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TWO PHASES STEFAN PROBLEM WITH SMOOTHED ENTHALPY*

M. AZAÏEZ[†], F. JELASSI[‡], M. MINT BRAHIM[§], AND J. SHEN[¶]

Abstract. The enthalpy regularization is a preliminary step in many numerical methods for the simulation of phase change problems. It consists in smoothing the discontinuity (on the enthalpy) caused by the latent heat of fusion and yields a thickening of the free boundary. The phase change occurs in a curved strip, i.e. the mushy zone, where solid and liquid phases are present simultaneously. The width ϵ of this (mushy) region is most often considered as the parameter to control the regularization effect. The purpose we have in mind is a rigorous study of the effect of the process of enthalpy smoothing. The melting Stefan problem we consider is set in a semi-infinite slab, heated at the extreme-point. After proving the existence of an auto-similar temperature, solution of the regularized problem, we focus on the convergence issue as $\epsilon \to 0$. Estimates found in the literature predict an accuracy like $\sqrt{\epsilon}$. We show that the thermal energy trapped in the mushy zone decays exactly like $\sqrt{\epsilon}$, which indicates that the global convergence rate of $\sqrt{\epsilon}$ cannot be improved. However, outside the mushy region, we derive a bound for the gap between the smoothed and exact temperature fields that decreases like ϵ. We also present some numerical computations to validate our results.

Key words. Stefan problem, phase change problems, enthalpy, convergence.

AMS subject classifications. 35B6, 65L20, 65N12, 80A20, 80A22.

1. Introduction

The two-phase Stefan problem is a basic model for melting (or solidification) of phase change materials. The unknowns are the temperature field and the location of the melting front delimiting the liquid and solid phases. The front, also called interphase or the free boundary, is dynamic and the moving velocity is given by the Stefan conditions which express the energy conservation and involve the latent heat of fusion absorbed during melting the mass. Mathematically, the resulting problem is non-linear, with an enthalpy jump along the liquid-solid interface. In spite of these complications, Stefan problem is widely used because of the availability of an analytical form of the exact solution in some standard geometries (see [2,15]). It is also a benchmark for testing and assessing mathematical and numerical methods developed for phase transition problems (cf. [2,6] and references therein).

The discontinuity of enthalpy is a source of difficulty for computation. Many numerical methods, especially those based on the enthalpy derivatives such as implicit time schemes with Newton type algorithms, start by embedding the original problem into a collection of regularized problems (see [2,4,5,9]). The enthalpy function becomes continuous and (piecewise) differentiable. As a result, the sharp front disappears and we have instead a mushy zone where solid and liquid phases are present simultaneously. We are interested in, first, the analysis of the smoothed version of Stefan problem, then we deal with the convergence of the regularized solution with respect to the width ϵ

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[†]I2M UMR 5295. Bordeaux INP, 16 Av Pey-Berland 33607 Pessac, France (azaiez@ipb.fr).

[‡]Sorbonne Universités, UTC, EA 2222, Laboratoire de Mathématiques Appliquées de Compiègne, F-60205 Compiègne, France (faten.jelassi@utc.fr).

[§]I2M UMR 5295. Bordeaux ENSAM, Esplanade des Arts et Métiers 33405 Talence cedex France and Sorbonne Universités, UTC, EA 2222, Laboratoire de Mathématiques Appliquées de Compiègne, F-60205 Compiègne, France (maimouna.mint-brahim@u-bordeaux.fr).

[¶]Fujian Provincial Key Laboratory on Mathematical Modeling & High Performance Scientific Computing and School of Mathematical Sciences, Xiamen University Xiamen, China 361005.
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of the mushy zone. We recall that this question has been addressed in the specialized literature where convergence results are established [8, 11]. They predict that the gap between the smoothed and the exact solutions decays like $\sqrt{\epsilon}$, in the energy norm. We aim at investigating the distribution of the error to have a better insight of the accuracy inherent to the regularizing process. In particular, we zoom in the mushy zone to show that it is responsible of 'slowing down' of the convergence to $\sqrt{\epsilon}$. Outside the mushy zone, we derive an order ϵ convergence rate. This sharp analysis is conducted for phase change problem in a semi-infinite slab. The substantial advantages of such a choice is the availability of analytical form of the (exact and smoothed) temperature fields, owing to Neumann similarity.

The outline of the paper is as follows. In Section 2, we set up the two-phase Stefan problem modeling a melting process in a semi-infinite slab. We describe how the enthalpy is smoothed to become a single valued function. In Section 3, we prove the existence of a Neumann auto-similar solution to the heat equation when arbitrary regularization is applied. Mathematical tools used here come from the theory of ordinary differential equation, easier than variational methods especially in unbounded domains. Using the Cauchy–Lipschitz theorem, we are able to derive useful qualitative features of the smoothed temperature and enthalpy fields. These properties are helpful in the convergence analysis conducted in Section 4 for piecewise linear enthalpy smoothing. We begin by showing that the mushy zone, of width ϵ, comes close to the free boundary with an accuracy of ϵ. Then, we prove that the thermal energy trapped in that mushy zone behaves exactly like $c\sqrt{\epsilon}$. This is an indication why the global convergence rate given in [8] can not be improved. We also provide a bound of order ϵ on the gap between regularized and exact temperature field outside the mushy region. We emphasize that the key of the study is the availability of analytical solutions to the regularized problems we deal with. Numerical experiments using SCILAB are presented at the end to validate the theoretical predictions.

Notation — Let $I \subset \mathbb{R}$ be an open interval. We denote by $L^2(I)$ the space of measurable and square integrable functions on X. The space $\mathscr{C}(I)$ contains the continuous functions on I and $\mathscr{C}^1(I)$ is for these space of functions that are continuously differentiable. To alleviate the presentation we use the symbols φ and $\psi\,(=1-\varphi)$ for the error and complementary error functions which were usually denoted by the symbols (erf) and (erfc) in the literature (see [1]).

2. Enthalpy smoothing

The two-phase Stefan problem can be expressed as a heat conduction problem in a semi-infinite slab geometrically represented by $I=(0,\infty)$. We set $Q=I\times]0,\infty[$. The generic point in I is denoted by x and the generic time is t. The slab is initially solid at the temperature $T(\cdot,0)=0$. It is then gradually melted by imposing the temperature $T(0,\cdot)$ to a fixed value T_1, larger than the melting temperature T_m. We have $T_1>T_m>0$. We therefore introduce the enthalpy function,

$$E(\theta)=\lambda\theta+Lf(\theta),$$

where $f(\theta)$ is the fraction of liquid phase at the temperature θ. There is a range of the possible values of f at the fusion temperature T_m. Hence, f is multi-valued and is defined by

$$f(\theta)=\begin{cases}0 & \theta<T_m\\ [0,1] & \theta=T_m\\ 1 & \theta>T_m\end{cases}.$$

We have set

$$\lambda=(\rho C)\kappa^{-1}, \qquad L=(\rho L_a)\kappa^{-1},$$

where L_a is the latent heat of fusion, the density ρ, the specific heat capacity C and the conductivity κ are to have the same values in the solid and liquid phases. This choice is made only by the desire to simplify the exposition. The overall results we develop here extend as well to account for different options, at the cost of more technical calculations.

