A Singular–Perturbed Two–Phase Stefan Problem Due to Slow Diffusion

J. STRUCKMEIER [1] and A. UNTERREITER [1]

[1] *Department of Mathematics, University of Kaiserslautern, P.O. Box 3049, 67653 Kaiserslautern, Germany*

(*Received*)

The asymptotic behavior of a singular–perturbed two–phase Stefan problem due to slow diffusion in one of the two phases is investigated. In the limit the model equations reduce to a one–phase Stefan problem. A boundary layer at the moving interface makes it necessary to use a corrected interface condition obtained from matched asymptotic expansions. The approach is validated by numerical experiments using a front–tracking method.

1 Introduction

This work concerns a one–dimensional, two–phase Stefan problem defined by the initial–boundary value problem on the interval $[0,1]$,

$$\frac{\partial u}{\partial t} = k_1 \frac{\partial^2 u}{\partial x^2}, \quad 0 < x < s(t)\,, \tag{1.1}$$

$$\frac{\partial v}{\partial t} = k_2 \frac{\partial^2 v}{\partial x^2}, \quad s(t) < x < 1\,. \tag{1.2}$$

Here, $s(t)$ denotes the position of the moving interface between the two phases. The initial and boundary conditions for $u = u(x,t)$ and $v = v(x,t)$ are given by

$$u(x,0) = u_0(x),\ u(0,t) = \alpha = u_0(0) > 0,\ v(x,0) = v_0(x),\ v(0,t) = \beta = v_0(1) < 0$$

and the equations (1.1), (1.2) are coupled via the usual interface conditions at $s(t)$, i.e.

$$u(s(t),t) = v(s(t),t) = 0, \quad k_2 \frac{\partial v}{\partial x}(s(t),t) - k_1 \frac{\partial u}{\partial x}(s(t),t) = \lambda \dot{s}(t)$$

where λ denotes the Stefan number.

A huge amount of mathematical research has been devoted to the analysis of the Stefan problem through the last decades. It would go far beyond the scope of this paper to give even a rough overview of the existing literature. Instead we refer the interested reader to [9] for an excellent review.

In the sequel we shall make extensive use of the fact that our model problem (1.1), (1.2) has a unique solution. This existence- and uniqueness result is well-known and a special case of much more general results [2, 3, 4].

We are interested in the case where the diffusion equations degenerate to a singularly perturbed problem due to slow diffusion in one of the two phases [7], e.g. $k_1 = \varepsilon \ll k_2 = 1$.

The one–dimensional two–phase Stefan problem with slow diffusion in one phase acts as model problem for complex multi–phase transport phenomena where the ratio of some physical parameters of the two phases is small. One of those problems which is of great interest in practical applications is the simulation of two–phase flows where the density ratio between the two fluids is small. We hope to reduce this problem to a one–phase problem such that the subsequent techniques apply.

Let us briefly recall the already available results for $k_1 = \varepsilon \to 0$, $k_2 = 1$. In [7] convergence (up to sub-sequences) of the solutions of the two-phase problem to a solution of a one-phase problem as $\varepsilon \to 0$ is proven. The argumentation is settled on a subtle combination of regularization arguments, compactness theorems and cutting techniques.

These rigoruos results cover one aspect of the limit $\varepsilon \to 0$. The other question is inspired by recent asymptotic investigations on singularly perturbed Stefan problems [10]: What are the qualitative properties of u and s for small values of ε ? Is there a numerically tractable and reliable one-phase approximation for small values of ε ?

It is the aim of this paper to deal with these two questions.

As $\varepsilon \to 0$ one may expect that the problem can be reduced to a one–phase Stefan problem for the single function $v(x,t)$ undergoing a diffusion process on a time scale of order $O(1)$.

However, if this reduction to a one–phase problem is settled on simply putting $\varepsilon = 0$, then one will get a wrong reference problem for small values of ε. A much better model is obtained from the employment of a corrected Stefan condition which results from matched asymptotic expansions in the slow diffusion region.

In the current investigation zeroth order expansions are performed. Higher order corrections seemingly require a new asymptotic approach for singular perturbed parabolic equations The development of these techniques is in progress [8].

The paper is organized as follows: in Section 2 we discuss the asymptotic behavior of the two–phase Stefan problem as $\varepsilon \to 0$. It is shown that the one–phase Stefan problem obtained by putting $\varepsilon = 0$ is not appropriate to describe the asymptotic behavior because this limit is dominated by a boundary layer in the slow diffusion region at the moving interface $x = s(t)$.

By matched asymptotic expansions we derive in Section 3 a corrected Stefan condition for the one–phase problem which guarantees the correct description of the limit $\varepsilon \to 0$. Numerical results based on a finite difference method combined with a front tracking algorithm are given in Section 4. We furthermore use the numerical simulations to demonstrate the existence of multiple time scales.

2 Asymptotic Behaviour of the Two–Phase Stefan Problem

Our aim is to investigate the asymptotic behaviour of the two–dimensional Stefan problem

$$\begin{cases} \dfrac{\partial u^\varepsilon}{\partial t} = \varepsilon \dfrac{\partial^2 u^\varepsilon}{\partial x^2}, \quad u^\varepsilon(x,0) = u_0(x), \quad 0 < x < s^\varepsilon(t)\,, \\ \dfrac{\partial v^\varepsilon}{\partial t} = \dfrac{\partial^2 v^\varepsilon}{\partial x^2}, \quad v^\varepsilon(x,0) = v_0(x), \quad s^\varepsilon(t) < x < 1\,, \\ u^\varepsilon(0,t) = \alpha, \quad v_\varepsilon(1,t) = \beta, \quad u^\varepsilon(s^\varepsilon(t),t) = v^\varepsilon(s^\varepsilon(t),t) = 0, \\ \dfrac{\partial v^\varepsilon}{\partial x}(s^\varepsilon(t),t) - \varepsilon \dfrac{\partial u^\varepsilon}{\partial x}(s^\varepsilon(t),t) = \lambda\, \dot{s}^\varepsilon(t) \end{cases} \tag{2.1}$$

in the limit as $\varepsilon \to 0$.

Remark 1 *For the sake of simplicity we assume that the initial conditions in (2.1) are consistent with the boundary conditions, i.e.* $\alpha = u_0(0)$ *and* $\beta = v_0(1)$. *Otherwise one should be aware of additional initial layers at the fixed boundaries.*

A first guess may be to consider the limit equations at $\varepsilon = 0$, i.e. the system

$$\begin{cases} \dfrac{\partial u}{\partial t} = 0, \quad u(x,0) = u_0(x), \quad s(t) < x < 1 \\ \dfrac{\partial v}{\partial t} = \dfrac{\partial^2 v}{\partial x^2}, \quad v(x,0) = v_0(x), \quad s(t) < x < 1 \\ u(0,t) = \alpha, \quad v(1,t) = \beta, \quad u(s(t),t) = v(s(t),t) = 0, \\ \dfrac{\partial v}{\partial x}(s(t),t) = \lambda\, \dot{s}(t), \end{cases} \tag{2.2}$$

This system decouples for $\varepsilon = 0$. We get a one–phase Stefan problem for the unknown function v,

$$\begin{cases} \dfrac{\partial v}{\partial t} = \dfrac{\partial^2 v}{\partial x^2}, \quad v(0,x) = v_0(x), \quad s(t) < x < 1 \\ v(t,s(t)) = 0, \quad \dfrac{\partial v}{\partial x}(t,s(t)) = \lambda\, \dot{s}(t), \quad v(t,1) = \beta, \end{cases} \tag{2.3}$$

and $u(x,t) = u_0(x)$ from the first equation in (2.2).

