Approximate Analytic Solution of the One Phase Superheated Stefan Problem

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Abstract
This paper presents an approximate analytic solution for a one phase Stefan problem involving a superheated solid over a finite spatial interval using, as far as the author is aware, a novel application of homotopy analysis. This problem is ill posed under certain initial conditions where the energy in the solid phase exceeds the energy required to melt it. To avoid this situation, the approximate analytic solution set out in this paper is developed subject to a set of assumptions that rule out this kind of behaviour (i.e., the analysis applies where there is incomplete melting of the solid as \( t \to \infty \)). In addition, the paper discusses the relationship between this approximation and the corresponding exact solution. As such, the problem analysed here is well posed for all \( t > 0 \) and this paper shows how the approximation may be made arbitrarily accurate by adding extra terms to the approximation to produce an exact analytic solution of the Stefan problem analysed herein.

Introduction
This paper outlines an analysis of a one phase Stefan problem for a superheated solid over a finite spatial interval through an application of homotopy analysis.2 This problem is ill posed under certain initial conditions where the energy in the solid phase exceeds the energy required to melt it. In these circumstances, the velocity of the moving boundary separating the liquid and solid phases shows finite time blow up; to avoid this situation, the approximate analytic solution set out in this paper is developed subject to a set of assumptions that rule out this kind of behaviour (i.e., where there is incomplete melting of the solid as \( t \to \infty \)) and ensures the problem is well posed (i.e., there is a unique solution that depends continuously on the initial data and exists for all \( t \geq 0 \)).

Various researchers have analysed this specific problem or variations of it using a range of techniques (including numerical and qualitative analysis), e.g., [1, 4, 5, 10] but have not, to the author’s knowledge, utilised the methods employed in this paper. A number of researchers have applied the homotopy analysis method to analyse single phase Stefan problems, e.g., [2, 6, 9] but have not, as far as the author is aware, considered its application to the specific problem analysed in this paper.

The remainder of this paper outlines the method including the characterisation of the solution for both the moving boundary and the underlying temperature profile as separate Taylor series along with the development of explicit expressions for the first two terms of both the Taylor series. Secondly, this paper briefly examines the issues of the existence, uniqueness, smoothness and convergence of the Taylor series solutions for the moving boundary and the underlying temperature profile as well as their relationship to the exact solution.

Nomenclature
\[ \alpha \] Stefan number where \( \alpha > 1 \)
\[ x \] space variable where \( 0 \leq x \leq s(t) \)
\[ t \] time variable where \( 0 \leq t < \infty \)
\[ u(x,t) \] temperature profile
\( s(t) \) position of the moving boundary
\( q \) embedding parameter
\( c_0 \) convergence control parameter

Outline of the Mathematical Problem
The mathematical problem analysed in this paper is as follows:

1. \( u(x,0) = 1 \) \( \quad (1) \)
2. \( u(x,t) = 0 \) \( \quad (2) \)
3. \( u(x,t) = 0 \) \( \quad (3) \)
4. \( u_s(t,0) = 0 \) \( \quad (4) \)
5. \( u_s(t) = \alpha s(t) \) \( \quad (5) \)
6. \( s(t) = 1 \) \( \quad (6) \)

where both \( u(x,t) \) and \( s(t) \) are unknown. The outer liquid phase (i.e., where \( x > s(t) \)) is taken to be at the melting temperature for \( t \geq 0 \) and, for convenience, the melting temperature is assumed to be equal to zero. Equation (5) is the Stefan condition which reflects the absorption of latent heat at the moving boundary as the superheated solid melts.

