

A First Order Singular Perturbation Solution
to a Simple One-Phase Stefan Problem with
Finite Neumann Boundary Conditions.

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Abstract

This paper examines the difference between infinite and finite domains of a Stefan Problem. It is pointed out that attributes of solutions to the Diffusion Equation suggest assumptions of an infinite domain are invalid during initial times for finite domain Stefan Problems. The paper provides a solution for initial and early times from an analytical approach using a perturbation. This solution can then easily be applied to numerical models for later times. The differences of the two domains are examined and discussed.

1 History of the Problem

1.1 Origins and Previous Work

Free boundary problems can be traced back to the design of artillery shells by Sir Isaac Newton in the 1600's [9]. However the Stefan problem began to take a more definitive shape when in 1831, Clapeyron and Lamé [7] examined the problem of a ball of water freezing and derived the well-known square root of time law for interface motion between the two phases of liquid water and solid ice.

A major breakthrough in the problem occurred in 1861 by Franz Neumann [8] who found a closed form solution for infinite and semi-infinite media. This is found in his class notes of the time.

In 1889, J. Stefan [15], whose name is attached to the problem, wrote four papers on the subject. In these papers he derived a large latent heat approximation and extended this approximation to include a time dependent surface temperature of the interface.

A very good collection of similarity solutions and references is to be found in Carslaw and Jaeger's 1959 book, *Conduction of Heat in Solids* [3]. Another very good book on the subject is by John Crank [8] in his definitive text *Free and Moving Boundary Problems* of 1984. In this book he states [8, page 101]:

“Very few analytical solutions are available in closed form. They are mainly for the one-dimensional cases of an infinite or semi-infinite region with simple initial and boundary conditions and constant thermal properties. These exact solutions usually take the form of functions of the single variable $x/t^{1/2}$ and are known as similarity solutions. Corresponding solutions which are functions of $r/t^{1/2}$ only are available in cylindrical and spherical coordinates.”

Some modern papers quote Ivantsov's work [10] on crystal growth in 1947, particularly Pelcé and Pomeau [12] in their paper on dendrites in 1986. And in 1990 Kim [11] described an application of a Stefan problem in the analytic valuations of American put options.

The late 1990's appear to have an upsurge in work on this problem. Chen, Merriman, Osher & Smereka [6] outline an attack to the problem using level sets in 1997 which shows great promise in understanding Stefan problems of higher dimension. In 1998 Riccardo Fazio [9] wrote a survey of similarity approaches to free boundary problems and concluded that some classes of these problems can be transformed to initial value problems. Fazio goes on to show that free boundary problems arise via a similarity analysis of moving hyperbolic problems and they can be obtained as approximations of boundary valued problems defined on infinite intervals. Also in 1998, Yi and Shih [16] proved the existence of a weak solution and uniqueness. They also obtained an error estimate for the approximating process.

In 1999 Rodrigues and Urbano [13] developed solutions to Stefan problems with convection in one of the phases. Charach and Fife [4] showed, also in 1999, thermodynamic consistency for diffuse interactions and implications for interface conditions in the associated sharp interface theories. Again in 1999 Elena Bonetti [2] established the existence and uniqueness of the solution to a diffusive phase transition problem for an integrodifferential energy balance equation of hyperbolic type. The related limiting case of the hyperbolic Stefan problem with memory was also examined.

In 2000, Beckett, Mackenzie and Robertson [1] developed a moving mesh finite element method for the solution of two-dimensional Stefan problems. This method involves the numerical solution of an enthalpy formulation. Again in 2000, Chen and Fife [5] continued their work on the thermodynamics of phase interfaces and derived relations of the Gibbs-Thomson type which entails surface tension at the interface. In their paper they suggest the use of perturbations to solve the Stefan problem, which we do here.

1.2 Motivation

This work stems from measurements of the diffusion coefficient of carbon dioxide into bitumen by Schmidt et al [14] which utilized a diffusion cell filled with bitumen coming into contact with carbon dioxide gas. The diffusion cell was a 1.6 cm wide tube, about 30 cm long, which was sectioned off into 10 sections at the end of the experiment. The concentration of carbon dioxide was measured in each section and a concentration profile for the tube of bitumen was interpolated and a diffusion coefficient then calculated. A

phenomenon noted at the end of the experiment was that the bitumen had swollen about half an inch up the diffusion tube and it was concluded the experiment consisted of a one-dimensional Stefan problem in diffusion.