Due to the singular nature of the two–phase problem, this solution will in general not satisfy the boundary condition $u(s(t),t) = 0$ at the moving interface. Hence, for small $\varepsilon \neq 0$, we can expect to have a boundary layer at $x = s(t)$, where the solution $u(x,t)$ is forced from $u_0(s(t))$ down to zero on a spatial distance of order $O(\varepsilon)$. Thus we expect that the derivative $\partial u/\partial x$ inside of the boundary layer is of order $O(1/\varepsilon)$ compensating the factor ε in front of the derivative $\partial u/\partial x$ in (2.1), i.e. $\varepsilon \partial u/\partial x = O(1)$.

If we accept this "'heuristic"' argument, one will doubt whether problem (2.3) is the correct limit, i.e. $(v^\varepsilon, s^\varepsilon) \to (v,s)$ as $\varepsilon \to 0$. As we will see later on, there is indeed the need to use a corrected Stefan condition to be substituted in the one–phase problem (2.3) as $\varepsilon \ll 1$.

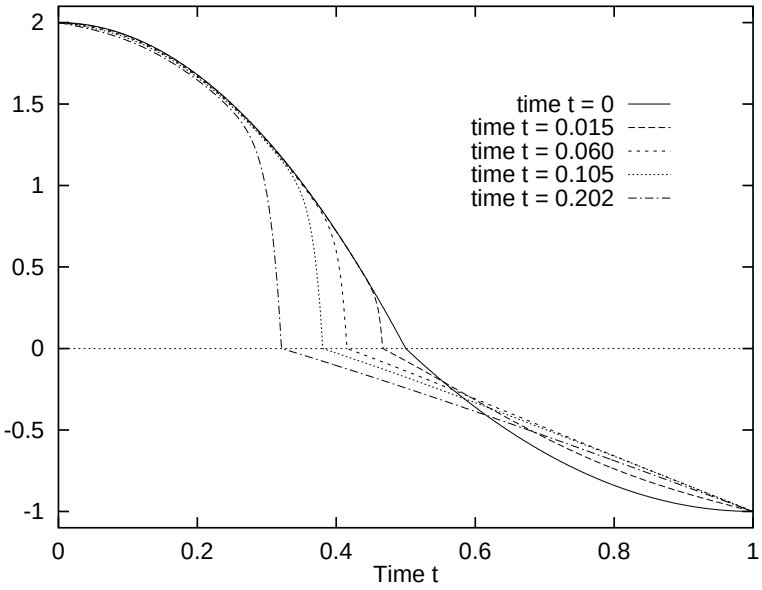

FIGURE 1. Solutions $u^\varepsilon(x,t)$ and $v^\varepsilon(x,t)$ at different times and $\varepsilon = 0.01$.

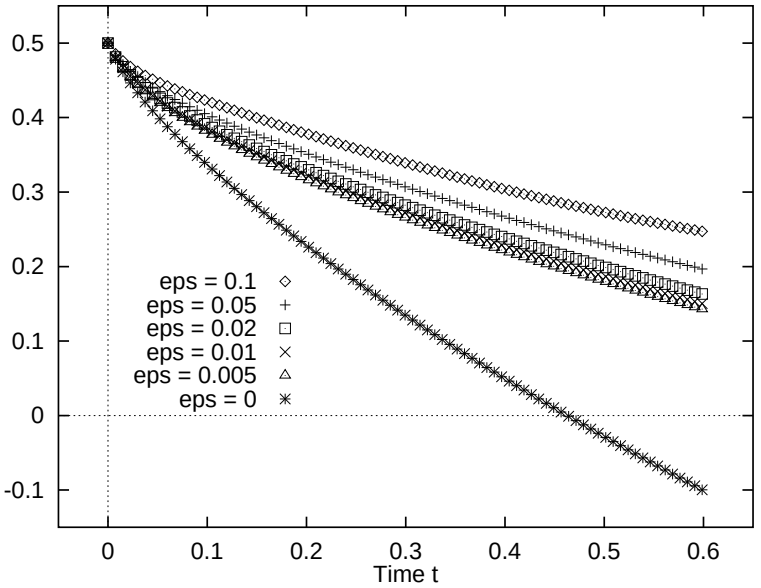

FIGURE 2. Position of the moving interface $s(t)$: $\varepsilon = 0$ denote a simulation based on the reduced one–phase problem, $\varepsilon > 0$ denote results from a two–phase simulation.

The existence of a boundary layer for small ε is confirmed by numerical simulations. Figure 1 shows results for the two–phase problem (2.1) with $\varepsilon = 0.01$ on the time interval $[0, 0.2]$. The initial conditions for u^ε and v^ε are parabolic profiles with $s(0) = 1/2$, $\lambda = 1$, $u^\varepsilon(0,t) = 2$ and $v^\varepsilon(1,t) = -1$. One observes the immediate formation of a boundary

layer on the left side of the moving interface as well as the nearly constant profile for $u^\varepsilon(x,t)$ outside the boundary layer.

A comparison between the two–phase problem given by (2.1) and the reduced one–phase problem (2.2) is given in figure 2, that shows the position $s(t)$ of the moving interface for both cases: $\varepsilon = 0$ denotes the simulation of the one–phase problem formulated in (2.3), whereas the results with $\varepsilon > 0$ are obtained from the two–phase system (2.1). One recognizes that the cases $\varepsilon = 0.01$ and $\varepsilon = 0.005$ are already quite close. This indicates that we are already close to the asymptotic limit $\varepsilon \to 0$. The simulation of (2.3) with $\varepsilon = 0$ yields an interface that moves faster than in the two–phase problem. Moreover, the interface crosses the point 0 in a finite time $T \approx 0.46$.

These numerical results indicate that the one–phase problem does not describe correctly the asymptotic limit, although we do not give results for parameters $\varepsilon < 0.005$. The numerical results are obtained by an explicit finite–difference approach on the interval $[0,1]$ combined with an explicit front–tracking scheme for the moving interface. This approach is obviously restricted to "moderately small" parameters ε: in order to describe the boundary layer at $x = s(t)$, one should use a spatial resolution, which is small enough to describe the boundary layer sufficiently accurate. For example, in the figures above we used a spatial resolution of order $O(10^{-3})$.