The temperature distribution is a solution of the following enthalpy problem: *Find* (T,H) *with* $H\in E(T)$ *and*

$$\begin{aligned} \partial_t H-\partial_{xx}T&=0 && \text{in } Q,\\ T(0,\cdot)=T_1, \qquad T(\infty,\cdot)&=0 && \text{on } (0,\infty),\\ T(\cdot,0)&=0 && \text{on } I. \end{aligned} \tag{2.1}$$

The notation $T(\infty,\cdot)$ should be taken in the sense of the limit $x\to\infty$. This is the two-phase Stefan problem that can be formulated as a free boundary problem. Considering $X(t)$ as the melted depth of the solid phase which is a function of time; the Stefan problem consists of finding (T,X) such that

$$\begin{aligned} \lambda\partial_t T-\partial_{xx}T&=0 && \text{in } (0,X(t))\times(0,\infty),\\ \lambda\partial_t T-\partial_{xx}T&=0 && \text{in } (X(t),\infty)\times(0,\infty),\\ X(0)=0, \quad T(X(t),t)=T_m, \quad L(\partial_t X)(t)&=[\partial_x T](X(t),t), && \text{in } (0,\infty),\\ T(0,\cdot)=T_1, \qquad T(\infty,\cdot)&=0 && \text{on } (0,\infty),\\ T(\cdot,0)&=0 && \text{on } I. \end{aligned} \tag{2.2}$$

The unknowns are the temperature field T and the moving interface position $X(\cdot)$. This problem has been solved analytically (cf., for instance, [6, 12, 16]). The auto-similar Neumann solution is given by

$$T(x,t)=u(\frac{x}{\sqrt{t}}), \qquad X(t)=\alpha\sqrt{t}.$$

Plugging these expression into problem (2.2), we come up with some differential equations. Solving them provides the solution

$$\begin{aligned} u(\zeta)&=A\phi(\omega\zeta)+T_1, && \forall\zeta\in[0,\alpha[,\\ u(\zeta)&=D\psi(\omega\zeta), && \forall\zeta\in]\alpha,\infty[, \end{aligned} \tag{2.3}$$

where

$$\omega=\frac{\sqrt{\lambda}}{2}, \qquad A=-\frac{T_1-T_m}{\phi(\omega\alpha)}, \qquad D=\frac{T_m}{\psi(\omega\alpha)}.$$

The coefficient $\alpha>0$, determining the melting front, is the unique positive solution of the following transcendental equation

$$\frac{T_1-T_m}{\phi(\omega\alpha)}-\frac{T_m}{\psi(\omega\alpha)}-\left(\frac{\sqrt{\pi}L}{4\omega}\right)\alpha e^{(\omega\alpha)^2}=0. \tag{2.4}$$

The multi-valued enthalpy function is usually smoothed for numerical and computational feasibility. The regularized value problem can be handled by means of standard functional tools for non linear partial differential equations, and its numerical approximation is easier than for differential inclusions (see [3]). Indeed, regularization is highly recommended when an implicit time scheme and a Newton method is used for the enthalpy.

Smoothing the enthalpy consists in replacing f by a single-valued smoothed function f_ϵ. We are therefore in the case of non-isothermal phase change (see, e.g. [7]). The function f_ϵ we select here is piecewise linear, as commonly used in the literature

$$f_\epsilon(\theta) = \begin{cases} 0 & \theta < (T_m)^- \\ \dfrac{1}{2\epsilon}(\theta - (T_m)^-) & \theta \in [(T_m)^-, (T_m)^+] \\ 1 & \theta > (T_m)_+ \end{cases}, \tag{2.5}$$

where we have set $(T_m)^\pm = T_m \pm \epsilon$. When close to zero, the parameter $\epsilon > 0$ controls the approximation of f by f_ϵ. The resulting enthalpy function is therefore

$$E_\epsilon(\theta) = \lambda\theta + L f_\epsilon(\theta) = \begin{cases} \lambda\theta & \theta < (T_m)^- \\ \lambda_\epsilon \theta + L_\epsilon & \theta \in [(T_m)^-, (T_m)^+] \\ \lambda\theta + L & \theta > (T_m)^+ \end{cases},$$

where we have set

$$\lambda_\epsilon = (\lambda + \frac{L}{2\epsilon}), \qquad L_\epsilon = -\frac{L}{2\epsilon}(T_m)^-.$$

The mushy zone is then defined by the range $(T_m)^- \leq \theta \leq (T_m)_+$.

REMARK 2.1. Many examples of smoothing enthalpy functions f_ϵ may be found in the literature and may be classified into two categories according to whether they agree with f away from T_m. In our case, we have that $f_\epsilon = f$ in $\mathbb{R} \backslash](T_m)^-, (T_m)^+[$. Here we provide some examples that do not coincide with f (away from T_m),

$$f_\epsilon(\theta) = \frac{1}{2}\left(1 + \frac{\theta - T_m}{\sqrt{(\theta - T_m)^2 + \epsilon^2}}\right), \qquad f_\epsilon(\theta) = \frac{1}{2}\left(1 + \tanh\frac{\theta - T_m}{\epsilon}\right). \tag{2.6}$$

Below, we plot, in the left panel, the exact fraction function f (dashed line) with $T_m = 0$ and the piecewise linear smoothed function f_ϵ (solid line). In the right panel, both examples in (2.6) are represented, the first with a dashed line and the second with a solid line.

The regularized boundary value problem is hence transformed into the following non-linear heat equation consisting in: *Find* (T_ϵ, H_ϵ) *such that* $H_\epsilon = E_\epsilon(T_\epsilon)$ *and solution*

$$\begin{aligned} \partial_t H_\epsilon - T_\epsilon'' &= 0 && \text{in } Q, \\ T_\epsilon(0,\cdot) = T_1, \qquad T_\epsilon(\infty,\cdot) &= 0 && \text{on } (0,\infty), \\ T_\epsilon(\cdot,0) &= 0 && \text{on } I. \end{aligned} \tag{2.7}$$

According to the auto-similarity of the solution for the melting Stefan problem given previously, one may ask whether the smoothed enthalpy problem has also an auto-similar solution. Basically, we aim to bring a positive answer to this question by establishing the existence of an auto-similar temperature field solution of this smoothed enthalpy problem. Although we are specifically interested on the piecewise linear smoothing of the enthalpy function, we address the issue of existence in the general frame of regularizing functions.