A transformation is required in order to reduce the problem in equations (1) – (6) to one involving fixed boundaries. The specific transformation involves the introduction of a new spatial variable, \( z \), defined such that \( z = x/s(t) \) and \( 0 \leq z \leq 1 \). The transformed boundary value problem (i.e., equations (1) – (6)) is as follows:

1. \( s(t)^2 u_z(z,t) = u_z(z,t) + z s_t(t) s_t(z) u_z(z,t) \) \( \quad (7) \)
2. \( u_z(0,t) = 0 \) \( \quad (8) \)
3. \( u_z(1,t) = \alpha s(t) s_t(t) \) \( \quad (9) \)
4. \( s(0) = 1 \) \( \quad (10) \)

Analytical Approximation to Equations (7) – (11) Using Homotopy Analysis
Consider now the following “generalised” PDE and associated boundary and initial conditions for the unknown functions for the temperature profile \( u(z,t;\varphi) \) and the position of the moving boundary \( s(t;\varphi) \):

\[ (1 - q_1) [u_z(z,t;\varphi) + z s_t(t;\varphi) s_t(z;\varphi) u_z(z,t;\varphi)] = c_0 \varphi [u_z(z,t;\varphi) + z s_t(t;\varphi) s_t(z;\varphi) u_z(z,t;\varphi)] - s(t;\varphi)^2 u_z(z,t;\varphi) \]

1 The corresponding supercooled single phase Stefan problem is mathematically equivalent to the problem analysed in this paper where \( u(x,t) \) is replaced by \( -u(x,t) \). See, for example, [4, 5].
2 For a detailed discussion of “homotopy analysis” including worked examples, see [7]. This paper provides a long list of applications of homotopy analysis to non-linear problems and sets out a comparison to both perturbation and non-perturbative methods.
3 Readers should note that the velocity of the moving boundary is unbounded at \( t = 0 \) but is finite for all \( t > 0 \).
The constant in equation (12), equal to s(t;0), is referred to as the “convergence control parameter” which is independent of changing q. By changing c₀, the rate of convergence of the Taylor series can be varied allowing the range of values of c₀ for which the Taylor series converges² to be identified.

Small Time Solution to Equations (1) – (6)

The starting point for the analysis is the development of an analytic solution applicable as \( t \to 0 \) (i.e., the “small time solution”). The small time solution to equations (1) – (6), which is denoted by \( f(x,t) \) for the temperature profile and \( s(t) \) for the moving boundary location, is as follows:

\[
\begin{align*}
    f(x,t) &= 1 - A \cdot \text{erfc}(1 - x/2t^{3/2}) \\
    s(t) &= 1 - 2A^2 
\end{align*}
\]

where \( A = 1/\text{erfc}(\lambda) \) and \( \lambda \) is the solution to the following transcendental equation: \( e^{\lambda^2} = \pi^2 \lambda \cdot \text{erfc}(\lambda) \).

Expressions for \( u(z,t;0) \) and \( s(t;0) \)

The next step in the analysis of equations (12) – (16) is to develop explicit expressions for the first term in each Taylor series for the moving boundary and the underlying temperature profile, namely \( u(z,t;0) \) and \( s(t;0) \). When \( q = 0 \), equations (12) – (16) are as follows²:

\[
\begin{align*}
    s(t;0)^2 \cdot u(z,t;0) &= s(t;0) \cdot u(z,t;0) + z \cdot s(t;0) \cdot s(t;0) \cdot u(z,t;0) \\
    u(1,t;0) &= 0 \text{ and } u(z;0;0) = 1 \\
    w(0,t;0) &= w(0,t;0) \\
    u(1,t;0) &= u(1,t;0) \\
    s(0;0) &= 1
\end{align*}
\]

While the homotopy analysis method allows for considerable flexibility in terms of the choice of \( u(z,t;0) \) and \( s(t;0) \), the choice made must match the initial conditions which apply to the problem being analysed (i.e., equations (1) – (6))². In the author’s view, the choice of \( u(z,t;0) \) and \( s(t;0) \) should also be a reasonable approximation to the actual solution over a wide range of values for \( z \) and \( t \) (including, of course, matching the solution and the corresponding Stefan condition exactly at \( t = 0 \)). Although the small time solution set out above is straightforward and matches the actual solution and the corresponding Stefan condition exactly at \( t = 0 \), the behaviour of the moving boundary for the small time solution is such that it becomes negative within a finite time (behaviour not exhibited by the moving boundary in the problem set out in equations (1) – (6)).

