenon we want to avoid, it is important to understand its occurrence and the relevant details will be discussed first in Sec. 3. For ease of exposition in the remainder of the paper, we will refer to (1.1)–(1.5) as the supercooled Stefan problem (SSP); (2.2)–(2.6) *without* the restriction of (2.9) as the unconstrained diffusion-consumption problem (UDCP), henceforth writing its solution as $c(x,t)$; and (2.2)–(2.6) *with* (2.9) as the constrained diffusion-consumption problem (CDCP), denoting its solution by $\bar{c}(x,t)$.

**3. Blow-up in (SSP) and in (UDCP).** We shall say that the solution of (SSP) or (UDCP) has essential (or proper) blow-up at $t = t^*$ if $s(t^*) > 0$, $\liminf_{t\to t^*-} \dot{s}(t) = -\infty$, and the solution cannot be continued beyond $t^*$.

Here we want to relate essential blow-up to the presence of a negativity set of $c(x,t)$.

First we prove that the onset of a negativity set for $c(x,t)$ leads to the occurrence of a singularity of $\dot{s}(t)$ after a finite time.

For $t \in (0,T)$, define

$$N(t) = \{x\colon 0 \le x < s(t),\ c(x,t) < 0\}.$$

We have the following

Proposition 3.1. If $N(t_1) \neq \emptyset$ then

(i) For any $t_2 \in (t_1, T) N(t_1) \subset\subset N(t_2)$, i.e. , the negativity set expands;

(ii) if for some $t^* > t_1$ the boundary $\partial N(t^*)$ touches the free boundary then $\dot{s}(t)$ is singular as $t \to T^*$;

(iii) the case above actually occurs.

*Proof*. The property (i) follows immediately from the fact that $c_t = u$ is negative for $0 \le x < s(t)$, $t > 0$.

Concerning (ii), if $s(t)$ is Lipschitz continuous at $t = t^*$ then $u_x$ is continuous at $(s(t^*), t^*)$ and $u, s$ are $C^\infty$ by a well-known argument. In such a case $c_t(s(t^*), t^*) = 0$, i.e., $c_{xx} > 0$ in a left-neighborhood of the free boundary, implying $c > 0$ in the same neighborhood and contradicting the fact that $(s(t^*), t^*)$ is a point of $\partial N(t^*)$.

To prove (iii) we note that the fact that the boundary of the negativity set of $c$ has to reach the free boundary in a finite time is a simple consequence of (i): we cannot have global existence (even if $Q \ge 0$) since $c$ would tend asymptotically to $c_\infty(x) = \frac{1}{2}(x - s(\infty))^2$ and this is not consistent with the persistence of any negativity point of $c$; for the same reason we can also infer that the free boundary does not reach $x = 0$ before it intersects $\partial N(t)$. □

At this point we can show that $(s(t^*), t^*)$ is indeed a point of essential blow-up and we can also characterize any such point as a boundary point of $\partial N(t^*)$.

We will need the following auxiliary result:

Proposition 3.2. For any $\bar{t} \in (0, T]$ the equation $u(x, \bar{t}) = -1$ cannot have infinitely many roots.

*Proof*. We reflect problem (1.1)–(1.5) about the $t$ axis and note that for $0 < \bar{t} < T$ the result follows from the analyticity w.r.t. $x$ of $u(x, \bar{t})$ in the interval $(-s(\bar{t}), s(\bar{t}))$ and the continuity in $(s(\bar{t}), \bar{t})$.

For $\bar{t} = T$ the proof is concluded by using the continuity of $u(x,t)$ for $t = T$ and $x \in (-s(T),\ s(T))$ and the maximum principle together with the result above. □

Now we prove

PROPOSITION 3.3. If $t^*$ is such that $(s(t^*), t^*) \in \partial N(t^*)$ then the solution cannot be continued for $t > t^*$. Conversely, if $(s(t^*), t^*)$ is a point of essential blow-up then it has to belong to $\partial N(t^*)$.

*Proof*. Assume $P^* \equiv (s(t^*), t) \in \partial N(t^*)$. Then $c(x, t^*) < 0$ in a left neighborhood of $P^*$. Indeed $P^*$ cannot be an accumulation point of zeros of $c(x,t^*)$ because otherwise also $c_{xx}(x,t^*)$ would vanish infinitely many times contradicting Proposition 3.2. Thus, recalling (2.1), any interval $(s(t^*) - \varepsilon, s(t^*))$ has to contain points where $u(x,t^*) < -1$. By virtue of Proposition 3.2 we can assert that $u(x,t^*) \leq -1$ in the whole interval for $\varepsilon$ sufficiently small. At this point, nonexistence for $t > t^*$ follows from [24].