The question then arose that since the diffusion cell was a finite length, are we permitted to assume it is infinite for short times and utilise the exact solution derived by Franz Neumann in 1861 or does the back wall of the cell influence the diffusion process even during short times and thereby alter the measurement of diffusion coefficients. Since the speed of propagation of the diffusion process is infinite there exists a suspicion that there would be some difference between a diffusion process in a finite domain as opposed to a semi-infinite domain. To answer this question we have used a perturbation approach for a finite but long one-dimensional domain of solvent having length " L " and Stefan number $1/\alpha$ with saturation concentration at the solvent-solute interface ψ^* , a constant. Here $\psi(t, x)$ is the concentration of solute measured as a weight fraction and $R(t)$ is the position of the gas-liquid interface which moves to the right.

It has been well established that a finite amount of solvent will eventually become saturated with solute and only swell a finite distance. Hence the classic square-root of time solution cannot be used over extended times for finite solvent domains since it predicts that the solvent-solute interface will swell an infinite distance. An analytic solution for such a situation has not yet been found and numeric models have been used extensively for investigations into this and similar phenomena. This is noted for example in the work of Schmidt et al and of Beckett et al [14] [1] There is, however, a problem with sharp initial interfaces in numerical models where the Neumann solution has been assumed for short times in order to initialise simulations. We present here a different solution for finite domains for short times.

As a result of our calculations we have found that it makes a difference in interface behaviour whether the media is semi-infinite or finite (even though the media is very large or we are considering only very short times). This difference becomes infinite as ψ^* approaches 1 if the solute is conserved.

2 Perturbation Solution with Neumann Boundary Conditions.

The diffusion equation:

$$\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2} \quad (1)$$

at the left boundary ...

$$\frac{\partial \psi}{\partial x} = 0 \text{ at } x = 0 \quad (2)$$

initial conditions ...

$$\psi(0, x) = 0 \quad (3)$$

$$R(0) = L \quad (4)$$

where L is the length of the solvent.

Conditions at the right moving boundary are ...

$$\psi = \psi^* \text{ at } x = R(t) \quad (5)$$

$$\alpha \frac{dR}{dt} = \frac{\partial \psi}{\partial x} \text{ at } x = R(t) \quad (6)$$

where ψ^* is a constant (the saturation level of the solution).

Nondimensionalizing with new variables:

$$\bar{x} = (x - L)/L \quad (7)$$

$$\bar{R} = (R - L)/L \quad (8)$$

$$\bar{\psi}(t, \bar{x}) = \psi(t, x) \quad (9)$$

Substitution yields ...

$$\frac{\partial \bar{\psi}}{\partial t} = \frac{1}{L^2} \frac{\partial^2 \bar{\psi}}{\partial \bar{x}^2} \quad (10)$$

$$\text{at } t = 0, \bar{\psi} = 0 \quad (11)$$

$$\text{at } \bar{x} = \bar{R}(t), \alpha \frac{d\bar{R}}{dt} = \frac{1}{L^2} \frac{\partial \bar{\psi}}{\partial \bar{x}} \quad (12)$$

$$\text{at } \bar{x} = -1, \frac{\partial \bar{\psi}}{\partial \bar{x}} = 0 \quad (13)$$

We now bring in a perturbation in the differential equation.

$$\text{Let } \epsilon = \frac{1}{L^2} \quad (14)$$

$$\frac{\partial \bar{\psi}}{\partial t} = \epsilon \frac{\partial^2 \bar{\psi}}{\partial \bar{x}^2} \quad (15)$$

Outer solution ...

$$\Rightarrow \frac{\partial \bar{\psi}}{\partial t} = 0 \quad (16)$$

$$\Rightarrow \bar{\psi} = g(\bar{x}) \quad (17)$$

$$\Rightarrow \bar{\psi} = 0 \text{ (initial conditions)} \quad (18)$$

Set up a boundary layer at the gas-liquid interface.

$$\tilde{x} = \frac{\bar{x} - \bar{R}(t)}{\epsilon^\gamma} \quad (19)$$

$$\frac{\partial \bar{\psi}}{\partial t} = \frac{\partial \tilde{\psi}}{\partial \tilde{x}} \frac{\partial \tilde{x}}{\partial t} + \frac{\partial \tilde{\psi}}{\partial t} \quad (20)$$

$$\frac{\partial \bar{\psi}}{\partial x} = \frac{1}{\epsilon^\gamma} \frac{\partial \tilde{\psi}}{\partial x} \quad (21)$$

Using the boundary layer variables ...