A better, but more complicated, choice for \( s(t;0) \) can be derived by developing a solution to a problem that approximates the underlying Stefan problem set out in equations (1) – (6) which: (i) embeds the small time solution within it; and (ii) approaches \( 0 \) from above as \( t \to \infty \) (i.e., for finite \( t \), \( 0 < s(t;0) < 1 \)). This can be achieved by replacing the function \( u(t) \) in equations (1) – (6) with the sum of the small time solution and an unknown function to be determined, \( e(x,t) \), and applying the boundary and initial conditions to yield the following boundary value problem for \( e(x,t) \):

\[
\begin{align*}
    e(x,t) &= e_{\infty}(x,t) \text{ where it is assumed}^9 \quad e(x,0) = 0 \\
    e(s(t),t) &= f(s(t),t) = A \cdot \text{erfc}(1 - s(t)/2t^{3/2}) - 1 \\
    e(0,t) &= f(0,t) = A \cdot e^{-1/4}(\pi)^{3/2} \\
    e(s(t),t) + f(s(t),t) &= A \cdot e^{-1/4}(\pi)^{3/2} - A \cdot e^{-1/4}(\pi)^{3/2} \alpha \cdot \text{erfc}(\lambda) \\
    e(x,t) &= e_{\infty}(x,t) \text{ as in the small time solution. Equation (28) can be solved using homotopy analysis through the following set up starting with the usual assumptions that the function } a(t;e) \text{ can be represented as a Taylor series in } q \text{ at the point } q = 0 \text{ and is convergent for } 0 \leq q \leq 1^{11}.
\end{align*}
\]

\[
\begin{align*}
    a(t;q) &= \sum_{n=0}^{\infty} \left[d^n a(t;0)/dq^n\right]q^n/\pi^{3/2} \\
    q \cdot A \cdot e^{-1/4}(\pi)^{3/2} &= A \cdot e^{-1/4}(\pi)^{3/2} \alpha \cdot a(t;q) \\
    a(t;q) &= A \cdot e^{-1/4}(\pi)^{3/2} \text{ as } t \to 0
\end{align*}
\]

When \( q = 1 \), the above ODE and associated initial condition (i.e., equations (30) – (31)) correspond to equation (28) and the small time behaviour of the moving boundary respectively and,

\[4\] Refer to [7] for a detailed discussion of the role of the convergence control parameter in the homotopy analysis method.

\[5\] The details of the small time solution set out above will be utilised in the development of the Taylor series for \( u(z,t;0) \) and \( s(t;0) \).

\[6\] This is sometimes referred to as the “Neumann solution”. Its variations of it are discussed at length in [3]. It matches equations (1) – (5), and (6) for all \( t \) but equation (4) only at \( t = 0 \).

\[9\] It is typical in problems where homotopy analysis is applied that the boundary and initial conditions (including the Stefan condition) are reflected in the first term of the Taylor series. In particular, at \( t = 0 \) both \( u(z,t;0) \) and \( s(t;0) \) must be an exact match with the solution \( u(z,t;0) \) and \( s(t;0) \).

\[10\] In other words, \( e(x,t) = A \cdot \text{erfc}(1 - x/2t^{3/2}) \).

\[11\] Put simply, the PDE for \( e(x,t) \) is approximated by its steady state counterpart by letting \( e_{\infty}(x,t) = e(x,0) = 0 \). This approach has been applied to other moving boundary problems. See, for example, [8] for an application dealing with a moving boundary problem in financial economics that applies a steady state approximation to the underlying governing PDE similar to the approach adopted here.

It emerges that the homotopy series generated from the above problem is convergent where the convergence control parameter is set equal to \( 1 \) and, therefore, the simplified approach to the problem outlined in equations (29) – (31) is justified.
accordingly, the series shown below is the solution to equations (24) – (28):

\[
    a(t; 1) = \sum_{n=0}^{\infty} \frac{[d^n a(t; 0)/dq^n]}{n!} \quad (32)
\]

The first two terms in the homotopy series for \( a(t; 1) \) are:

\[
    a(t; 0) = 1 - 2\lambda^{2/3} \quad (33)
\]

\[
    a(t; 0) = A t^{1/4} \int_{0}^{\infty} k^{1/2} e^{-t/k} q/(q^3) dq \quad (34)
\]