The proof of the converse statement is also easy: if in $(s(t^*), t^*)$ we have essential blow-up, then the inequality $u(x,t^*) > -1$ cannot be satisfied in any interval $(s(t^*) - \varepsilon,\ s(t^*))$, otherwise the solution would be continuable [24]. Then, by Proposition 3.2 $c \leq 0$, $c \not\equiv 0$ for any $\varepsilon$ sufficiently small. □

It is of some importance to distinguish the role played in the theory by the set of inner points where $c = 0$ and the set of the points where $u = -1$.

It is easy to see that when a negativity set of $c$ is present, a curve $u = -1$ of inflection points of $c(x,t)$ must lie between it and the free boundary. Then a point of essential blow-up is reached both by a curve $c = 0$ bounding the negativity set, and by a curve $u = -1$.

However in Proposition 3.4 below we show more generally that when a curve $u = -1$ reaches the free boundary, then $\dot{s}$ is singular at the meeting point, although, as we shall see later, this does not necessarily imply the existence of a negativity set of $c$ and essential blow-up.

PROPOSITION 3.4. Let $t_0 \in (0, T]$ and assume that in $D_{t_0}$ either the set $\{(x,t)\colon u(x,t) = -1\}$ is empty or it has a positive distance from the free boundary. Then $\dot{s}$ is bounded for any $t \leq t_0$. If on the contrary this set reaches the free boundary at $t = t_0$, then $\lim_{t \to t_0 -} \dot{s}(t) = -\infty$.

*Proof*. The first statement is proved in [5]. The second result follows from the fact that as long as $\dot{s}$ is bounded the solution of (SSP) is smooth in the vicinity of the free boundary. □

We conclude our analysis of the possible singularities of the free boundary by showing that the free boundary can actually have isolated singularities, which do not prevent the continuation of the solution.

PROPOSITION 3.5. There are initial data such that problem (2.2)–(2.6) admits global solutions with $\lim_{t \to t_0} \dot{s}(t) = -\infty$ for some $t_0 > 0$.

*Proof*. We construct a specific example. Let us consider the following set of initial data for (1.1)–(1.5):

$$u_0(x) = \begin{cases} -M, & 0 < x < a, \\ -N, & a < x < b, \\ 0, & b < x < 1, \end{cases}$$

where $M$ and $N$ are nonnegative constants. From (2.7) we have

$$c_0(x) = \frac{1}{2}(x-1)^2 + \begin{cases} -\frac{1}{2}N(a-b)^2 - N(a-b)(x-a) - \frac{1}{2}M(x-a)^2, & 0 < x < a, \\ -\frac{1}{2}N(x-b)^2, & a < x < b, \\ 0, & b < x < 1. \end{cases}$$

Thus

$$Q = 1 - N(b-a) - Ma,$$
$$c_0(0) = \frac{1}{2} - \frac{1}{2}N(b-a)^2 - Na(b-a) - \frac{1}{2}Ma^2.$$

We show that both of the conditions $Q > 0$ and $c_0(0) \leq 0$ can be satisfied by a suitable choice of the parameters. Setting $\delta = b - a$, this means that

$$1 - N\delta - Ma > 0, \tag{3.1}$$
$$N\delta(\delta + 2a) + Ma^2 - 1 \geq 0. \tag{3.2}$$

In the quarter-plane $M \geq 0, N \geq 0$ the two half-planes represented by (3.1), (3.2) have a nonvoid intersection $I$ if and only if

$$2a + \delta = a + b > 1. \tag{3.3}$$

It is easily seen that $M < 1$ and $N > 1$ in $I$, so that two level curves $u = -1$ exist in $D_T$ for data satisfying (3.1), (3.2). Now we select $M = 0, a = \frac{1}{2}, b = \frac{3}{4}$ and we consider the whole family of problems parameterized by $N$. For $N \leq 1$ we have global existence, $u$ being greater than $-1$ everywhere. For $N = 0$ the solution is stationary. For increasing values of $N$ the free boundaries are monotonically ordered because of the maximum principle, as long as $c \geq 0$. More precisely, if $N_1 < N_2$ we can say that $s_1 > s_2$ and $c_1 > c_2$ at least until $x = s_2(t)$ crosses the negativity set of $c_1$. For $N$ satisfying (3.1), (3.2), e.g., $N = \frac{7}{2}$, a negativity set of $c$ is present from the beginning and essential blow-up will take place. It is important to observe that for no values of $N \in [0, 4)$ can finite extinction occur, since $Q > 0$ (because of (3.1)).