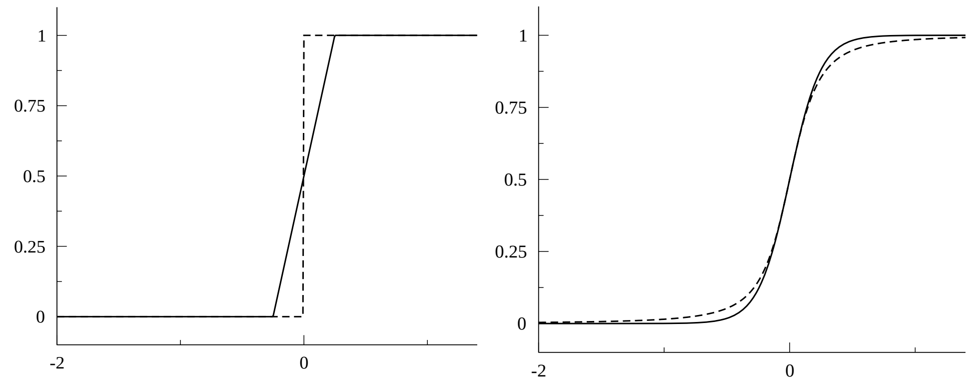

FIG. 2.1. *Examples of the liquid fraction functions f and f_ϵ.*

We need some additional assumptions. Suppose that E_ϵ is continuous and piecewise continuously differentiable. The function E'_ϵ has a finite number of jumps and T_1 is not among the discontinuity points of it. Moreover, we assume that

$$\lambda \leq E'_\epsilon(\cdot) \leq \mu_\epsilon = \frac{\mu}{\epsilon}, \qquad \text{a.e. in } \mathbb{R}. \tag{2.8}$$

This means in particular that the liquid fraction function f_ϵ is non-decreasing and has a bounded derivative.

3. Auto-similarity

For the sake of simplicity, we shall omit the index ϵ from the notations in this section. We denote $J_\xi = [0,\xi[$. To look for an auto-similar solution for the smoothed enthalpy equation, we write T and H (i.e., T_ϵ and H_ϵ) under the following form,

$$T(x,t) = u(\frac{x}{\sqrt{t}}), \qquad H(x,t) = e(\frac{x}{\sqrt{t}}) = E(u)(\frac{x}{\sqrt{t}}).$$

Notice that E is actually E_ϵ which is a continuous single-valued function. Moreover, we wrote u instead of u_ϵ. Substituting in (2.7), making necessary calculations and after introducing the new variable ξ (for $\frac{x}{\sqrt{t}}$) we arrive at the following reduced boundary value problem

$$\begin{aligned} -\frac{1}{2}\xi e'(\xi) - u''(\xi) = 0 \qquad \forall \xi \in J_\infty, \\ u(0) = T_1, \qquad u(\infty) = 0. \end{aligned} \tag{3.1}$$

for all $\gamma \in \mathbb{R}$, we define (u_γ, e_γ), with $e_\gamma = E(u_\gamma)$, as the solution of the ordinary differential equation

$$\begin{aligned} -\frac{1}{2}\xi e'_\gamma(\xi) - u''_\gamma(\xi) = 0 \qquad \forall \xi \in J_\infty, \\ u_\gamma(0) = T_1, \qquad u'_\gamma(0) = \gamma. \end{aligned} \tag{3.2}$$

Then, we consider the algebraic problem: *Find γ such that*

$$u_\gamma(\infty) = 0. \tag{3.3}$$

If this equation is solved for some γ_*, then u_{γ_*} is solution of (3.1).

The main task of this section is to prove that this problem has only one solution.

3.1. The differential equation. We focus here on the problem (3.2). We start by rewriting the differential equation in the principal unknown u_γ,

$$\begin{aligned} -\frac{1}{2}\xi E'(u_\gamma)u'_\gamma - u''_\gamma = 0 \qquad \text{in } J_\infty, \\ u_\gamma(0) = T_1, \qquad u'_\gamma(0) = \gamma. \end{aligned} \tag{3.4}$$

Various obstacles have to be surmounted for a satisfactory existence and uniqueness result. The first one is the discontinuity of E'. We have thus to cope with the question of determining accurately $E'(u_\gamma)$. The other is that, even if E' is continuous, and hence the function $E'(u_\gamma)$ makes sense, one may possibly use the Cauchy–Peano existence theorem (see [10]), but the uniqueness is not ensured and this may be troublesome. To bypass these complications, we integrate this equation to obtain that

$$\begin{aligned} -\frac{1}{2}\xi E(u_\gamma) + \frac{1}{2}\int^{\xi} E(u_\gamma)(\zeta)\,d\zeta - u'_\gamma = 0 \qquad \text{in } J_\infty, \\ u_\gamma(0) = T_1, \qquad u'_\gamma(0) = \gamma. \end{aligned}$$

Checking the equivalence between this differential equation and the equation (3.4) is straightforward. If now we introduce the new unknown w_γ for the integral term, then we get the following differential system

$$\begin{aligned} u'_\gamma &= -\frac{1}{2}\xi E(u_\gamma) + w_\gamma, && \text{in } J_\infty, \\ w'_\gamma &= \frac{1}{2}E(u_\gamma), && \text{in } J_\infty, \\ u_\gamma(0) &= T_1, \qquad w_\gamma(0) = \gamma. \end{aligned} \tag{3.5}$$

That $(\xi,u) \mapsto \xi E(u)$ is Lipschitz continuous on any bounded interval J_{ξ_*} allows us to apply the Cauchy-Lipschitz theorem. As a result we have a unique maximum solution which is global.

LEMMA 3.1. *The differential system* (3.5) *has a unique solution* $(u_\gamma, w_\gamma) \in \mathscr{C}^1(J_\infty, \mathbb{R}^2)$.

The well-known Gronwall's lemma results in the continuous dependence of the solution upon the initial conditions. The proof of the following can be found in [10].

COROLLARY 3.1. *Forall* $\xi_* > 0$, *there exists a constant* $C = C(\xi_*) > 0$ *such that the following bound holds*

$$\|u_\gamma - u_{\gamma_*}\|_{\mathscr{C}(J_{\xi_*},\mathbb{R})} + \|w_\gamma - w_{\gamma_*}\|_{\mathscr{C}(J_{\xi_*},\mathbb{R})} \le C|\gamma - \gamma_*|.$$

3.2. Shooting problem. The objective here is to use the shooting method to solve (3.3). Denoting $d_\gamma = u'_\gamma$, we can rewrite equation (3.3) in an equivalent form

$$\int_0^\infty d_\gamma(\zeta)\,d\zeta = -T_1. \tag{3.6}$$

We shall first show that the integral term depends continuously upon γ, and then use the classical intermediate value theorem.

PROPOSITION 3.1. *The following function is continuous on* $\mathbb{R}$,

$$S:\gamma\mapsto\int_0^\infty d_\gamma(\zeta)\,d\zeta. \tag{3.7}$$

The proof of this proposition requires an intermediary result on the behavior of d_γ in a neighborhood of $+\infty$.

LEMMA 3.2. *There holds that*

$$|d_\gamma(\xi)|\le|\gamma|e^{-\frac{\lambda}{4}\xi^2},\qquad \forall\xi\in J_\infty.$$

Moreover, if $\gamma>0$ *then* $d_\gamma<0$.