$$-\bar{R}_t \epsilon^{-\gamma} \tilde{\psi}_{\tilde{x}} + \tilde{\psi}_t = \epsilon^{1-2\gamma} \tilde{\psi}_{\tilde{x}\tilde{x}} \quad (22)$$

$$\alpha \bar{R}_t = \epsilon^{1-\gamma} \tilde{\psi}_{\tilde{x}} \quad (23)$$

Combining 22 and 23 to eliminate $\bar{R}(t)$ yields ...

$$\tilde{\psi}_t = \frac{\epsilon^{1-2\gamma}}{\alpha} \tilde{\psi}_{\tilde{x}}^2 + \epsilon^{1-2\gamma} \tilde{\psi}_{\tilde{x}\tilde{x}} \quad (24)$$

Boundary conditions

$$\tilde{\psi} = \psi^* \text{ at } \tilde{x} = 0 \quad (25)$$

$$\tilde{\psi} \rightarrow 0 \text{ at } \tilde{x} \rightarrow -\infty \quad (26)$$

and matching yields $\gamma = 1/2$

Dropping the tilde notation we have the PDE ...

$$\psi_t = \frac{\psi_x^2}{\alpha} + \psi_{xx} \quad (27)$$

Using a similarity solution ...

$$\psi = f(x/t^\beta) \quad (28)$$

$$\psi_t = -\frac{x\beta}{t^{\beta+1}}f' \quad (29)$$

$$\psi_x = \frac{1}{t^\beta}f' \quad (30)$$

$$\psi_{xx} = \frac{1}{t^{2\beta}}f'' \quad (31)$$

Hence ...

$$-\frac{x\beta}{t^{\beta+1}}f' = \frac{1}{\alpha t^{2\beta}}(f')^2 + \frac{1}{t^{2\beta}}f'' \quad (32)$$

From which we obtain

$$\beta = 1/2 \quad (33)$$

Letting

$$z = x/\sqrt{t} \quad (34)$$

and substituting back we have the ODE ...

$$f'' + \frac{(f')^2}{\alpha} + \frac{z}{2}f' = 0 \quad (35)$$

Let

$$v = f' \quad (36)$$

Then

$$v' + \frac{v^2}{\alpha} + \frac{z}{2}v = 0 \quad (37)$$

Using the transformation ...

$$v = e^{-z^2/4}w \quad (38)$$

along with ...

$$v' = \left(\frac{-z}{2}w + w'\right)e^{-z^2/4} \quad (39)$$

we obtain ...

$$\left(\frac{-z}{2}w + w'\right)e^{-z^2/4} + \frac{w^2}{\alpha}e^{-z^2/2} + \frac{z}{2}we^{-z^2/4} = 0 \quad (40)$$

Simplifying ...

$$\alpha w' + w^2 e^{-z^2/4} = 0 \quad (41)$$

Rearranging ...

$$\frac{w'}{w^2} = \frac{-e^{-z^2/4}}{\alpha} \quad (42)$$

Integrating both sides ...

$$-\frac{1}{w} = -\frac{1}{\alpha} \int e^{-z^2/4} dz + C \quad (43)$$

$$w = \frac{\alpha}{2 \operatorname{erf}(z/2) + C} \quad (44)$$

Solving for v we have

$$v(z) = \frac{\alpha e^{-z^2/4}}{2 \operatorname{erf}(z/2) + C} \quad (45)$$

and

$$f' = v \quad (46)$$

Solving for f we have ...

$$f = \int_0^z v(\sigma) d\sigma + C_2 \quad (47)$$

As $z \rightarrow -\infty$, $v \rightarrow 0$ so ...

$$C_2 = \int_{-\infty}^0 v(\sigma) d\sigma \quad (48)$$

Combining the two

$$f = \int_{-\infty}^z v(\sigma) d\sigma \quad (49)$$

and

$$\psi^* = f(0) = \alpha \int_{-\infty}^0 \frac{e^{-z^2/4}}{2 \operatorname{erf}(z/2) + C} dz \quad (50)$$

From which we can find the value of C .

Substituting back we have ...

$$\tilde{\psi} = \frac{\alpha\sqrt{\pi}}{2} \ln\left(\frac{2 \operatorname{erf}(\frac{\tilde{x}}{2\sqrt{t}}) + C}{C - 2}\right) \quad (51)$$

giving ...

$$\frac{d\bar{R}}{dt} = \frac{\sqrt{\epsilon} e^{-\frac{\tilde{x}^2}{4t}}}{\sqrt{t}(2 \operatorname{erf}(\frac{\tilde{x}}{2\sqrt{t}}) + C)} \quad (52)$$

Setting

$$\tilde{x} = 0 \quad (53)$$

we have

$$\bar{R} = 2 \frac{\sqrt{\epsilon t}}{C} \quad (54)$$

where

$$C = \frac{2e^{2\psi^*/(\alpha\sqrt{\pi})}}{e^{2\psi^*/(\alpha\sqrt{\pi})} - 1} \quad (55)$$

This approximation is valid for times up to $O(1/\epsilon)$ or $O(L^2)$.