Denoting by $\Gamma_{-1}$ the set $\{u = -1\}$ and by $\Gamma_0$ the free boundary, we define

$$d_N = \operatorname{dist}(\Gamma_{-1}, \Gamma_0) \quad \text{for } N > 1,$$
$$d_N = 1 \quad \text{for } N \leq 1.$$

For each $N$ let $(T_N, s_N, u_N)$ denote the corresponding solution of (SSP). We remark that $d_N > 0$ implies $T_N = +\infty$ and $c_N \geq 0$ by Proposition 3.1.

Let us consider $N_0 = \sup\{N \colon d_N > 0\}$. Then (using the continuous dependence theorem of [3, I]) $u_N$ converges monotonically to $u_{N_0}$ in $D_{T_{N_0}}$ as $N \uparrow N_0$ and $c_{N_0} \geq 0$. Since $d_{N_0} = 0$, the interval $(0, T_{N_0})$ in which (1.1)–(1.5) has a classical solution is finite and $\dot{s}_{N_0}(t)$ is singular for $t \to T_{N_0}$. Since $c_{N_0}(x, T_{N_0}) \geq 0$ and no more than two curves $\{u_{N_0} = -1\}$ exist in $D_{T_{N_0}}$, we have $u_{N_0}(x, T_{N_0}) > -1$ for $0 < x < s_{N_0}(T_0)$. Hence taking $u_{N_0}(x, t_{N_0})$ as new initial data, (SSP) is globally solvable for $t > T_{N_0}$.

We can remark that while the point $(s(T_{N_0}), T_{N_0})$ is a singularity point for (SSP) it is not to be considered such for (CDCP) since for the latter problem the free boundary is not required to be differentiable.[1] Hence the proof is concluded. □

REMARK 3.6. Note that the fact that $u < 0$, as we are assuming, is essential only in the proof of parts (i) and (iii) of Proposition 3.1. □

REMARK 3.7. There are three ways in which a negativity set may first appear: firstly, $c_0(x)$ may be negative somewhere; secondly, $c(0, t)$ may become negative with $c_x(0, t)$
$= -Q > 0$ as in Fig. 1; thirdly, $c_0(x)$ may have an interior minimum ($c_0' = 0$) which subsequently decreases through zero (Fig. 2). Only the third case is possible if $Q > 0$, but all three can occur (and at lease one has to) if $Q < 0$.

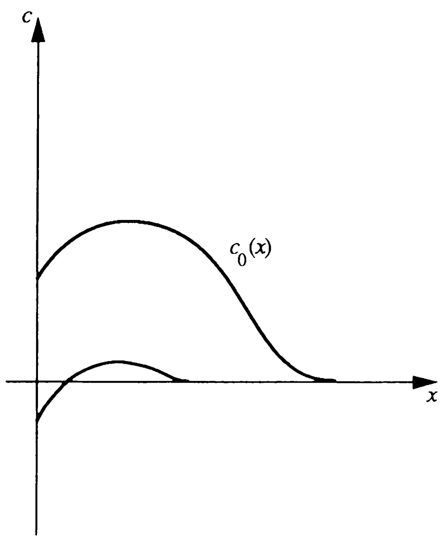


FIG. 1

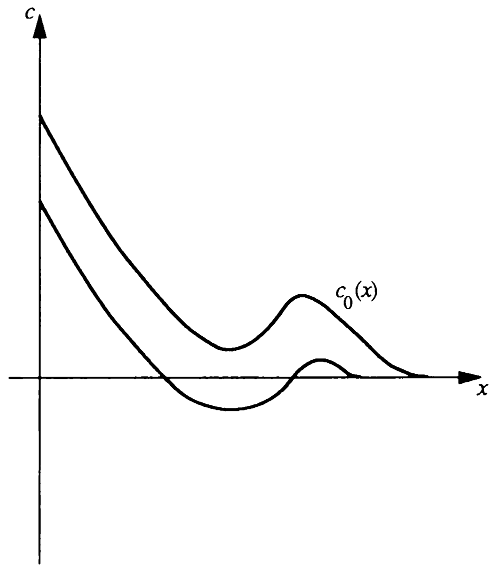


FIG. 2

Figures (3a, b) illustrate the case (UDCP)≡(CDCP) with $Q > 0$, showing the asymptotic values $s_\infty = Q$, $c_\infty = \frac{1}{2}(x - Q)^2, u_\infty = 0$. □

**4. Further remarks on the Stefan problem and on the oxygen diffusion-consumption problem.** In view of the results obtained in Sec. 3 many facts in the theory of the Stefan problem and of the oxygen consumption problem can be given an immediate interpretation, providing a basis for the material to be discussed in Sec. 5.