Figure 1 below shows the plot of the solution to the above approximate ODE for the moving boundary using a single step Euler method (with step size = 0.001) where \( \alpha = 2 \), \( \lambda = 0.432751599 \) and \( A = 1.8500116728 \) along with the corresponding one and two-term approximations of the homotopy series representation of \( a(t; 1) \):

\[
    \text{Figure 1: Approximate Boundary Position } a(t; 1) - \text{Euler Single Step v. HAM Approximations}
\]

Figure 1 indicates that, for the above parameters, the first two terms of the homotopy series for \( a(t; 1) \) are sufficient to ensure convergence (or nearly so) to the actual solution\(^{12} \) for \( t \leq 2 \).

In determining a suitable choice for \( u(z,t;0) \), it is easier to work in a different spatial variable, denoted in the remainder of this section by \( x \), rather than \( z \). The corresponding expression for \( u(z,t;0) \) (which is denoted by the function, \( w(x,t) \), in the remainder of this section) can be found by solving the following boundary value problem over: \(-\infty < x < a(t;1)\) and \(0 \leq t < \infty\):

\[
    w(x,t) = w_{x}(x,t) \quad (35)
\]

\[
    w(x,0) = 1 \quad (36)
\]

\[
    w(a(t;1),t) = 0 \quad (37)
\]

The substitution \( r = a(t;1) - x \) transforms equations (35) – (37) and the associated initial and boundary conditions into the following:

\[
    w(r,t) = w_{x}(r,t) - a(t;1)w(r,t) \text{ where } 0 \leq r < \infty \text{ and } 0 \leq t < \infty \quad (38)
\]

\[
    w(r,0) = 1 \quad (39)
\]

\[
    w(0,t) = 0 \quad (40)
\]

\( ^{12} \)\footnote{Based on a numerical analysis of the homotopy series for \( a(t;1) \) the first five terms are sufficient to ensure convergence for \( t \leq 15 \) for the same parameter values.}\)

\( ^{13} \)\footnote{Using \( a(t;1) \) to define the right hand limit of the spatial boundary for equations (35) – (37) ensures \( u(z,t;0) \) is consistent with the behaviour of \( a(t;1) \) while the change of spatial coordinates reflected in equations (35) – (37) has been made to facilitate the solution of equations (19) – (23). The solution of equations (19) – (23), \( u(z,t;0) \), is obtained by making the substitution \( x = z s(t;0) \) where \( s(t;0) = a(t;1) \) to the solution to equations (35) – (37) derived in this section.}

The term involving the first spatial derivative in equation (38) presents difficulties given that there is only a single left hand boundary condition (i.e., equation (40)) but it can also be solved through the following set up starting with the usual assumption that the function \( w(r,t;q) \) can be represented as a Taylor series in \( q \) about the point \( q = 0 \) and is convergent for \( 0 \leq q \leq 1 \):

\[
    w(r,t;q) = \sum_{n=0}^{\infty} [d^n w(r,t;0)/dq^n] q^n/n! \quad (41)
\]

\[
    w(r,t;q) = w_{0}(r,t;0) - q A(t;1) w_{2}(r,t;0) - (1 - q) A(t;0) w_{0}(r,t;0) \quad (42)
\]

\[
    w(0,t;q) = 0 \quad (43)
\]

\[
    w(0,t;q) = 0 \quad (44)
\]

When \( q = 1 \), the above PDE’s and associated boundary and initial conditions (i.e., equations (42) – (44)) correspond to the equations (38) – (40) and, accordingly, the series shown below is the solution equations (38) – (40):

\[
    w(r,t;1) = \sum_{n=0}^{\infty} [d^n w(r,t;0)/dq^n] q^n/n! \quad (45)
\]

The first term (i.e., \( w(r,t;0) \)) corresponds to the small time solution as \( t \to 0 \) because of the requirement that \( u(z,t;0) \) and \( s(t;0) \) match the behaviour of the exact solution as \( t \to 0 \):

\[
    w(r,t;0) = 1 - A \text{erfc}([1 - a(t;0) + a(t;1) - x]/2t^{1/2}) \quad (46)
\]

\[
    w(r,t;0) = 1 - A \text{erfc}([1 - a(t;0) + a(t;1) - x]/2t^{1/2}) \quad (47)
\]

\[
    w(r,t;0) = 1 - A \text{erfc}([1 - a(t;0) + a(t;1) - x]/2t^{1/2}) (48)
\]