In the following we will show that the one–phase problem provides no appropriate description of the limit $\varepsilon \to 0$. To check this let us first of all have a look at the steady–state system of the two–phase problem:

$$\begin{cases} \dfrac{\partial^2 u_\infty}{\partial x^2} = 0, \qquad u_\infty(0) = \alpha, \qquad u_\infty(s_\infty) = 0 \\ \dfrac{\partial^2 v_\infty}{\partial x^2} = 0, \qquad v_\infty(s_\infty) = 0, \qquad v_\infty(1) = \beta \\ \dfrac{\partial v_\infty}{\partial x}(s_\infty) - \varepsilon \dfrac{\partial u_\infty}{\partial x}(s_\infty) = 0 \end{cases} \tag{2.4}$$

whose solution is

$$\begin{cases} u_\infty(x) = \dfrac{\beta - \varepsilon\alpha}{\varepsilon} x + \alpha \\ u_\infty(x) = (\beta - \varepsilon\alpha)x + \varepsilon\alpha \\ s_\infty = \dfrac{\varepsilon\alpha}{\varepsilon\alpha - \beta} \end{cases}$$

Hence, as long as $\varepsilon > 0$, the moving interface will run into the point $s_\infty = \varepsilon\alpha/(\varepsilon\alpha - \beta) > 0$ as $t \to \infty$. Moreover, in the limit as $t \to \infty$ and $\varepsilon \to 0$ we have $s^\varepsilon \searrow 0$.

Now let us consider the one-phase Stefan problem

$$\begin{cases} \dfrac{\partial v}{\partial t} = \dfrac{\partial^2 v}{\partial x^2}, \qquad v(0,x) = v_0(x) \\ v(t,s(t)) = 0, \quad \dfrac{\partial v}{\partial x}(t,s(t)) = \lambda\, \dot{s}(t), \quad v(t,1) = \beta, \end{cases} \tag{2.5}$$

The question is whether (v,s) is a "good" approximation of $(v^\varepsilon, s^\varepsilon)$, at least for "small" values of ε. The simple answer, already indicated by the numerical simulations given above, is "no" and this can be seen as follows.
By Taylor's formula we have

$$\begin{aligned} v(x,t) &= v(s(t),t) + \frac{\partial v}{\partial x}(s(t),t)\,(x-s(t)) + \int_{s(t)}^{x} \frac{\partial^2 v}{\partial x^2}(\xi)\,(x-\xi)\,d\xi \\ &= 0 + \lambda\,\dot s(t)\,(x-s(t)) + \int_{s(t)}^{x} \frac{\partial v}{\partial t}(\xi)\,(x-\xi)\,d\xi \\ &= \lambda\,\dot s(t)\,(x-s(t)) + \frac{\partial}{\partial t}\left[\int_{s(t)}^{x} v(\xi,t)\,(x-\xi)\,d\xi\right] + \dot s(t)\,v(s(t),t)\,(x-s(t)) \\ &= \frac{\partial}{\partial t}\left[\frac{\lambda}{2}\,s(t)\,(2x-s(t))\right] + \frac{\partial}{\partial t}\left[\int_{s(t)}^{x} v(\xi,t)\,(x-\xi)\,d\xi\right] \\ &= \frac{\partial}{\partial t}\left[\frac{\lambda}{2}\,s(t)\,(2x-s(t)) + \int_{s(t)}^{x} v(\xi,t)\,(x-\xi)\,d\xi\right], \end{aligned}$$

such that we get for $x=1$ the conservation law

$$\frac{dL}{dt} = \frac{d}{dt}\left[-2\,\beta\,t + \lambda\,s(t)\,(2-s(t)) + 2\int_{s(t)}^{1} v(\xi,t)\,(1-\xi)\,d\xi\right] = 0,$$

i.e. we have for all t

$$L(0) = L(t) = -2\,\beta\,t + \lambda\,s(t)\,(2-s(t)) + 2\int_{s(t)}^{1} v(t,\xi)\,(1-\xi)\,d\xi. \tag{2.6}$$

According to the maximum principle we have $|v| \leqslant c_1 := \max\{1, \sup\{|v_0(x)| : s(0) < x < 1\}\}$. But this implies that $s(t)$ can not be bounded! Indeed, if $s(t)$ were bounded then it followed from (2.6) that t is bounded and this yields a contradiction.

Now let us assume $\beta < 0$ and $-c \leqslant v_0 \leqslant 0$ with $c \in (0,\infty)$. Then $-\max\{1,c\} \leqslant v \leqslant 0$ and $\dot s \leqslant 0$. From (2.6) we get lower and upper estimates for the maximal time-interval $[0, T_{\max}]$ for which $0 \leqslant s(t)$, $t \in [0, T_{\max}]$ holds, namely

$$\max\left\{0, \frac{L(0)}{2\,|\beta|}\right\} \leqslant T_{\max} \leqslant \frac{L(0) + \max\{1,c\}}{2\,|\beta|}$$

For example, with $s(0) = 1/2$ and $v_0(x) = 4\,(1-x)^2 - 1$, $1/2 \leqslant x \leqslant 1$, $\beta = -1$, we get $L(0) = (6\,\lambda - 3)/8$ and therefore

$$\max\left\{0, \frac{6\,\lambda - 3}{16}\right\} \leqslant T_{\max} \leqslant \frac{6\,\lambda + 5}{16}.$$

For $t > T_{\max}$ we have the (ε-independent !) estimate $s(t) < 0$, while for all $\varepsilon > 0$ and $t > 0$ the estimate $0 < s^\varepsilon(t)$ holds, i.e. v is not an acceptable approximation for v^ε for all $t > T_{\max}$.

Remark 2 *We may check the estimates for $T_{\max}$ at which the moving interface of problem (2.3) crosses the zero using our numerical simulations given in figure 2: the estimate*

$0.1875 = 3/16 \leqslant T_{\max} \leqslant 11/16 = 0.6875$ *should be compared with the numerical result* $T_{\max} \approx 0.46$ *for the case* $\varepsilon = 0$.

3 Asymptotic Expansion Techniques

In the following we will derive a corrected Stefan condition for the one–phase problem formulated in (2.3), which is based on an asymptotic expansion of the slow diffusion region $0 < x < s(t)$. Thus, we will consider the parabolic equation $\partial u^\varepsilon/\partial t = \varepsilon \partial^2 u^\varepsilon/\partial x^2$ with initial condition $u^\varepsilon(x,0) = u_0(x)$ and boundary condition $u^\varepsilon(0,t) = \alpha$, $u^\varepsilon(s(t),t) = 0$, where we assume that the position of the moving interface $s(t)$ is known.

We expect a boundary layer at $x = s(t)$. Hence we should derive an outer expansion valid outside of the boundary layer. In a second step, we should calculate an inner expansion based on a stretching of the boundary layer and in the final step we should match both expansions to determine the asymptotic behavior along the whole interval $0 < x < s(t)$.