Proof. Let us first assume that the function $E'(u_\gamma)$ is defined almost everywhere. This means that

$$\Xi=\big\{\xi\in J_\infty;\ E' \text{ is discontinuous at } u_\gamma(\xi)\big\} \tag{3.8}$$

is a negligible set. Considering the first equation in (3.5), it is easily seen that

$$d_\gamma'=-\frac{1}{2}\xi E'(u_\gamma)d_\gamma=-\varphi'(\xi)d_\gamma,\qquad \text{in } J_\infty,$$

with $\varphi'=-\frac{1}{2}\xi E'(u_\gamma)$. Integrating this equation yields that

$$d_\gamma(\xi)=\gamma e^{-\varphi(\xi)},\qquad \forall\xi\in J_\infty. \tag{3.9}$$

Now, using the assumption (2.8) on E' yields the desired result.

It remains to show that the (Lebesgue) measure of the set Ξ defined in (3.8) cannot be positive. In fact, it is a discrete set and all its points are isolated. We shall prove this statement by contradiction.
Ξ is obviously a closed set and let $\Xi'(\subset\Xi)$ denote the set of its limit points. If the statement is false, then Ξ has at least one limit point and the set Ξ' is not empty. According to [13, Chapter 2, Exercice 6], $\Xi'\subset J_\infty$ is a closed set and has therefore a minimum value we denote by $\xi_\flat$. We set $T_\flat=u_\gamma(\xi_\flat)$; it is a jumping point for the function E'. Then, there exists a sequence $(\xi_n)_{n\ge0}$ converging towards $\xi_\flat$ and $u_\gamma(\xi_n)=T_\flat$. This yields in particular that $d_\gamma(0)=u_\gamma'(\xi_\flat)=0$. Next, as $E'(u_\gamma)$ is defined a.e in $J_{\xi_\flat}$, we deduce that the expression (3.9) is valid for d_γ at least in $J_{\xi_\flat}$. Passing to the limit of d_γ at $\xi_\flat$ shows that it is positive and cannot be zero, unless we have that $\lim_{\xi\to\xi_\flat}\varphi(\xi)=+\infty$ which cannot be true. Hence, Ξ is negligible. ∎

Proof. (Proposition 3.1.) Using Corollary 3.1 and referring once again to the first equation in (3.5), the map $\gamma\mapsto d_\gamma$ is a continuous (and even Lipschitz-continuous) mapping from $\mathbb{R}$ into $\mathscr{C}(J_{\xi_*},\mathbb{R})$, for all $\xi_*>0$. As a result,

$$\lim_{\gamma\to\gamma_*}\int_0^{\xi_*}|d_\gamma-d_{\gamma_*}|(\zeta)\,d\zeta=0.$$

To obtain the desired result, we use the bound of Lemma 3.2. Indeed, we have that

$$\int_{\xi_*}^\infty|d_\gamma-d_{\gamma_*}|(\zeta)\,d\zeta\le\frac{1}{\omega}\psi(\omega\xi_*)\,(|\gamma|+|\gamma_*|),$$

where $\omega = \frac{1}{2}\sqrt{\lambda}$. Finally, the triangular inequality gives that

$$|S(\gamma) - S(\gamma_*)| = \left| \int_0^{\infty} (d_\gamma - d_{\gamma_*})(\zeta)\, d\zeta \right| \leq \int_0^{\xi_*} |d_\gamma - d_{\gamma_*}|(\zeta)\, d\zeta + \frac{1}{\omega}\psi(\omega\xi_*)(|\gamma| + |\gamma_*|).$$

The term in ψ can be made arbitrary small, provided that ξ_* is chosen large enough. Moreover, the integral term tends towards zero as $\gamma \to \gamma_*$, which implies that the function S is continuous. □

REMARK 3.1. According to (3.9), forall $\gamma < 0$ we have $d_\gamma < 0$. As a result the solution u_γ is decreasing, and we have

$$T_1 + \frac{\gamma}{\omega}\psi(\omega\xi) \leq u_\gamma(\xi) \leq T_1, \qquad \forall \xi \in J_\infty.$$

The function u_γ has therefore a limit when $\xi \to +\infty$. Notice that, if $\gamma > 0$, then $d_\gamma \geq 0$, u_γ is increasing and (3.6) cannot be satisfied.

PROPOSITION 3.2. *Problem* (3.6) *has at least one solution γ which is negative. The corresponding function u_γ is then decreasing.*

Proof. Following Remark 3.1, any solution γ is necessarily negative. We look for a solution γ in $]-\infty,0]$. Proceeding like in the proof of Lemma 3.2, we can derive

$$\gamma\sqrt{\frac{\pi}{\lambda}} \leq \int_0^{\infty} d_\gamma(\xi)\, d\xi \leq \gamma\sqrt{\frac{\pi}{\mu}} \leq 0.$$

As a result, the 'shooting' function S is continuous from $]-\infty,0]$ into $]-\infty,0]$. By the intermediate values theorem, it takes at least once the negative value $(-T_1)$. The fact that u_γ is decreasing is ensued from the negativity of $d_\gamma = u'_\gamma$ according to (3.9). The proof is complete. □

3.3. Uniqueness. The uniqueness may be reached by establishing the monotonicity of the function (3.7). To this end, consider γ and γ_* be two real-numbers with $\gamma < \gamma_* \leq 0$. We intend to show that $u_\gamma(\infty) > u_{\gamma_*}(\infty)$. To proceed, we denote

$$g = \frac{u_\gamma - u_{\gamma_*}}{\gamma - \gamma_*}, \qquad k = \frac{w_\gamma - w_{\gamma_*}}{\gamma - \gamma_*}, \qquad F = \frac{E(u_\gamma) - E(u_{\gamma_*})}{u_\gamma - u_{\gamma_*}}.$$

Both functions g and k are continuously-differentiable on J_∞ while F is measurable with

$$0 < \lambda \leq F(\xi) \leq \mu, \qquad \forall \xi \in J_\infty.$$

It is easily checked that (g,k) is the unique solution of the linear system

$$\begin{aligned} g' &= -\frac{1}{2}\xi F g + k, && \text{in } J_\infty, \\ k' &= \frac{1}{2} F g, && \text{in } J_\infty, \\ g(0) &= 0, \qquad k(0) = 1. \end{aligned} \tag{3.10}$$

Notice that according to Remark 3.1, the limit of u_γ (and of u_{γ_*}) at infinity exists and is finite. As a result, the limit $g(\infty)$ exists and is finite.

The next lemma, which indicates that $g(\infty) > 0$, yields the desired result.

LEMMA 3.3. *We have that*

$$g(\xi) > 0, \qquad k(\xi) > 1, \qquad \forall \xi \in J_\infty.$$

Moreover, the following holds

$$\lim_{\xi \to +\infty} g(\xi) > 0$$

and the function (3.7) *is increasing.*

Proof. We start by noticing that $g'(0) = 1$. Hence, g is increasing in a neighborhood of $\xi = 0$, and $g(\xi) > 0$ in some interval $]0, \xi_0[$, with $\xi_0 > 0$. Next, we prove by contradiction that $\xi_0 = +\infty$.