The next term, \( w(r,t;0) \), is the solution to a standard heat transfer problem over \( 0 \leq r < \infty \) where \( w(r,t;0) = w_{0}(r,t;0) = 0 \) with a source term corresponding to the product of the time derivative of \(- a(t;1) + a(t;0) \), i.e., \(- a(t;1) - \lambda\lambda^{2} \), and the first spatial derivative of \( w(r,t;0) \) in the homotopy series for \( w(r,t;1) = u(x,t;0) \). The solution, keeping in mind that \( r = a(t;1) - x \), is:

\[
    w_{0}(r,t;0) = \left[ \int_{0}^{\infty} \int_{0}^{\infty} w_{0}(y,k;0) [a_{0}(k;1) + \lambda^{2} k^{2}] \right] [e^{-r^{2}/[4(t-k)^{2}]} - e^{-x^{2}/[4(t-k)^{2}]}]/(2\pi(t-k)^{5/2}) dy dk \quad (49)
\]

The coefficients for the remaining terms involve a series of standard heat transfer problems over \( 0 \leq r < \infty \) where \( d^{n} w(r,t;0)/dq^{n} = d^{n} w(r,t;0)/dq^{n} = 0 \) and a source term corresponding to the product of: (i) \(- n \); (ii) the time derivative of the known approximate boundary function, i.e., \( a(t;1) \); and (iii) the first spatial derivative of the preceding term in the homotopy series for \( w(r,t;1) \). The solution, keeping in mind that \( r = a(t;1) - x \) for the \( n^{th} \) term of the Taylor series for \( w(r,t;1) \) for \( n \geq 2 \) is:

\[
    d^{n} w(r,t;0)/dq^{n} = \left[ \int_{0}^{\infty} \int_{0}^{\infty} \left[ \int_{0}^{\infty} \int_{0}^{\infty} w_{0}(y,k;0)/dq^{n-1} \right] [a_{0}(k;1) \times [e^{-r^{2}/[4(t-k)^{2}]} - e^{-x^{2}/[4(t-k)^{2}]}]/(2\pi(t-k)^{5/2}) dy dk \quad (50)
\]

Insofar as the behaviour of \( w(r,t;1) \) is concerned, note that \( a(t;1) \) (which equals \( s(t;0) \)) is always greater than or equal to \( a(t;0) = 1 - 2\lambda \sqrt{t} \) and, as \( t \to \infty \), \( a(t;1) \) approaches a finite limit of \( 0 \). Since the small time solution and the corresponding fixed boundary problem (i.e., where \( s(t;1) = 1 \) for all \( t \)) for equations (1) – (6) are well posed for all \( t \), the corresponding PDE and boundary / initial conditions for \( w(r,t;1) \) will also be well posed.\(^{14} \) As noted in Footnote 13, the required function, \( u(z,t;0) \), is obtained by making the substitution \( x = z s(t;0) \) where \( s(t;0) = a(t;1) \).

\( ^{14} \)\footnote{The equivalence of equations (38) – (40) and equations (42) – (44) when \( q = 1 \) coupled with the fact that the problem for \( w(r,t) \) is well posed implies the smoothness and convergence of the Taylor series solution for \( w(r,t;1) \).}
Expressions for $u_q(z,t;0)$ and $s_q(t;0)$

The development of explicit expressions for the second term in each Taylor series for $u(z,t;1)$ and $s(t;1)$, namely $u_q(z,t;0)$ and $s_q(t;0)$, begins by differentiating equations (12) – (16) once with respect to $q$ and setting $q$ equal to zero to yield the following:

$$u_q(z,t;0) = 0$$  \hspace{1cm} (51)
$$u_q(0,t;0) = -u(0,0,t;0)$$  \hspace{1cm} (52)
$$u_q(1,t;0) = 0$$  \hspace{1cm} (53)
$$u_q(0,0,0,0) = 0$$  \hspace{1cm} (54)