(a) In the classical one-phase Stefan problem the implications $u_0(x) \geq 0 \Rightarrow u(x, t) \geq 0 \Rightarrow c(x, t) > 0$ show that this is a trivial case of global existence. □

[1] A similar phenomenon of continuation beyond a blow-up point has been found in unsteady Hele-Shaw problems and for one-parameter families of two-dimensional obstacle problems in [23, 27].

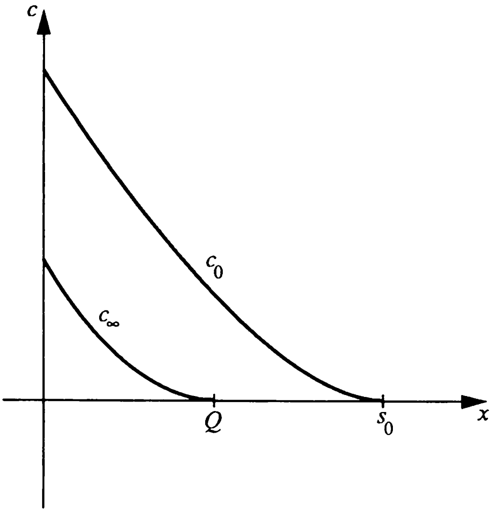


FIG. 3a

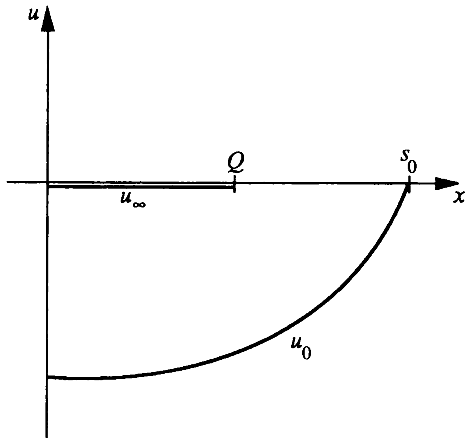


FIG. 3b

(b) Consider a Stefan problem with a given volumetric heat source in the framework of the enthalpy formulation. When a mushy region advances towards a solid region under the action of the heat source the temperature $\theta$ in the solid (see [20]) is such that the quantity $c = -\theta$ solves (UDCP). Therefore, since superheating is not allowed and $\theta < 0$, there will be no blow-up. $\square$

(c) Concerning (UDCP), the implication $Q < 0 \Rightarrow$ *essential blow-up* can be explained very easily as follows. The assumption $-\|u_0\| \leq u < 0$ implies $|c_{xx}| \leq 1 + \|u_0\| \equiv K$. Therefore the length of the interval $(0, x)$ in which $c_x$ decreases from $-Q$ (at $x = 0$) to 0 (at $x = s$) must exceed $|Q|/K \equiv S$, i.e., $s(t) > S$. Consequently, finite time extinction being excluded, global existence would be inconsistent with $c_x(0, t) > 0$. $\square$

(d) If (CDCP) is formulated classically, with a new free boundary appearing each time $c$ becomes zero, then we always have finite time extinction.

Indeed, let $t_0$ be such that $c(x_0, t_0) = 0$ for some $0 < x_0 < s(t_0)$. Then for $x > x_0$, $t > t_0$ the solution of (CDCP), i.e., the triple $(\sigma, \bar{s}, \bar{c})$, (if it exists) satisfies

$$
\begin{aligned}
&\bar{c}_{xx} - \bar{c}_t = 1, \qquad \sigma(t) < x < \bar{s}(t), \qquad t > t_0,\\
&\sigma(t_0) = x_0, \qquad \bar{s}(t_0) = s(t_0),\\
&\bar{c}(x, t_0) = c(x, t_0), \qquad x_0 < x < s(t_0),\\
&\bar{c}(\sigma(t), t) = \bar{c}_x(\sigma(t), t) = 0, \qquad t > t_0,\\
&\bar{c}(\bar{s}(t), t) = \bar{c}_x(\bar{s}(t), t) = 0, \qquad t > t_0.
\end{aligned}
\tag{4.1}
$$

Another free boundary will be generated at the left of $x = \sigma(t)$ (see points $(e, f)$ below). We can see as follows that the curves $x = \sigma(t)$ and $x = \bar{s}(t)$ must meet each other in a finite time.