Assume that $\xi_0 < +\infty$ and $g(\xi_0) = 0$. This yields $g'(\xi_0) \leq 0$. From the first equation of (3.10), we obtain that $k(\xi_0) \leq 0$. This cannot be true since we derive from the second equation of (3.10) that $k'(\xi) > 0$ in $]0, \xi_0[$. Hence $k(\xi_0) > k(0) = 1$. By contradiction, we have $g > 0$ in $]0, +\infty[$. Thus $k' > 0$ and k is increasing, which shows that $k > 1$ in $]0, +\infty[$. ∎

Combining the above results, we have proved the main result of this section showing existence and uniqueness together with the 'uniform' stability of the solution.

THEOREM 3.1. *Problem* (3.1) *has an unique solution* (e_ϵ, u_ϵ)*. The temperature field* T *is decreasing, and it holds that*

$$\|e_\epsilon\|_{L^2(J_\infty)} + \|u'_\epsilon\|_{L^2(J_\infty)} \leq C|T_1|,$$

where the constant C *does not depend on* ϵ*. Moreover, the solution* u_ϵ *is decreasing in* J_∞*, from* T_1 *towards* 0.

4. Convergence

In this section, we carry out the convergence analysis for the piecewise linear smoothing enthalpy problem. The issue has been tackled in [8] (see also [11]), where variational techniques is used in bounded domains. The smoothed temperature T_ϵ is proved to approximate the exact T, solution to the Stefan problem. The convergence rates with respect to L^2-norm and H^1-norm are of order $\sqrt{\epsilon}$. Our purpose is to find out what exactly happen locally in the slab. Is the accuracy of $\sqrt{\epsilon}$ uniformly distributed (in the slab) or is it only concentrated in the mushy zone? How does the temperature field T_ϵ (or equivalently of u_ϵ) behave in the solid and liquid regions? To answer these questions, we zoom into the mushy zone and undertake a detailed analysis based on the analytic form of the solution to the smoothed enthalpy problem.

According to Theorem 3.1, the auto-similar temperature u_ϵ decreases towards zero from T_1 in the slab. This suggests that the enthalpy form changes twice. Different ions are related to the events: $u_\epsilon \geq (T_m)^+$, $(T_m)^- \leq u_\epsilon \leq (T_m)^+$, and $u_\epsilon \leq (T_m)^-$. Then, there exist two real-numbers $0 < a_\epsilon < b_\epsilon$ such that $u_\epsilon(a_\epsilon) = (T_m)^+$ and $u_\epsilon(b_\epsilon) = (T_m)^-$. The interfaces $X_\epsilon(t) = a_\epsilon \sqrt{t}$ and $Y_\epsilon(t) = b_\epsilon \sqrt{t}$ enclose the mushy zone that separates the solid and liquid phases. They are expected to come close to each other and to eventually coincide with the sharp interface $X(t) = \alpha\sqrt{t}$, at the limit $\epsilon \to 0$. This will be the central point of the analysis. Splitting the whole interval into three subintervals $J^f = (0, a_\epsilon)$, $J^\epsilon = (a_\epsilon, b_\epsilon)$, and $J^s = (b_\epsilon, +\infty)$, and solving the smoothed problem in the three subintervals gives the following solution u_ϵ,

$$u_\epsilon(\zeta) = \begin{cases} A_\epsilon \phi(\omega\zeta) + T_1 & \forall \zeta \in J^f \\ B_\epsilon \phi(\omega_\epsilon \zeta) + C_\epsilon & \forall \zeta \in J^\epsilon, \\ D_\epsilon \psi(\omega\zeta) & \forall \zeta \in J^s, \end{cases}$$

where $\omega_\epsilon = \frac{\sqrt{\lambda_\epsilon}}{2}$. Recall that J^f and J^s are the liquid and solid zones respectively while J^ϵ is the mushy zone.

All the constants are dependent upon ϵ. For simplicity we choose henceforth to drop off the index ϵ in some places and put it back only when necessary.

Using the fact that $u_\epsilon(a_\epsilon) = (T_m)^+$ and $u_\epsilon(b_\epsilon) = (T_m)^-$, we derive

$$A = -\frac{T_1 - (T_m)^+}{\phi(\omega a_\epsilon)}, \qquad D = \frac{(T_m)^-}{\psi(\omega b_\epsilon)}. \tag{4.1}$$

The continuity of u_ϵ at both points a_ϵ and b_ϵ results in

$$B = \frac{2\epsilon}{\phi(\omega_\epsilon a_\epsilon) - \phi(\omega_\epsilon b_\epsilon)}, \qquad C = (T_m)^+ - B\phi(\omega_\epsilon a_\epsilon). \tag{4.2}$$

To fully solve the problem, we need to enforce the flux conservation at points a_ϵ and b_ϵ which leads to

$$\begin{aligned} A\omega e^{-(\omega a_\epsilon)^2} &= B\omega_\epsilon e^{-(\omega_\epsilon a_\epsilon)^2}, \\ -D\omega e^{-(\omega b_\epsilon)^2} &= B\omega_\epsilon e^{-(\omega_\epsilon b_\epsilon)^2}. \end{aligned} \tag{4.3}$$

Plugging in (4.3), the coefficients A, D as given in (4.1) and B as in (4.2), results in a non-linear algebraic system of two equations for two unknowns a_ϵ and b_ϵ. A direct consequence of the foregoing analysis is that this system has a unique solution (a_ϵ, b_ϵ) with $b_\epsilon > a_\epsilon > 0$.

Next we would like to show that the sequences $(a_\epsilon)_{\epsilon>0}$ and $(b_\epsilon)_{\epsilon>0}$ converge and share the same limit α, the solution of the transcendental equation (2.4). We aim also to exhibit an accurate convergence rate.

LEMMA 4.1. *The sequences $(a_\epsilon)_{\epsilon>0}$ and $(b_\epsilon)_{\epsilon>0}$ are uniformly bounded away from zero, i.e., there exist two constants α_L and α_R with $0 < \alpha_L < \alpha_R < \infty$ such that*

$$\alpha_L \le a_\epsilon < b_\epsilon \le \alpha_R, \qquad \forall \epsilon < \min(T_m, T_1 - T_m).$$

Proof. These results are consequences of the uniform bound on $\|u_\epsilon'\|_{L^2(J_\infty)}$ of Theorem 3.1. Indeed, if for instance a_ϵ goes to zero, it can be checked that $\|u_\epsilon'\|_{L^2(J^f)}$ will blow up for small ϵ. ∎

LEMMA 4.2. *It holds that*

$$(b_\epsilon - a_\epsilon) \le K\epsilon,$$

for some positive constant K.