The zeroth order term of the outer expansion is simply given by $u^0(x,t) = u_0(x)$. To get an inner expansion, we perform the rescaling $x = s(t) - \varepsilon\xi$ and define the function $w^\varepsilon(\xi,t)$ by

$$w^\varepsilon(\xi,t) = u^\varepsilon(s(t) - \varepsilon\xi, t)$$

The differential equation inside the boundary layer is

$$\frac{\partial w^\varepsilon}{\partial t} + \frac{\dot{s}}{\varepsilon}\frac{\partial w^\varepsilon}{\partial \xi} = \frac{1}{\varepsilon}\frac{\partial^2 w^\varepsilon}{\partial \xi^2}$$

the boundary condition is $w^\varepsilon(0,t) = 0$ and the initial condition is $w^\varepsilon(\xi,0) = u_0(s(0) - \varepsilon\xi)$. The solution of the zeroth order equation $\dot{s}\partial w^0/\partial\xi = \partial^2 w^0/\partial\xi^2$ with boundary condition $w^0(\xi,t)$ is given by

$$w^0(\xi,t) = C(\exp(\dot{s}\xi) - 1)$$

where $C = C(t)$ is not determined yet. $C(t)$ will be used to perform the matching between inner and outer expansion.
The matching of $u^0(x,t)$ and $w^0(\xi,t)$ may be done using either an intermediate variable $\eta = \xi\varepsilon^{\alpha-1}$, $0 < \alpha < 1$, or with Van Dyke's matching rule (see [5]). Using, e.g., the intermediate variable η we have to require $u^0(s(t) - \varepsilon^{2-\alpha}\eta, t) = w^0(\eta\varepsilon^{1-\alpha}, t)$ to be satisfied up to zeroth order. An asymptotic expansion with η fixed and $\varepsilon \to 0$ gives

$$\begin{aligned} u^0(x,t) &= u_0(x) = u_0(s(t) - \varepsilon^{2-\alpha}\eta) \approx u_0(s(t)) \\ w^0(\xi,t) &= C(\exp(\dot{s}\xi) - 1) = C(\exp(\dot{s}\eta\varepsilon^{1-\alpha}) - 1) \approx -C \end{aligned}$$

The matching condition determines C:

$$C(t) = -u_0(s(t))$$

Hence, the inner expansion in the spatial variable x is

$$\hat{w}^0(x,t) = w^0\Big(\frac{s(t)-x}{\varepsilon}, t\Big) = -u_0(s(t))\Big(\exp(\dot{s}\frac{s(t)-x}{\varepsilon}) - 1\Big) \tag{3.1}$$

Using (3.1) we are able to formulate a corrected Stefan condition for our one–phase problem on $s(t) < x < 1$: the two–phase Stefan condition at $x = s(t)$ is of the form

$$\frac{\partial v}{\partial x} - \varepsilon \frac{\partial u}{\partial x} = \lambda \dot{s} \tag{3.2}$$

Calculating the gradient $\partial u/\partial x$ at the interface $x = s(t)$ yields the zeroth order expression

$$\frac{\partial u^0}{\partial x} = \frac{\partial \hat{w}^0}{\partial x} = u_0(s(t)) \frac{\dot{s}}{\varepsilon}$$

which gives together with (3.2) the corrected Stefan condition

$$\frac{\partial v}{\partial x} = \Big(\lambda + u_0(s(t))\Big) \dot{s} \; .$$

Hence, instead of the one–phase Stefan problem formulated in (2.3), one should use the corrected one–phase Stefan problem for $s(t) < x < 1$ given by

$$\begin{cases} \dfrac{\partial v}{\partial t} = \dfrac{\partial^2 v}{\partial x^2}, & v(0,x) = v_0(x) \\ v(t,s(t)) = 0, \quad \dfrac{\partial v}{\partial x}(t,s(t)) = \Big(\lambda + u_0(s(t))\Big)\, \dot{s}(t), & v(t,1) = \beta, \end{cases} \tag{3.3}$$

The zeroth order expansion (3.3) for the two–phase Stefan problem terminates as soon as the position of the moving interface reaches the fixed left boundary $x = 0$. From this time T_0 on the zeroth order expansion no longer exists, because the term $u_0(s(t))$ arising in the Stefan condition is defined only for $s(t) \in [0,1]$.

However, as shown Section 2 the steady–state position of the interface for (2.1) and $\varepsilon > 0$ is given by $s_\infty = \varepsilon\alpha/(\varepsilon\alpha - \beta)$, such that an expansion of s_∞ around $\varepsilon = 0$ yields

$$s_\infty = -\varepsilon \frac{\alpha}{\beta} + O(\varepsilon^2)$$

This means that $s(T_0) = 0$ is a correct zeroth order approximation for the steady–state solution and we can expect that even the solution $v(x,T_0)$ with $s(T_0) = 0$ is a zeroth order approximation of the steady–state solution of (2.1). This we will validate by numerical simulations in Section 4.

Remark 3 *From the numerical results given in figure 1 we can observe that the solution $v(x,t)$ is already at time $t = 0.2$ close to a linear profile, although the interface still moves to the left. Hence, we may guess the velocity of the moving interface, when it reaches the fixed left boundary to be*

$$\dot{s}(T_0) = \frac{\beta}{\lambda + \alpha}.$$

Let us prove that $s(t)$ of (3.3) will reach the left boundary in finite time. First of all we verify in analogy to Section 2 the conservation law

$$\begin{aligned} L_0(0) &= L_0(t) \\ &= -2\,\beta\, t + \lambda\, s(t)\,(2 - s(t)) + 2\,U_1(s(t)) - 2\,U_2(s(t)) + 2\int_{s(t)}^{1} v(\xi,t)\,(1-\xi)\,d\xi, \end{aligned}$$

where

$$U_1(s) := \int_0^s u_0(\xi)\, d\xi, \quad U_2(s) := \int_0^s \xi\, u_0(\xi)\, d\xi.$$

If we assume $\alpha > 0$, $u_0 \geqslant 0$, $\beta < 0$ and $-c \leqslant v_0 \leqslant 0$ with $c \in (0, \infty)$, then we will have $U_1 \geqslant U_2$ and we will get from the maximum principle lower and upper estimates for T_0:

$$T_0 \geqslant \max\left\{0, \frac{L(0) + 2\,U_1(s(0)) - 2\,U_2(s(0))}{2\,|\beta|}\right\},$$

$$T_0 \leqslant \frac{L(0) + 2\,U_1(s(0)) - 2\,U_2(s(0)) + \max\{1, c\}}{2\,|\beta|},$$

where L is as in Section 2. For example, with $s(0) = 1/2$, $\alpha = 2$, $u_0(x) = -8\,x^2 + 2$, $0 \leqslant x \leqslant 1/2$, $\beta = -1$, $v_0(x) = 4\,(1-x)^2 - 1$, $1/2 \leqslant x \leqslant 1$ we get

$$T_{max} = \frac{18\,\lambda + 15}{48} < \frac{18\,\lambda + 17}{48} \leqslant T_0 \leqslant \frac{18\,\lambda + 41}{48},$$

such that the zeroth order approximation definitely terminates after the naive approximation of Section 2.