3 Simplified Neumann Solution for Semi-infinite Domain

Here everything is the same as in the previous chapter except that at $x = -\infty$, $\frac{\partial\psi}{\partial x} = 0$. Or, to write out the equations for a semi-infinite domain:

The diffusion equation:

$$\frac{\partial\psi}{\partial t} = \frac{\partial^2\psi}{\partial x^2} \quad (56)$$

At the left boundary ...

$$\frac{\partial\psi}{\partial x} = 0 \text{ at } x = -\infty \quad (57)$$

Initial conditions ...

$$\psi(0, x) = 0 \quad (58)$$

$$R(0) = 0 \quad (59)$$

Conditions at the right moving boundary are ...

$$\psi = \psi^* \text{ at } x = R(t) \quad (60)$$

$$\alpha \frac{dR}{dt} = \frac{\partial \psi}{\partial x} \text{ at } x = R(t) \quad (61)$$

Using the Boltzmann substitution we have a solution of:

$$\psi = \theta \left(1 + \operatorname{erf} \left(\frac{x}{2\sqrt{t}} \right) \right) \quad (62)$$

and

$$R(t) = \phi_\infty \sqrt{t} \quad (63)$$

Where it can be shown that ...

$$\phi_\infty = \frac{\psi^* 2e^{-\phi_\infty^2/4}}{\alpha \sqrt{\pi} (1 + \operatorname{erf}(\phi_\infty/2))} \quad (64)$$

and ϕ_∞ can be found through an iterative search and ...

$$\theta = \frac{\psi^*}{1 + \operatorname{erf}(\phi_\infty/2)} \quad (65)$$

For our following observation we consider the solute to be conserved throughout the dissolving process. In this case we have

$$\alpha = 1 - \psi^* \quad (66)$$

Now it becomes possible to compare the behaviour of interface motions for short times between finite and semi-infinite domains for conservation of solute. Using the FZERO function of Matlab it is seen that ϕ_∞ tends to ∞ as ψ^* tends to 1. This means the semi-infinite domain blows up with very high saturation concentrations. In the extreme case of the interface being completely saturated with solute the interface moves to the right an infinite distance with an infinite speed.

Consider the finite domain. Here C tends to 2 as ψ^* tends to 1 (or α tends to 0). In which case the interface moves as the square root of time, or $R(t) = L + \sqrt{t}$. In other words, the interface does not blow up and its position has finite values over time. Therefore the difference between the interface positions for finite and semi-infinite domains increases with ψ^* until the difference is infinite.

Further investigation shows that the two situations, finite and semi-infinite, become identical for lower saturation concentrations. Various figures are included to demonstrate this.

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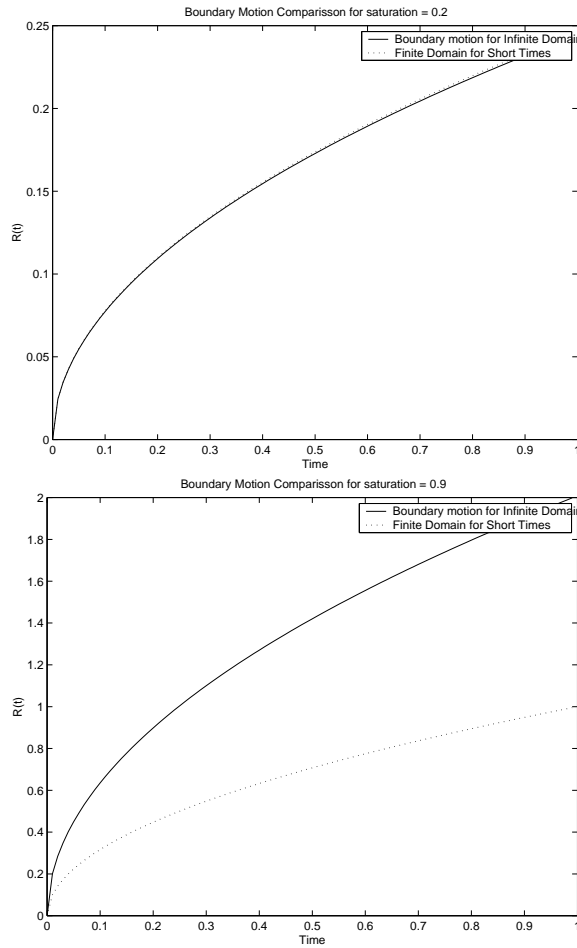


Figure 1: Comparison of interface motion versus time for saturation levels $\psi^* = 0.2$ for the upper figure and below that, $\psi^* = 0.9$. At a smaller saturation level we see the two interface behaviours are nearly identical while at a saturation level of 0.9 the semi-infinite domain has an interface motion about twice as fast as the finite domain over short times.