Proof. We derive from (4.3) that

$$e^{-\omega_\epsilon^2(b_\epsilon^2 - a_\epsilon^2)} = -\frac{D}{A} e^{-\omega^2(b_\epsilon^2 - a_\epsilon^2)}.$$

Using the expressions of A and D as in (4.1), we obtain

$$e^{\frac{L}{8}\frac{(b_\epsilon^2 - a_\epsilon^2)}{\epsilon}} = \frac{T_1 - (T_m)^+}{(T_m)^-} \frac{\psi(\omega b_\epsilon)}{\phi(\omega a_\epsilon)}. \tag{4.4}$$

Now, Lemma 4.1 implies that the term on the right-hand side is uniformly bounded in ϵ. As a result, we have that

$$(b_\epsilon^2 - a_\epsilon^2) \leq K\epsilon,$$

for some constant $K > 0$. The lemma is then a consequence of the boundedness of a_ϵ and b_ϵ. ∎

The next step is to show that $(a_\epsilon)_{\epsilon>0}$ and $(b_\epsilon)_{\epsilon>0}$ are convergent. We prove that each of them has α as the only accumulation point. By Bolzano–Weierstrass theorem, the boundedness of $(a_\epsilon)_{\epsilon>0}$ and $(b_\epsilon)_{\epsilon>0}$ yields that each sequence has at least an accumulation point. There exist then two convergent subsequences we still call $(a_\epsilon)_{\epsilon>0}$ and $(b_\epsilon)_{\epsilon>0}$, with a slight abuse of notation. According to Lemma 3.2, both sequences share the same limit which we denote by a. The last step is to prove that the only possible value for a is α, the solution of (2.4).

Lemma 4.3. *The (whole) sequences $(a_\epsilon)_{\epsilon>0}$ and $(b_\epsilon)_{\epsilon>0}$ converge toward α, the solution of the transcendental equation* (2.4).

Proof. Let $(a_\epsilon)_{\epsilon>0}$ and $(b_\epsilon)_{\epsilon>0}$ be convergent subsequences with the limit $a > 0$. Using equalities (4.1) results in

$$-A\omega e^{-(\omega a_\epsilon)^2} - D\omega e^{-(\omega b_\epsilon)^2} = -B\omega_\epsilon (e^{-(\omega_\epsilon a_\epsilon)^2} - e^{-(\omega_\epsilon b_\epsilon)^2}).$$

Replacing B as in (4.2) leads to

$$-A\omega e^{-(\omega a_\epsilon)^2} - D\omega e^{-(\omega b_\epsilon)^2} = 2\epsilon\omega_\epsilon \frac{e^{-(\omega_\epsilon a_\epsilon)^2} - e^{-(\omega_\epsilon b_\epsilon)^2}}{\phi(\omega_\epsilon b_\epsilon) - \phi(\omega_\epsilon a_\epsilon)}. \tag{4.5}$$

The term on the right-hand side can be bounded above and below as [1])

$$2\epsilon\omega_\epsilon(\sqrt{\pi}\omega_\epsilon a_\epsilon) \leq 2\epsilon\omega_\epsilon \frac{e^{-(\omega_\epsilon a_\epsilon)^2} - e^{-(\omega_\epsilon b_\epsilon)^2}}{\phi(\omega_\epsilon b_\epsilon) - \phi(\omega_\epsilon a_\epsilon)} \leq 2\epsilon\omega_\epsilon(\sqrt{\pi}\omega_\epsilon b_\epsilon). \tag{4.7}$$

Passing to the limit ($\epsilon \to 0$) shows that the three sequences have the common limit $\frac{1}{4}\sqrt{\pi}La$.

Returning to equation (4.5). After passing to the limit, we get that a is a solution of the same instance of equation (2.4), which implies $a = \alpha$ by uniqueness. ∎

Next, we establish the convergence rate of $(a_\epsilon)_{\epsilon>0}$ and of $(b_\epsilon)_{\epsilon>0}$ towards α.

Proposition 4.1. *There exists a constant K such that*

$$|a_\epsilon - \alpha| + |b_\epsilon - \alpha| \leq K\epsilon.$$

Proof. Let us introduce the function

$$G(\varrho) = \frac{T_1 - T_m}{\phi(\omega\varrho)} - \frac{T_m}{\psi(\omega\varrho)} - \left(\frac{\sqrt{\pi}L}{4\omega}\right)\varrho e^{(\omega\varrho)^2}$$

[1] Using the double inequality

$$\sqrt{\pi}x(\phi(y) - \phi(x)) \leq e^{-x^2} - e^{-y^2} \leq \sqrt{\pi}y(\phi(y) - \phi(x)), \qquad 0 \leq x \leq y. \tag{4.6}$$

It is smooth and decreasing in $]0,\infty[$. Moreover, α is the unique root of G in $]0,\infty[$, that is

$$G(\alpha) = 0. \tag{4.8}$$

On the other hand, let us consider the following perturbed function

$$G_\epsilon(\varrho) = \frac{T_1 - (T_m)^+}{\phi(\omega\varrho)} - \frac{(T_m)^-}{\psi(\omega\varrho)} - \left(\frac{\sqrt{\pi}L}{4\omega}\right)\varrho e^{(\omega\varrho)^2}.$$

According to (4.5), the point a_ϵ may be seen as solution of

$$G_\epsilon(a_\epsilon) = r_\epsilon, \tag{4.9}$$

where

$$r_\epsilon = \left[2\epsilon\frac{\omega_\epsilon}{\omega}\frac{e^{-(\omega_\epsilon a_\epsilon)^2} - e^{-(\omega_\epsilon b_\epsilon)^2}}{\phi(\omega_\epsilon b_\epsilon) - \phi(\omega_\epsilon a_\epsilon)} - \left(\frac{\sqrt{\pi}L}{4\omega}\right)a_\epsilon\right]e^{(\omega a_\epsilon)^2} + \left[\frac{e^{-(\omega b_\epsilon)^2}}{\psi(\omega b_\epsilon)} - \frac{e^{-(\omega a_\epsilon)^2}}{\psi(\omega a_\epsilon)}\right](T_m)^- e^{(\omega a_\epsilon)^2}. \tag{4.10}$$

Let $[\alpha_L, \alpha_R]$ be contained in $]0,\infty[$, we can derive immediately from

$$G_\epsilon(\varrho) - G(\varrho) = \epsilon\left(-\frac{1}{\phi(\omega\varrho)} + \frac{1}{\psi(\omega\varrho)}\right).$$

that

$$\sup_{\varrho\in[\alpha_L,\alpha_R]} |G_\epsilon(\varrho) - G(\varrho)| \le K\epsilon.$$

We can show (cf. Appendix A) that

$$|r_\epsilon| \le K\epsilon. \tag{4.11}$$

Now, we derive from (4.9) and (4.8) that

$$G(\alpha) - G(a_\epsilon) = (G_\epsilon(a_\epsilon) - G(a_\epsilon)) - r_\epsilon.$$

This implies that

$$|G(\alpha) - G(a_\epsilon)| \le |G_\epsilon(a_\epsilon) - G(a_\epsilon)| + |r_\epsilon| \le K\epsilon.$$

Calling for the mean value theorem we derive that $|\alpha - a_\epsilon| \le K\epsilon$. Of course, the constant K depends on $\min_{\varrho\in[\alpha_L,\alpha_R]} |G'(\varrho)| > 0$. The proof is complete. □

The first and major consequence of this result is the optimal convergence of u_ϵ towards u outside the mushy region. To state the accuracy result, let us set $(a_\epsilon)^- = \min(a, a_\epsilon)$ and $(b_\epsilon)^+ = \max(\alpha, b_\epsilon)$.