Remark 4 *We may check the estimates for T_0 with the numerical simulations given in figure 5: the estimate $0.72916 < 35/48 \leqslant T_0 \leqslant 59/48 < 1.22917$ should be compared with the numerical result $T_0 \approx 1.003$ for the case $\varepsilon = 0$.*

The reason why our zeroth order approximation has to terminate is that our previous scalings will break down: if the position of the moving interface $s^\varepsilon(t)$ is itself of the order $O(\varepsilon)$, then the boundary layer at the interface will interact with the fixed left boundary and it does not make any sense to consider an outer expansion.

Thus, defining $s^\varepsilon(t) = \varepsilon\sigma^\varepsilon(t)$, we should substitute if $s^\varepsilon(t) = O(\varepsilon)$ the equation for $u^\varepsilon(x,t)$ in the slow diffusion region by

$$z^\varepsilon(\xi, t) = u^\varepsilon(\varepsilon\xi, t)$$

and study the problem

$$\left\{\begin{array}{l} \varepsilon\dfrac{\partial z^\varepsilon}{\partial t} = \dfrac{\partial^2 z^\varepsilon}{\partial \xi^2}, \quad z^\varepsilon(\xi, 0) = u_0(\varepsilon\xi) \\ z^\varepsilon(0,t) = \alpha, \quad z^\varepsilon(\sigma^\varepsilon(t)) = 0 \end{array}\right.$$

Then, the zeroth order approximation is given by

$$\frac{\partial^2 z^0}{\partial \xi^2} = 0, \quad z^0(0,t) = \alpha, \quad z^0(\sigma^0(t), t) = 0\,,$$

such that

$$z^0(\xi, t) = -\frac{\alpha}{\sigma^0(t)}\xi + \alpha$$

Computing the gradient gives $\partial z^0/\partial\xi = -\alpha/\sigma^0(t)$ and the two–phase interface condition

will read

$$\frac{\partial v}{\partial x} + \frac{\alpha}{\sigma^0} = \varepsilon\lambda\dot{\sigma}^0 \tag{3.4}$$

Taking again the zeroth order approximation for (3.4) we get

$$v^0(x,t) = -\frac{\alpha}{\sigma^0(t)}$$

and assuming that $\sigma^0(t) \approx s_\infty/\varepsilon$ we have

$$v^0(x,t) \approx -\beta\,,$$

which exactly defines a zeroth order approximation of the steady–state solution v_∞ from Section 2. Even this analysis confirms that at the time T_0, at which the corrected one–phase problem (3.3) will terminate, we have a zeroth order approximation for the two–phase problem.

4 Numerical Results

In this section we give some further results on the numerical simulation of the one–dimensional Stefan problem with slow diffusion. One of the aims is to validate the corrected Stefan condition derived in Section 3.

First we present the numerical algorithm based on a front–tracking method on a fixed finite–difference grid. This technique is a standard approach for the two–phase Stefan problem and suffices to validate the asymptotic expansion of the slow diffusion region. Hence, we even restrict ourselves to an explicit finite–difference scheme, except in the neighbourhood of the moving interface.

In Section 4.2 we validate the corrected one–phase problem (3.3). The results show that this problem is an appropriate approximation for small values of ε. Some additional results on the original two–phase Stefan problem are given in Section 4.3.

4.1 Numerical Approach Using Front Tracking

The numerical results given in the following use a standard front tracking method applied to a fixed finite difference grid, see [1]: given an equidistant spatial grid $x_0 = 0 < x_1 < \cdots < x_{m-1} < x_m = 1$ on the interval $[0,1]$ with resolution $h = 1/m$, $x_i = i/m$, we use an explicit finite difference method for the diffusion equations as well as an explicit time marching procedure for the moving interface $s(t)$. Some special care is taken for the grid points in the neighbourhood of the moving interface as well as if the moving interface crosses a grid point:

- in order to ensure the standard stability restriction of an explicit scheme, we use the weighted average method [6] with $\theta \geqslant 1/2$ to include implicit formulas close to the moving interface,
- if the interface is too close to a grid point, we use an interpolation formula instead of finite differences,
- if the moving interface crosses a grid point, we use an implicit difference formula for

the second grid point in the direction of the movement as well as an interpolation formula for the first point.

With the standard notations for the numerical approximates, $u_i^n \approx u(x_i, t_n)$, $v_i^n \approx v(x_i, t_n)$, $t_n = n \cdot k$, $x_i = i \cdot h$, $r = k/h^2$, the whole algorithm is formulated as follows:

1) Let i_s denote the index such that $x_{i_s} < s(0) < x_{i_s+1}$ and put $p^0 = (s(0) - x_{i_s})/h \neq 0$. Moreover, given the initial conditions $u_0(x)$ and $v_0(x)$ at time $t = 0$ as well as the position of the interface $s(0)$, we initialize our numerical approximates as follows:

$$u_i^0 = u_0(x_i), \quad i = 0, \ldots, i_s, \quad v_i^0 = v_0(x_i), \quad i = i_s + 1, \ldots, m,$$

2) for $n = 0, \ldots, n_{max}$ perform the following steps

   a) compute the position of the interface at time t_{n+1}:

$$\begin{aligned}(\partial_x u)^n &= \frac{p^n}{1+p^n}\, u_{i_s-1}^n - \frac{1+p^n}{p^n}\, u_{i_s}^n \\ (\partial_x v)^n &= \frac{2-p^n}{1-p^n}\, v_{i_s+1}^n - \frac{1-p^n}{2-p^n}\, v_{i_s+2}^n \\ p^{n+1} &= p^n + r\Big((\partial_x v)^n - (\partial_x u)^n\Big)/\lambda \end{aligned} \tag{4.1}$$

   b) fix the left and right boundary values:

$$u_0^{n+1} = \alpha, \quad v_m^{n+1} = \beta$$

   c) compute the new values on the left and right of the moving interface:

$$\begin{aligned} u_i^{n+1} &= u_i^n + \varepsilon r(u_{i-1}^n - 2u_i^n + u_{i+1}^n), \quad i = 1, \ldots, i_s - 1 \\ v_i^{n+1} &= v_i^n + r(v_{i-1}^n - 2v_i^n + v_{i+1}^n), \quad i = i_s + 2, \ldots, m-1 \end{aligned}$$

   d) compute the new values at the moving interface:

if $p^{n+1} \geqslant 0$ and $p^{n+1} \leqslant 1$ then $\quad \backslash *$ *interface remains in* $[x_{i_s}, x_{i_s+1}]$ $*\backslash$

if $p^{n+1} \leqslant \delta$ then $\quad \backslash *$ *interface is too close to* x_{i_s} $*\backslash$

$$u_{i_s}^{n+1} = \frac{p^{n+1}}{1+p^{n+1}}\, u_{i_s-1}^{n+1} \tag{4.2}$$

$$v_{i_s+1}^{n+1} = \frac{1-p^{n+1}}{1-p^{n+1}+2\theta r} \cdot \tag{4.3}$$

$$\Big(v_{i_s+1}^n + 2\theta r \frac{v_{i_s+2}^{n+1}}{2-p^{n+1}} + 2(1-\theta)r\Big(\frac{v_{i_s+2}^n}{2-p^n} - \frac{v_{i_s+1}^n}{1-p^n}\Big)\Big) \tag{4.4}$$