Indeed we can introduce a function $\phi(x) \geq \bar{c}(x, t_0)$ such that $\phi(x_0) = 0, \phi(s(t_0)) = \phi'(s(t_0)) = 0, \phi$ is symmetric with respect to the centre of the interval $(x_0,\ s(t_0))$, and

$\phi''$ vanishes at only two points. On the basis of the results of [5] we can say that the symmetric left and right free boundaries for (CDCP) with initial data $\phi$ have to meet in a finite time. Hence the same has to happen to the curves $x = \sigma(t), x = \bar{s}(t)$. □

(e) When a new free boundary is generated for (CDCP) it starts with infinite speed. Let $\bar{u} = \bar{c}_t$ where $\bar{c}$ is the solution to (4.1). Then the fact that $\lim_{x\to x_0+} \bar{u}(x, t_0) < 0$ implies that $\dot{\sigma}(t)$ cannot be bounded in the vicinity of $t = t_0$. □

(f) The solution of (4.1) exists. Since by assumption $c(x, t_0) > 0$ for $x_0 < x < s(t_0)$, there must be points in a small neighborhood $(x_0, x_0 + \varepsilon)$ in which $\bar{u}(x, t_0) > -1$, where $\bar{u}(x, t_0)$ coincides with $\lim_{t_0-} u(x, t), u$ solving (SSP) for $t \le t_0$. Using once more Proposition 3.2 and [24], existence and uniqueness are guaranteed. □

If $x_0 = 0$ we modify the boundary conditions at $x = 0$ for $t > t_0$ introducing a waiting time $\tau$ as described in Sec. 5, Case 2, so that (4.1) is to be solved for $t > t_0 + \tau$ with some initial data $\bar{c}(x, t_0 + \tau)$ such that $\bar{c}_x(0, t_0 + \tau) = 0$. For such a problem the conclusions under (d), (f) remain valid.

**5. Regularization of the blow-up SSP.** We begin with the most straightforward case.

CASE 1. $Q = 0$, $c_0 \ge 0$.

This implies that $c_x(0, t) = 0$ and, as mentioned earlier, blow-up can only occur if an interior minimum of $c$ reaches $c = 0$. We suppose that the first place at which $c$ vanishes away from $x = s(t)$ is at $x = \hat{x}$, when $t = \hat{t}; 0 \le \hat{x} < s(\hat{t})$. Up to $t = \hat{t}$, (UDCP) $\equiv$ (CDCP), i.e., $c \equiv \bar{c}$, and $u \equiv c_t = \bar{c}_t$. In this case the (CDCP) evolves as in Fig. 4a (see points $e, f$ of the previous section), compared to the (UDCP) (Fig. 4b), and $\bar{c}_t$ evolves as in Fig. 4c.

At each of the two new phase boundaries, the Stefan condition (1.5) is satisfied by $\bar{c}_t$, but this solution for $u$ differs from the time derivative $c_t$ of the (UDCP) for $t > \hat{t}$.