Corollary 4.1. *The following estimate holds*

$$\|u - u_\epsilon\|_{L^\infty(0,(a_\epsilon)^-)} + \|u - u_\epsilon\|_{L^\infty((b_\epsilon)^+,\infty)} \le K\epsilon.$$

Proof. Since

$$\|u-u_\epsilon\|_{L^\infty(0,(a_\epsilon)^-)} \le |A_\epsilon - A| = \left|\frac{T_1-(T_m)^+}{\phi(\omega a_\epsilon)} - \frac{T_1-T_m}{\phi(\omega\alpha)}\right|,$$
$$\|u-u_\epsilon\|_{L^\infty((b_\epsilon)^+,\infty)} \le |D_\epsilon - D| = \left|\frac{(T_m)^-}{\psi(\omega b_\epsilon)} - \frac{T_m}{\psi(\omega\alpha)}\right|.$$

The desired results then follow from Proposition 4.1. ∎

Corollary 4.1 provides the convergence rate of u_ϵ towards u, away from the mushy portion of the slab. Next, to assess the behavior of u_ϵ within the mushy zone we need to sharpen the estimate of Lemma 4.1.

LEMMA 4.4. *We have that*

$$\lim_{\epsilon\to 0}\frac{b_\epsilon - a_\epsilon}{\epsilon} = \rho > 0.$$

Proof. We prove first that $C = \inf_{\epsilon>0}\frac{b_\epsilon - a_\epsilon}{\epsilon} > 0$. We proceed by contradiction. Assume that $C=0$. Then, $\frac{b_\epsilon - a_\epsilon}{\epsilon}$ converges towards zero (modulo a subsequence). Passing to the limit in (4.4), we derive that

$$\frac{T_1-T_m}{T_m}\frac{\psi(\omega\alpha)}{\phi(\omega\alpha)} = 1.$$

This yields that

$$\phi(\omega\alpha) = \frac{T_1-T_m}{T_1}, \qquad \psi(\omega\alpha) = \frac{T_m}{T_1}.$$

Replacing in (2.4) gives that $\alpha = 0$. This cannot occur since $T_m < T_1$. Now, we claim that $\frac{b_\epsilon - a_\epsilon}{\epsilon}$ has only one accumulation point. This is because, if we take (4.4) to the limit, we have

$$\lim_{\epsilon\to 0}\frac{b_\epsilon - a_\epsilon}{\epsilon} = \frac{4}{L\alpha}\ln\left[\left(\frac{T_1}{T_m}-1\right)\left(\frac{1}{\phi(\omega\alpha)}-1\right)\right] > 0.$$

∎

PROPOSITION 4.2. *There exists a constant such that*

$$\|u_\epsilon\|_{L^2(a_\epsilon,b_\epsilon)} = \mathcal{O}(\sqrt{\epsilon}), \qquad \|u'_\epsilon\|_{L^2(a_\epsilon,b_\epsilon)} = \mathcal{O}(\sqrt{\epsilon}).$$

Proof. We start from the double bound

$$(T_m)^- \le u_\epsilon(\zeta) \le (T_m)^+, \qquad \forall \zeta \in (a_\epsilon, b_\epsilon).$$

After integration we obtain

$$(T_m)^-\sqrt{b_\epsilon - a_\epsilon} \le \|u_\epsilon\|_{L^2(a_\epsilon,b_\epsilon)} \le (T_m)^+\sqrt{b_\epsilon - a_\epsilon}.$$

Invoking Lemma 4.4 results in the first estimate.

Next, we integrate

$$u'_\epsilon(\zeta) = B_\epsilon \omega_\epsilon e^{-(\omega_\epsilon \zeta)^2}$$

to get

$$\|u'_\epsilon\|^2_{L^2(a_\epsilon,b_\epsilon)} = (2\sqrt{2}\omega_\epsilon \epsilon^2)\,\frac{\phi(\sqrt{2}\omega_\epsilon b_\epsilon) - \phi(\sqrt{2}\omega_\epsilon a_\epsilon)}{(\phi(\omega_\epsilon b_\epsilon) - \phi(\omega_\epsilon a_\epsilon))^2}.$$

Applying the double inequality (4.6) twice and carrying out some calculations will lead to

$$\|u'_\epsilon\|_{L^2(a_\epsilon,b_\epsilon)} = \mathcal{O}(\epsilon\sqrt{\omega_\epsilon}) = \mathcal{O}(\sqrt{\epsilon}).$$

The proof is complete. $\square$

REMARK 4.1. One can get more information about the solution u_ϵ within the mushy zone. In fact, one can check readily that

$$\lim_{\epsilon\to 0} \frac{\|u_\epsilon\|_{L^2(a_\epsilon,b_\epsilon)}}{\sqrt{\epsilon}} = T_m \rho, \qquad \lim_{\epsilon\to 0} \frac{\|u'_\epsilon\|_{L^2(a_\epsilon,b_\epsilon)}}{\sqrt{\pi\epsilon}} = \frac{L\alpha}{4}\coth\left(\frac{L\alpha}{8}\rho\right).$$

Here, ρ is the limit provided in *Lemma 4.4*.

5. Numerical results

To compute α, one has to numerically solve the transcendental equation (4.5), and to obtain (a_ϵ, b_ϵ), one has to solve the algebraic system (4.4) and (4.5). Equation (4.5) may be rewritten in such a form that $\omega\alpha$ depends only on two dimensionless numbers: Stefan numbers St_F and St_S. They are provided as the ratio of the sensible and the latent heats in the liquid and in the solid phases,

$$St_L = \frac{\lambda}{L}(T_1 - T_m) = \frac{C}{La}(T_1 - T_m), \qquad St_S = \frac{\lambda}{L}T_m = \frac{C}{La}T_m.$$

Numerical examples are performed using SCILAB to assess the theoretical findings in the previous sections about the gaps $(a_\epsilon - \alpha)$ and $(b_\epsilon - \alpha)$. Nonlinear equations are solved by Newton's algorithm.