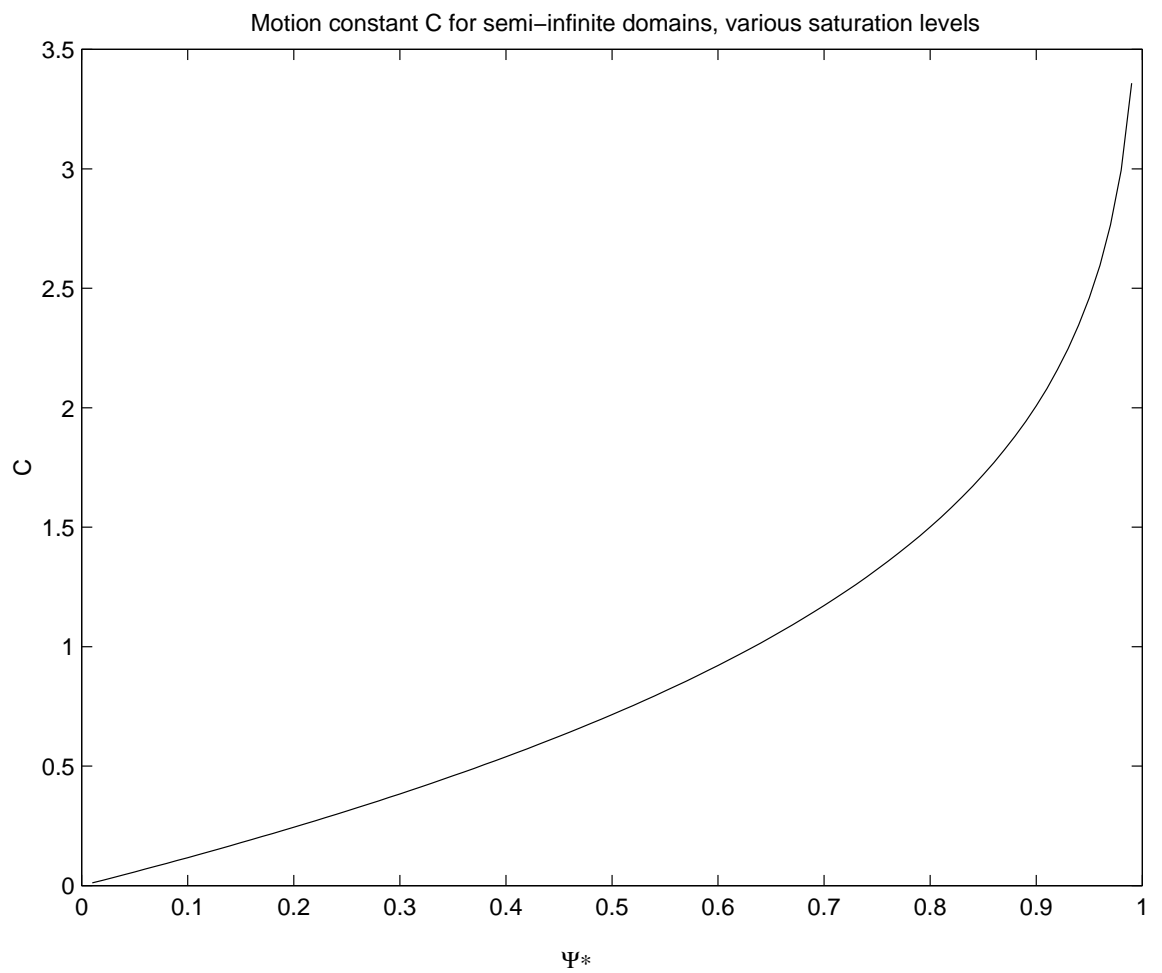


Figure 2: Graph showing the blowup of C where $R_\infty(t) = C\sqrt{t}$ as $\psi^* \rightarrow 1$. We see that $R(t)$ is well-behaved for most values of ψ^* but increases drastically should there be close to total saturation levels at the interface.