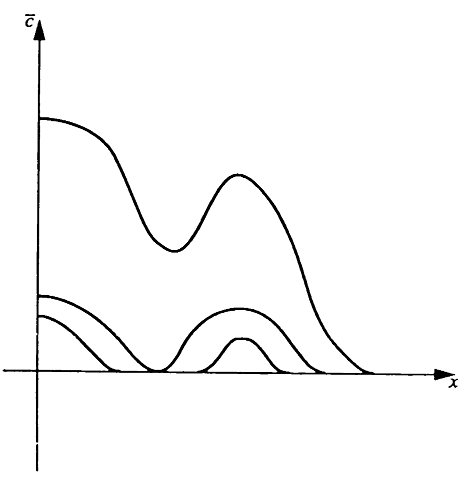


FIG. 4a

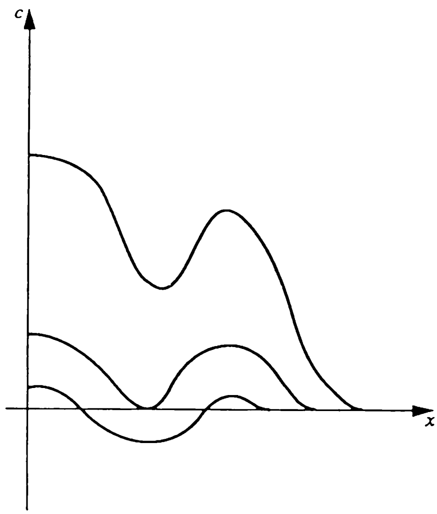


FIG. 4b

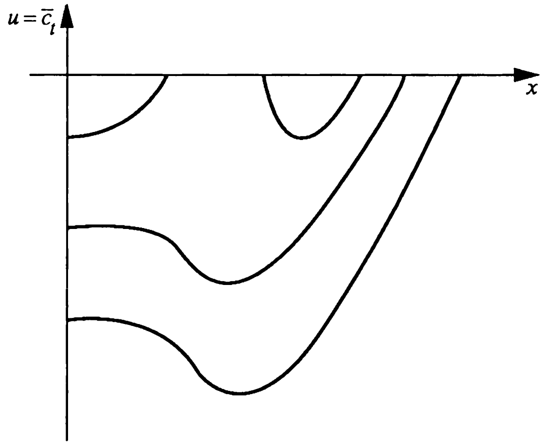


FIG. 4c

There is no change in the "energy" $\int_0^{s(\hat{t})} u(x,\hat{t})\,dx$ but the creation of the new phase boundaries rearranges the energy fluxes in such a way that the blow-up that would have occurred because of the deficit near $x = s(t)$ (counterbalanced by a surplus near $x = 0$) does not occur. Of course, if $\bar{c}$ subsequently falls to zero at another point, we must again nucleate two new free boundaries as before.

Lastly we mention that we might allow $c$ to become negative on an interval before nucleating as in Case 3 below, but the case given here corresponds to the earliest possible removal of negativity sets for the (UDCP), so it may be called a "least nucleation principle."

CASE 2. $Q < 0, c_0 \geq 0$.

Now $c_x(0,t) = -Q > 0$ for $t > 0$, and we only consider the case where, as in Fig. 5a, $c$ first falls to zero away from $x = s(t)$ at $x = 0, t = \hat{t}$ (otherwise, Case 1 applies). For $0 < t < \hat{t}$ we define $u = c_t = \bar{c}_t$, as before but now the (SSP) has an energy deficit $Q$ which must be removed in order to prevent blow-up.

To maintain positivity of $\bar{c}$, we must change the boundary condition at $x = 0$. This we may do in several ways, even if we do it at the earliest possible time $\hat{t}$. Two possibilities are as follows.

(a) Perhaps the most physically natural procedure is to "pin" $\bar{c}$ at zero and allow $\bar{c}_x$ to relax to zero in some finite time $\bar{t}$ (Fig. 5a). We may achieve this mathematically by applying the Signorini boundary condition

$$\bar{c}(\bar{c}_x + Q) = 0, \qquad \bar{c} \geq 0, \qquad \bar{c}_x + Q \leq 0.$$

The consequence of this choice is that the temperature $u = \bar{c}_t$ is reduced to zero at $x = 0, t = \hat{t}$, and also "pinned" at that value for $\hat{t} < t < \hat{t} + \bar{t}$, but that no phase change occurs until $t = \hat{t} + \bar{t}$ when nucleation occurs at $x = 0$ (Fig. 5b). The deficit of energy $-Q$ is removed from the (SSP) via the sink at $x = 0$ during the time interval $\hat{t} < t < \hat{t} + \bar{t}$.

(b) An alternative to this option is the relaxation of the boundary condition $\bar{c}_x + Q = 0$ at $x = 0$, and its replacement by the zero-flux condition $\bar{c}_x = 0$ (corresponding