elseif $1 - p^{n+1} \leqslant \delta$ then $\quad$ * *interface is too close to* x_{i_s+1} **

$$u_{i_s}^{n+1} = \frac{p^{n+1}}{p^{n+1} + 2\varepsilon\theta r} \cdot \left(u_{i_s}^n + 2\varepsilon\theta r \, \frac{u_{i_s-1}^{n+1}}{p^{n+1}+1} + 2\varepsilon(1-\theta) r \Big(\frac{u_{i_s-1}^n}{p^n+1} - \frac{u_{i_s}^n}{p^n} \Big) \right)$$

$$v_{i_s+1}^{n+1} = \frac{1-p^{n+1}}{2-p^{n+1}} \, v_{i_s+2}^{n+1}$$

else $\quad$ * *use weighted average method* **

$$u_{i_s}^{n+1} = \frac{p^{n+1}}{p^{n+1} + 2\varepsilon\theta r} \cdot \left(u_{i_s}^n + 2\varepsilon\theta r \, \frac{u_{i_s-1}^{n+1}}{p^{n+1}+1} + 2\varepsilon(1-\theta) r \Big(\frac{u_{i_s-1}^n}{p^n+1} - \frac{u_{i_s}^n}{p^n} \Big) \right)$$

$$v_{i_s+1}^{n+1} = \frac{1-p^{n+1}}{1-p^{n+1} + 2\theta r} \cdot \left(v_{i_s+1}^n + 2\theta r \frac{v_{i_s+2}^{n+1}}{2-p^{n+1}} + 2(1-\theta) r \Big(\frac{v_{i_s+2}^n}{2-p^n} - \frac{v_{i_s+1}^n}{1-p^n} \Big) \right)$$

elseif $p^{n+1} > 1$ then $\quad$ * *interface crossed grid point* x_{i_s+1} **

$$u_{i_s}^{n+1} = \frac{p^{n+1}}{p^{n+1} + 2\varepsilon\theta r} \cdot \left(u_{i_s}^n + 2\varepsilon\theta r \, \frac{u_{i_s-1}^{n+1}}{p^{n+1}+1} + 2\varepsilon(1-\theta) r \Big(\frac{u_{i_s-1}^n}{p^n+1} - \frac{u_{i_s}^n}{p^n} \Big) \right)$$

$$u_{i_s+1}^{n+1} = \frac{p^{n+1}-1}{p^{n+1}} \, u_{i_s}^{n+1}$$

$$i_s \leftarrow i_s + 1$$

$$p^{n+1} \leftarrow p^{n+1} - 1$$

else $\quad$ * *interface crossed grid point* x_{i_s} **

$$v_{i_s+1}^{n+1} = \frac{1-p^{n+1}}{1-p^{n+1} + 2\theta r} \cdot \left(v_{i_s+1}^n + 2\theta r \frac{v_{i_s+2}^{n+1}}{2-p^{n+1}} + 2(1-\theta) r \Big(\frac{v_{i_s+2}^n}{2-p^n} - \frac{v_{i_s+1}^n}{1-p^n} \Big) \right)$$

$$v_{i_s}^{n+1} = \frac{p^{n+1}}{p^{n+1}-1} \, v_{i_s+1}^{n+1}$$

$$i_s \leftarrow i_s - 1$$

$$p^{n+1} \leftarrow p^{n+1} + 1$$

end if

e) recompute the position of the moving interface:

$$s^{n+1} = (p^{n+1} + i_s) \cdot h$$

Remark 5 *Equations like (4.2) are interpolation formulas whereas equations like (4.3)*

are derived from finite difference approximations on non–equidistant grids based on Lagrange interpolation [1].

The algorithm above is modified in a straightforward way to a scheme for one–phase problems: one simply deletes all expressions involving the numerical approximtes u_i^n. Moreover, for the corrected one phase problem of Section 3, one should substitute Eq. (4.1) by the formula

$$p^{n+1} = p^n + r\Big((\partial_x v)^n - (\partial_x u)^n\Big)/\Big(\lambda + u_0(s^n)\Big)$$

For one–phase problems, the left boundary is defined by the moving interface itself and therefore the problem is not restricted to the unit interval $[0,1]$ (as it is for the two–phase problem). According to figure 2 the system (2.3) yields negative values for $s(t)$ even in finite times. Hence, we should extend the algorithm above to possibly negative grid points and negative indices i_s.

In the following two sections we always use the set of parameters

$$h = 1/1001, \quad r = 1/2, \quad \theta = 1, \quad \delta = 10^{-1}$$

to run the scheme as well as a Stefan number $\lambda = 1$. This means that we use a fully implicit difference approximation at the moving interface. The boundary conditions are choosen like in Section 2, i.e. $\alpha = 2$ and $\beta = -1$, the interface is located at the beginning at $s(0) = 1/2$ and the initial conditions are the parabolic profiles

$$u_0(x) = -\alpha\left(\frac{x}{s(0)}\right)^2 + \alpha, \qquad 0 \leqslant x \leqslant s(0)$$

$$v_0(x) = -\beta\left(\frac{1-x}{1-s(0)}\right)^2 + \beta, \qquad s(0) \leqslant x \leqslant 1$$

4.2 Comparison with One–Phase Simulations

In this section we will validate the corrected one–phase problem from Section 3. According to figure 2 the moving interface computed from problem (2.3) already gets negative at a time $T \approx 0.46$, where the exact interface of the two–phase problem with $\varepsilon \ll 1$ is located at $s^\varepsilon(0.46) \approx 0.19$ and therefore stays – with respect to the parameter ε – significantly away from the left boundary $x = 0$.

In figure 3 we include the results from a numerical simulation of the corrected one–phase problem (3.3). One observes the good agreement of the positions of the moving interface for the two–phase problem with $\varepsilon = 0.01$ with the corrected one–phase problem. This validates the zeroth order expansion from Section 3. The same holds for the solution $v^\varepsilon(x,t)$ (see figure 4): the agreement between the two–phase and the corrected one–phase problem is excellent, whereas the simple one–phase problem (2.3) shows strong deviations from the exact solution.

The zeroth order approximation (3.3) shown in figure 3 can be extended up to the time, where the moving interface $s(t)$ becomes zero: this occurs in the numerical simulation at time $T_0 \approx 1.003$, see figure 5. At this time, the interface $s^\varepsilon(t)$ of the two–phase problem is of the order $O(\varepsilon)$ and hence already close to the steady–state $s_\infty = \varepsilon\alpha/(\varepsilon\alpha - \beta)$.