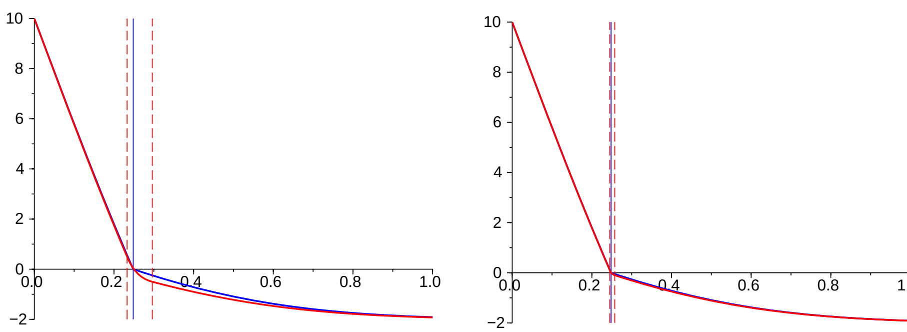

FIG. 5.1. *Auto-similar functions u and u_ϵ with $\epsilon = 0.5$ (left) and $\epsilon = 0.1$ (right). $T_{(\epsilon)}(x,t) = u_{(\epsilon)}(\frac{x}{\sqrt{t}})$.*

Example one — In the first test, we fix the parameters with $\lambda = 10$ and $L = 250$ with $T_0 = -2$, $T_1 = 10$, and $T_m = 0$. Stefan numbers are therefore given by $St_L = 0.4$ and

$\epsilon=$	1	0.1	0.01
$(a_\epsilon-\alpha)$	-1.21×10^{-1}	-1.26×10^{-2}	-1.27×10^{-3}
$(b_\epsilon-\alpha)$	4.10×10^{-1}	3.74×10^{-2}	3.72×10^{-3}

TABLE 5.1. *Errors on the position of the melting front coefficient* α.

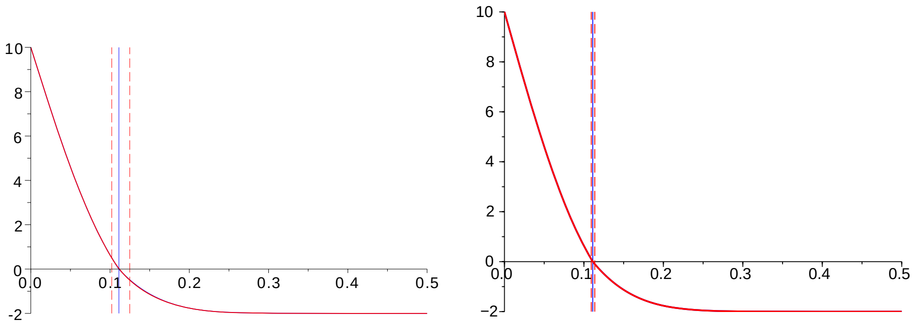

FIG. 5.2. *Functions u and u_ϵ with $\epsilon=0.5$ (left) and $\epsilon=0.1$ (right).*

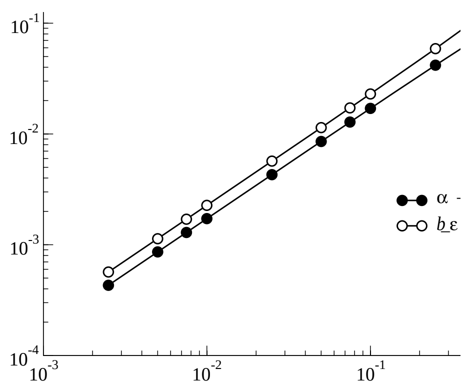

FIG. 5.3. *Convergence curves of the melting front coefficient* α.

$St_S=0.08$. Initially the slab is frozen at the temperature $T_0=-2$. A melting process starts at the origin $x=0$, because the temperature at that point is brought to $T_1=10$, above the melting level $T_0=0$. The auto-similar solutions u and u_ϵ are represented in Figure 5.1, with $\epsilon=0.5$ and $\epsilon=0.1$. Recall that $T_{(\epsilon)}(x,t)=u_{(\epsilon)}(\frac{x}{\sqrt{t}})$. The vertical lines indicate the location of α (solid line) and the positions of a_ϵ and b_ϵ (dashed lines). The regularized solution is close to the exact one, and becomes closer for smaller ϵ. Moreover, results recorded in Table 5.1 illustrate the order one decaying of the error, with respect ϵ. Observe also that the exact α lays within the mushy zone, and for smaller ϵ the mushy zone shrinks around the melting front.

Example two — We keep all the parameters unchanged except setting $\lambda=250$. This means that the specific heat capacity C of the slab is higher, and the ratio of sensible/latent heat is increased. Stefan numbers are given by $St_F = 10$ and $St_S = 2$. The exact and regularized auto-similar representations of the temperature, u and u_ϵ, are depicted in Figure 5.2, for $\epsilon = 0.5$ and $\epsilon = 0.1$. Gaps between them are small, especially for $\epsilon = 0.1$. In, Figure 5.3, the convergence history is plotted, confirming the order one convergence rate of the melting font location with respect to ϵ.

6. Conclusion

We considered the melting free-boundary Stefan problem set in a semi-infinite slab. The effects of the smoothing procedure applied to the enthalpy equation, in phase transition models, are investigated semi-analytically. We obtained detailed estimates of order $\sqrt{\epsilon}$ (ϵ being the width of the mushy zone) within the mushy zone and of order ϵ outside of the mushy zone.

A direct consequence is that the (global) estimate obtained in [8] is optimal and cannot be improved. The limitation is due to the energy trapped within that mushy region. A careful investigation outside this zone shows that the regularized enthalpy and temperature converge towards their exact counterparts like ϵ. We emphasize that the analysis developed here may be conducted as well for many other non-linear models where a closed form for the solution is available (see [14, 15]).

Appendix A. We sketch below the proof of (4.11) which is necessary for the proof of Proposition 4.1.

Proof. The residual r_ϵ is composed of two contributions $(r_\epsilon)_1$ and $(r_\epsilon)_2$ in (4.10). Using the double inequality (4.7), we find

$$\left[\frac{2\sqrt{\pi}}{\omega}\epsilon(\omega_\epsilon)^2 - \left(\frac{\sqrt{\pi}L}{4\omega}\right)\right] a_\epsilon e^{(\omega a_\epsilon)^2} \le (r_\epsilon)_1 \le \left[\frac{2\sqrt{\pi}}{\omega}\epsilon(\omega_\epsilon)^2 b_\epsilon - \left(\frac{\sqrt{\pi}L}{4\omega}\right) a_\epsilon\right] e^{(\omega a_\epsilon)^2}.$$

Recalling that

$$(\omega_\epsilon)^2 = \frac{\lambda_\epsilon}{4} = \frac{\lambda}{4} + \frac{L}{8\epsilon} = \omega^2 + \frac{L}{8\epsilon},$$

from which we derive

$$[2\sqrt{\pi}\omega\epsilon] a_\epsilon e^{(\omega a_\epsilon)^2} \le (r_\epsilon)_1 \le \left[2\sqrt{\pi}\omega\epsilon a_\epsilon + \left(\frac{\sqrt{\pi}L}{4\omega}\right)(b_\epsilon - a_\epsilon)\right] e^{(\omega a_\epsilon)^2}.$$

The boundedness of the sequence $(a_\epsilon)_\epsilon$ together with the bound obtained in Lemma 4.2 yields the desired estimate on $(r_\epsilon)_1$.
The bound for $(r_\epsilon)_2$ can be obtained by applying the mean value theorem to the inverse of the scaled complementary error function

$$\rho \mapsto \frac{e^{-\rho^2}}{\psi(\rho)},$$

and another use of Lemma 4.2. □

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