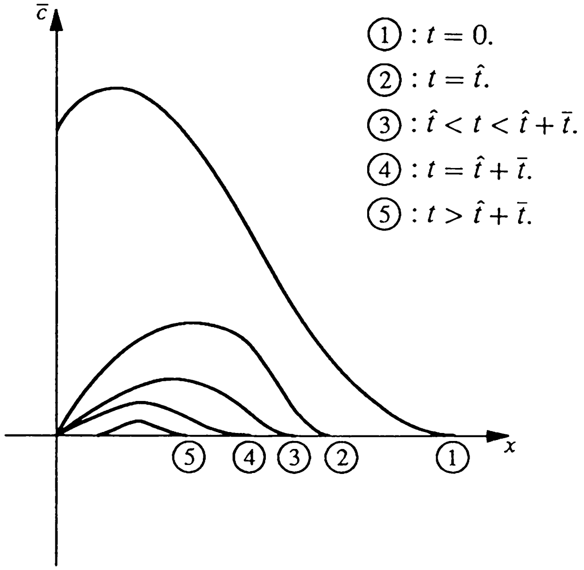


FIG. 5a

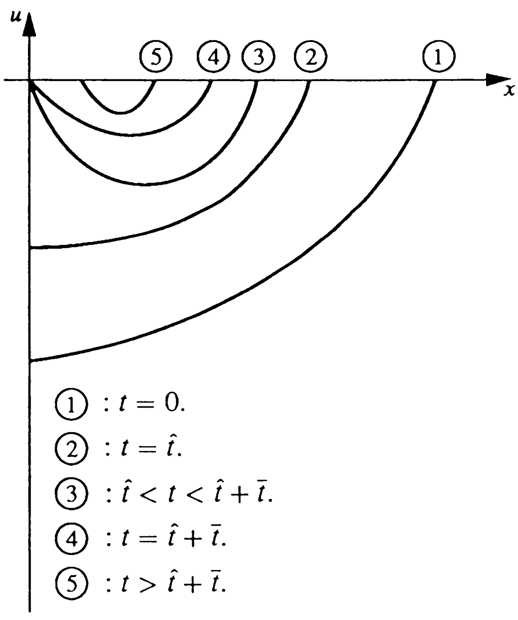


FIG. 5b

to zero-flux in the (SSP)). Then $\bar{c}$ would evolve with $\bar{c}(0,t) > 0$ but $\bar{c}_x(0,t) = 0$ for $t > \hat{t}$ (Fig. 6a). This would imply a more dramatic energy change for $u = c_t$, with $u$

being measure-valued at $t = \hat{t}$, since

$$\left[\int_0^{s(t)} [u(x,t)+1]\,dx\right]_{t=\hat{t}^-}^{t=\hat{t}^+} = [\bar{c}_x(0,t)]_{t=\hat{t}^-}^{t=\hat{t}^+} = -Q,$$

so that

$$u(x,\hat{t}^+) = u(x,\hat{t}^-) - Q\delta(x).$$

However, the subsequent evolution of $u$ would include a nonsupercooled region $u > 0$ separated from the supercooled region $u < 0$ by a zero isotherm which is not a phase boundary (Fig. 6b); in view of our requirement that $u \leq 0$ we do not pursue this point further, except to mention that when $\bar{c}(0,t)$ again falls to zero, a new phase boundary appears at $x = 0$.

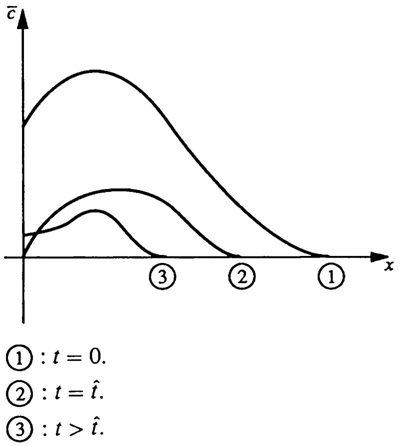


FIG. 6a

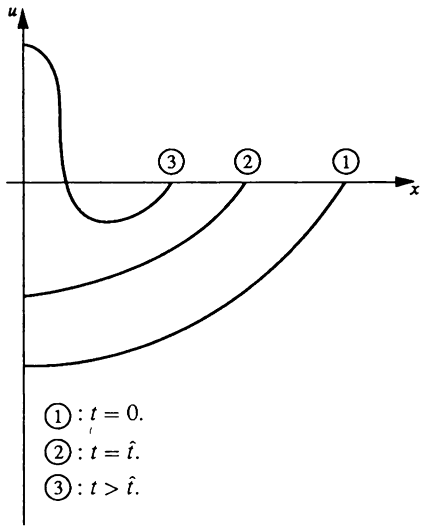


FIG. 6b

For sake of completeness, we will also consider the case in which the initial data is such that $c_0(x)$, defined according to (2.7), has intervals of negativity in [0,1), although such a situation could never exist in practice if the nucleation assumption holds.

CASE 3. $c_0(x)$ negative for some $x \in [0,1)$.

For simplicity, we just consider the configuration in Fig. 7a where $c_0 < 0$ for $0 < x < x_0$. Now the earliest removal of the negativity set is to prescribe $\bar{c}(x, 0^+) = 0$ in $0 < x < x_0$, thereby instantaneously solidifying the whole interval $[0, x_0)$ in the (SSP), but analogously to Case 2 we have two possibilities for $t > 0$.

(a) Pin $\bar{c} = 0$ at $x = x_0$ until $\bar{c}_x$ also vanishes at $x = x_0$, and then allow a new free boundary to form in the (CDCP). This again corresponds to pinning $u = \bar{c}_t$ without change of phase at $x = x_0$, and subsequently nucleating the point $x = x_0$ at the appropriate time (Figs. 7b, c).

(b) Relax the condition $\bar{c} = 0$ at $x = x_0$ and allow $\bar{c}$ to evolve as the (CDCP) with a free boundary emanating from $x = x_0$ at $t = 0$. This new free boundary advances into $x < x_0$ for some positive times.[2]

In the corresponding (SSP) with $u = c_t$, this free boundary is a phase boundary between unsupercooled liquid and solid at $u = 0$; between this and the supercooled phase boundary $x = s(t)$ is a zero isotherm at which no phase change occurs (see Figs. 7d, e). As in Case 2 above, this contravenes the requirement that $u \le 0$.