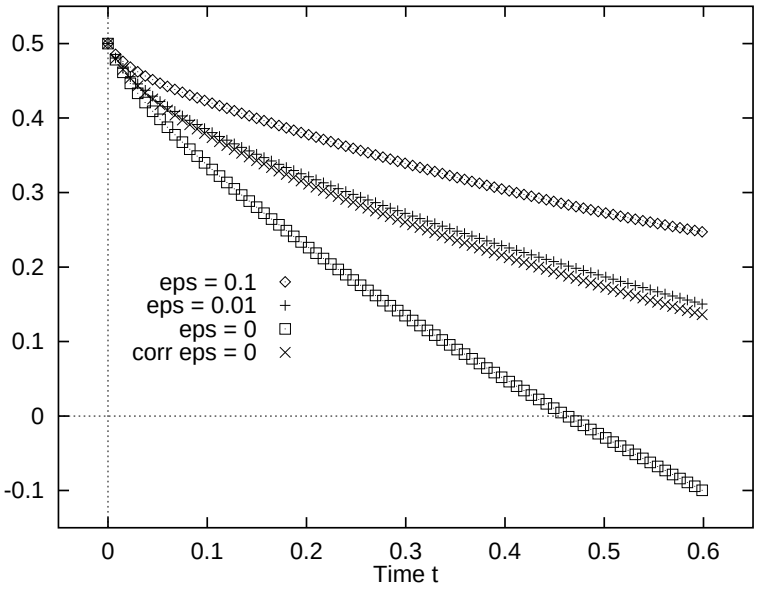

FIGURE 3. Position of the moving interface $s(t)$: corr $\varepsilon = 0$ denote a simulation based on the corrected one–phase problem.

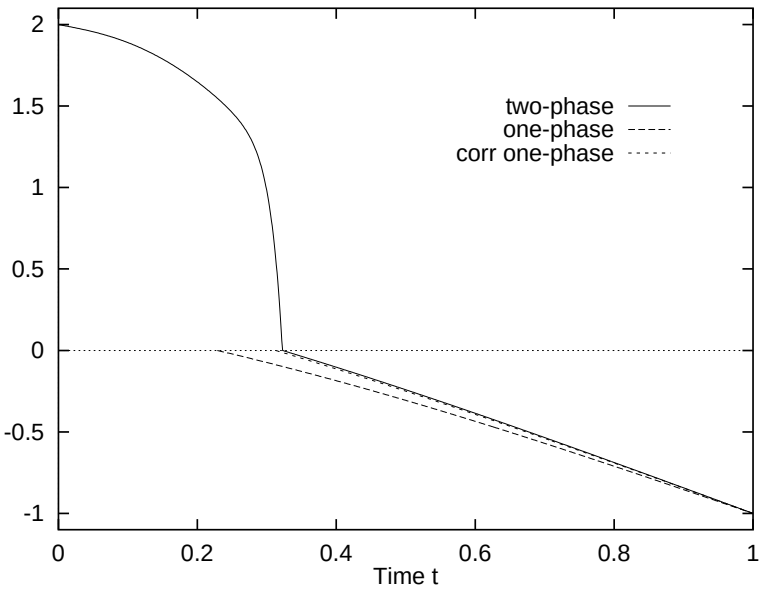

FIGURE 4. Solutions $u^\varepsilon(x,t)$ and $v^\varepsilon(x,t)$ at time $t \approx 0.2$ and $\varepsilon = 0.01$, compared with the one–phase problems.

Moreover, the profiles itself are close to the steady–state solutions given in Section 2, close in the sense that even the solution of (3.3) is the correct zeroth order expansion (see also figure 6).

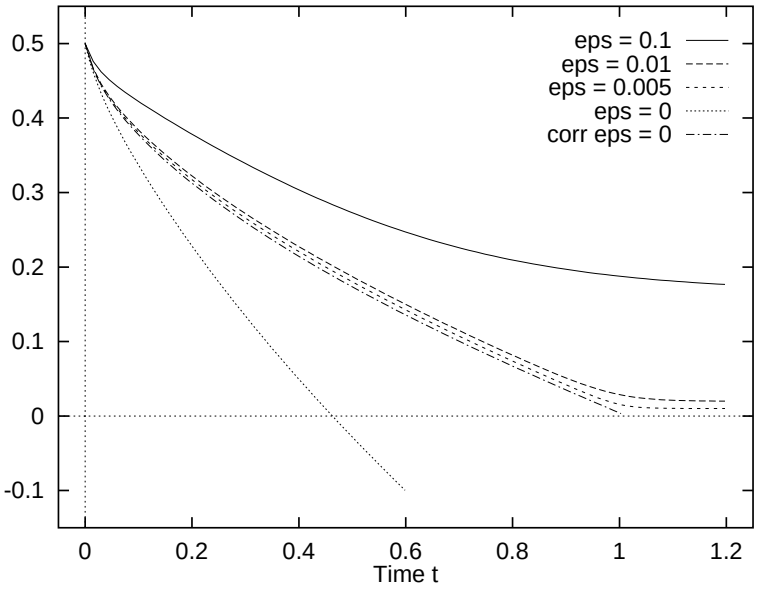

FIGURE 5. Position of the moving interface $s(t)$.

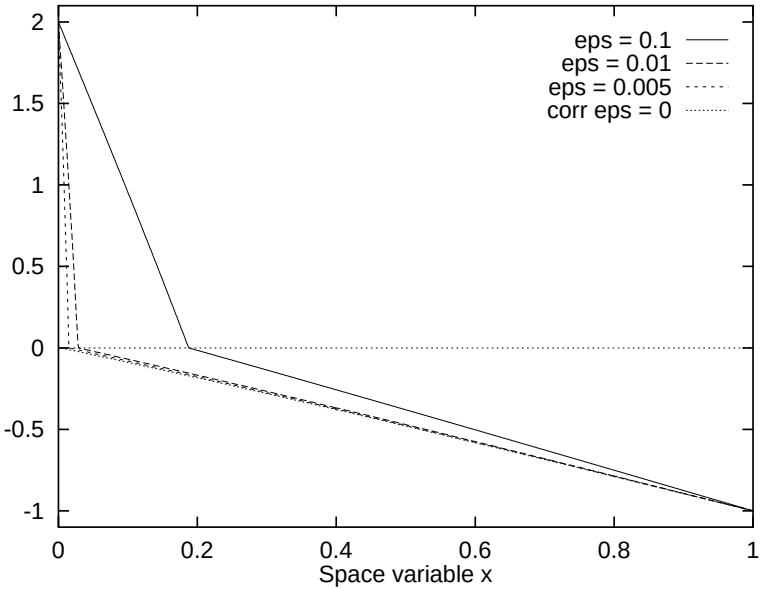

FIGURE 6. Solutions $u^\varepsilon(x,t)$ and $v^\varepsilon(x,t)$ at time $t = 1.003$, just before the corrected one–phase problems terminates with $s(T) = 0$.

4.3 Additional Results for the Two–Phase Problem

In addition to the numerical validation of the corrected Stefan condition we will give some further results on the two–phase problem as $\varepsilon \to 0$.