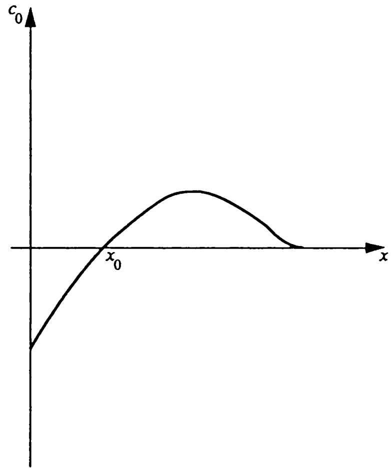


FIG. 7a

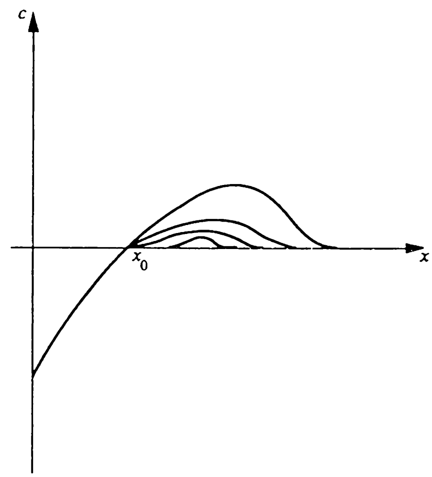


FIG. 7b

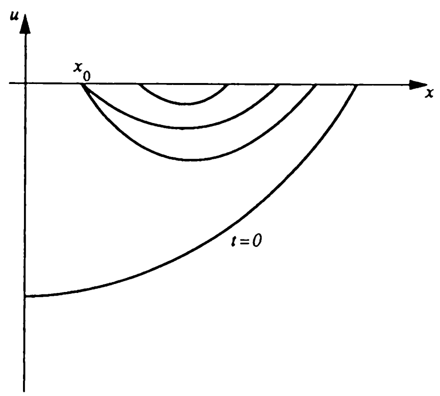


FIG. 7c

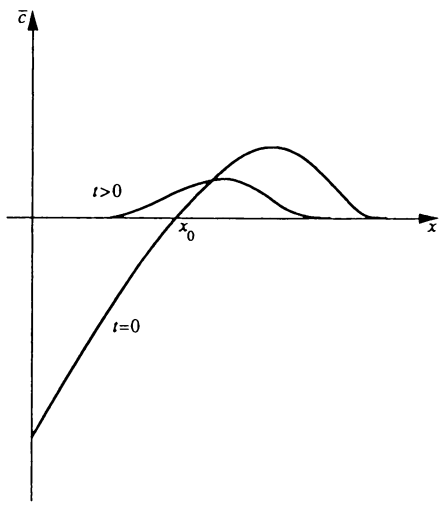


FIG. 7d

[2]We note that such "advancing" free boundaries would occur in the original (CDCP) [18] if the initial data $c(x, 0)$ had finite nonzero slope at $x = 1$. If $c_0'(1) = 0$ the sign of $c_0''(x) + 1|_{x=1}$ determines the direction of motion of this free boundary (advancing or receding).

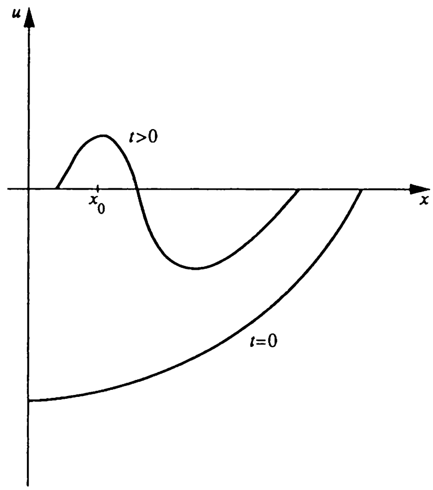


FIG. 7e

**Conclusion.** We have described a purely mathematical way of modifying (UDCP)'s which are associated with (SSP)'s in such a way that no finite-time blow-up occurs. The corresponding (CDCP)'s and regularized (SSP)'s have also been linked. The proposed regularization procedure is based on the analysis of the possible singularities of (SSP)'s. Even though there may have been little physical significance except perhaps in the Case 1, it is interesting to note that in all the situations considered here there is an earliest time at which the negativity set of $c$ can naturally be excised, and that this excision can be thought of as a "least nucleation" principle for the (SSP).

It is possible that similar ideas can be worked through in more dimensions but the negativity sets for $c_0$ may involve $c_0 \to -\infty$; for example in Case 3 with radial symmetry, $c(r, 0)$ has a delta function behaviour at $r = (x^2 + y^2)^{1/2} = 0$.

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