In figure 2 one realizes the formation of a boundary layer at the moving interface. In figure 6 solution profiles at time $T_0 = 1.003$ (at this time the zeroth order approximation

terminates) are given. Now, we like to investigate in more detail the solution $u^\varepsilon(x,t)$ in the slow diffusion region, where we can detect different time scale effects during the transient computation. Hence, we will look at the scaled function $\hat{u}^\varepsilon(y,t) = u^\varepsilon(ys^\varepsilon(t),t)$, such that the scaled variable $y = x/s^\varepsilon(t)$ runs at each time on the interval $[0,1]$.

Remark 6 *Because we are using a fixed finite–difference grid the number of points used to approximate the solution $\hat{u}^\varepsilon(y,t)$ changes with time: based on the resolution $h \approx 10^{-3}$, we have initially about 500 points, in the limit $t \to \infty$ we remain with about 10 points, because $s_\infty = \varepsilon\alpha/(\varepsilon\alpha - \beta)$ (see Section 2).*

Figure 7 shows a sequence of profiles for $\varepsilon = 0.005$ from the time interval $[0, 1.153]$, where the eight profiles are choosen from an equidistant grid on $[0, 1.153]$. At the beginning of the computation, there is a rapid formation of the boundary layer at $y = 1$, shown in the first two profiles at $t = 0$ and $t = 0.165$. Then, between $t = 0.165$ and $t = 0.494$ the profile outside of the boundary layer starts to grow up close to maximal value at the left boundary $\hat{u}^\varepsilon(0,t) = 2$. Later on, between $t = 0.494$ and $t = 0.823$ the boundary layer starts to increase significantly to the right and therefore forms a profile, which is quite similar to the initial condition $u_0(x)$. In the next picture ($t = 0.988$), we see that the solution has rapidly changed close to the steady–state solution; a linear profile, which is then completely built at time $t = 1.153$.

We therefore detect several time scales in the transient behavior:

- a fast time scale at the beginning with a rapid formation of a boundary layer at $x = s(t)$. This is confirmed by the large gradient $\dot{s}$ in figure 5 close to $t = 0$,
- a slow time scale, where the profile outside the boundary layer increases to the maximal value and the boundary layer starts to move to the left. In this region, the gradient $\dot{s}$ stays nearly constant,
- a fast time scale, where the profile rapidly drops down close to the steady–state profile. In figure 5, this region is found at the sharp bend around $t = 1$,
- a slow time scale, where the profile finally reaches the steady–state solution u_∞. Here, one detects this region as the plateau for $t > 1$, where $\dot{s}$ is approximately zero.

5 Conclusion

In this paper a singular–perturbed two–phase Stefan problem due to slow diffusion in one of the two phases has been investigated. We showed the necessity to use a corrected interface condition, which takes into account the formation of a boundary layer in the slow diffusion region.

The modified interface condition has been obtained from a zeroth order matched asymptotic expansion in the slow diffusion region. The reduced one–phase problem has been validated by numerical experiments, which are based on a front–tracking method on a fixed finite–difference grid. Moreover, we investigated in detail the transient behavior in the slow diffusion region, where several time scale phenomena can be detected.

The investigated system acts as a model problem for multi–phase transport phenom-

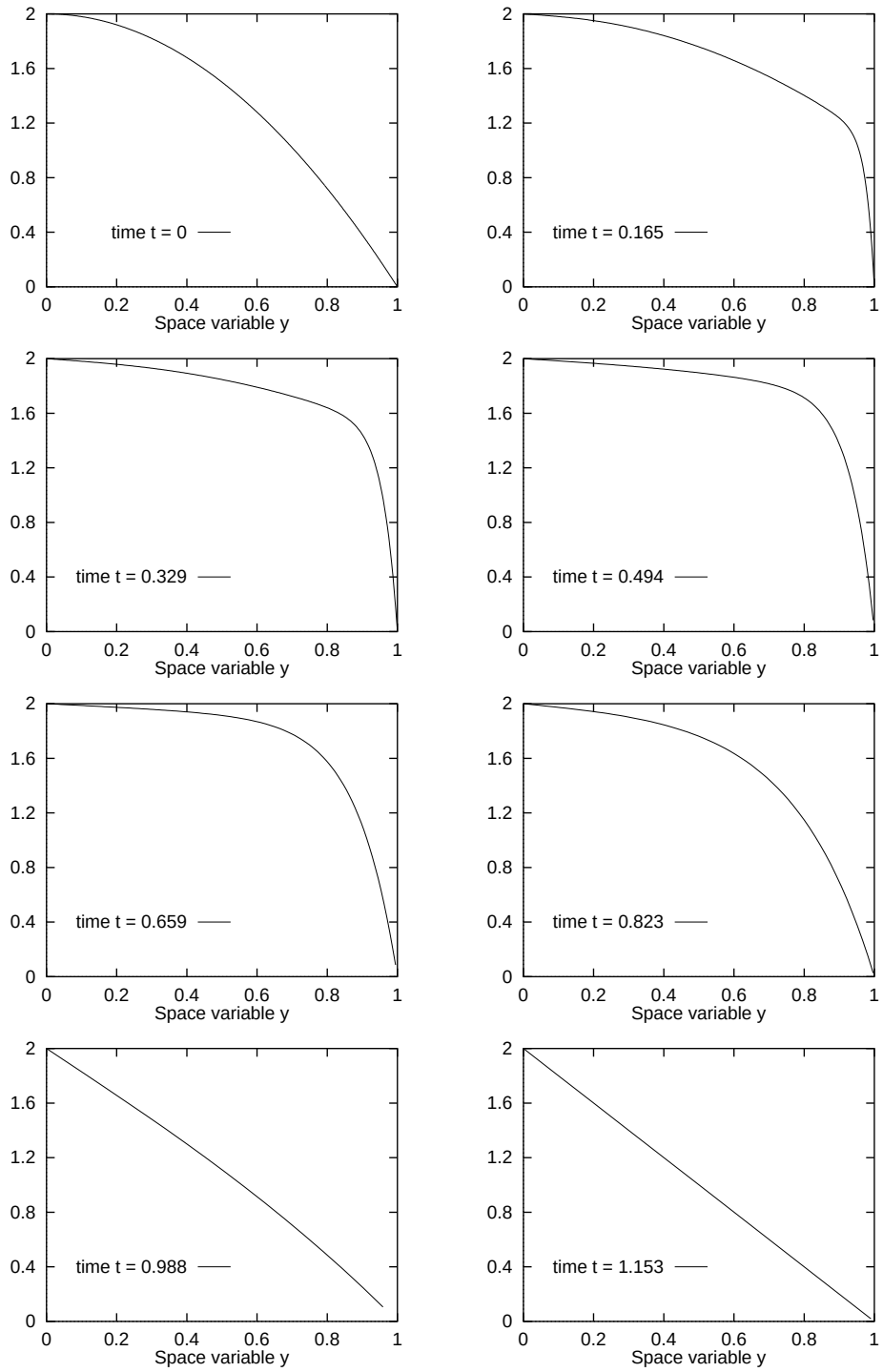

FIGURE 7. Transient behavior of the scaled function $\hat{u}^{\varepsilon}(y,t)$.

ena with small parameters. Some future work will be concerned with the application of asymptotic expansion techniques to those problems.

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