The development of explicit expressions for the second term in each Taylor series for $u(z,t;1)$ is following general form (i.e., for higher order terms for the moving boundary position are of the form $u(z,t;1) = d\alpha s(t;0).s_q(t;0) - u(1,t;0) + \alpha s(t;0).s_q(t;0)$ for further research).

$$s_q(t;0) = 0$$  \hspace{1cm} (55)

The solution to equation (51) (which is a second order linear ODE) subject to the conditions set out in equations (52) – (53) is

as follows:

$$u(z,t;0) = u(0,t;0), [1 - z]$$  \hspace{1cm} (56)

Taking this result and substituting it into equation (54) yields a first order linear ODE for $s_q(t;0)$ subject to the condition in equation (55). This is easily solved given that $s(0,t;0)$, $s(t,0,0), u(0,t;0), u(1,t;0)$ and $u_q(1,t;0)$ are already known:

$$s(t;0) = s(t;0) - s(t;0) \int_0^1 s(k,t;0) [(u_1(k;0) - u_1(0,k;0))/(\alpha s(k;0)) - s_1(k;0)]dk + ...$$  \hspace{1cm} (57)

Accordingly, the two term approximation for the temperature profile in terms of the variables $z$ and $t$ is:

$$u(z,t;1) = u_1(t;0) + u_1(t;0), [1 - z] + ...$$  \hspace{1cm} (58)

and the two term approximation for the moving boundary is:

$$s(t;1) = s(t;0) + s(t;0) - u_1(0,k;0))/((\alpha s)(k;0)) - s_1(k;0)]dk + ...$$  \hspace{1cm} (59)

Higher Order Terms, Approximate and Exact Solutions

The steps outlined in the section immediately above can be repeated to allow for the derivation of higher order terms within each Taylor series expression for $u(z,t;1)$ and $s(t;1)$. The subsidiary PDE’s and associated boundary and initial conditions for all the higher order terms for the temperature profile are of the following general form (i.e., for $n \geq 2$):

$$d^n(d^n u(z,t;0)/dq^n)/dz^n = g_{q}(z,t,c)|_{q=0}$$  \hspace{1cm} (60)

where $g_{q}(z,t,c)|_{q=0}$ is: (i) the $n^{th}$ derivative with respect to $q$ evaluated at $q = 0$ of a suitably rearranged equation (12) excluding the second order spatial derivative; and (ii) calculated from the results for the previous terms for the Taylor series for each of $u(z,t;1)$ and $s(t;1)$ that have already been determined. The corresponding boundary conditions are $d^n u(z = 0,t;0)/dq^n = 0$ and $d^n u(z = 1,t;0)/dq^n = 0$ and the initial condition is $d^n u(z,t = 0)/dq^n = 0$. Furthermore, the subsidiary ODE’s for all the higher order terms for the moving boundary position are of the following general form (i.e., for $n \geq 2$): $d^n d^n u(z,t;0)/dq^n/\alpha s_q(t;0) = g_{q}(z,t,c)|_{q=0}$ evaluated at $q = 0$ and are subject to the initial condition $d^n s(t;0)/dq^n = 0$.

If the Taylor series for each of $u(z,t;1)$ and $s(t;1)$ is truncated at a finite number of terms, the result will be a fully analytic approximation of the solution to the original boundary problem (as represented by equations (7) – (11)). Subject to the comments in the following section regarding the convergence control parameter, $c_0$, this approximation may be made arbitrarily more accurate by the addition of extra terms in each Taylor series to produce an exact analytic solution. To recover the solution to the temperature profile in the original spatial variable, $x$, the substitution, $z = x(s(t;1))$ must be made.

Existence, Uniqueness, Smoothness and Convergence

As noted above, the one phase superheated Stefan problem analysed here is well posed where the Stefan number, $\alpha$, is $> 1$. This fact and the equivalence, when $q = 1$, of equations (12) – (16) and equations (7) – (11) collectively imply the smoothness and convergence of the Taylor series solutions for both $u(z,t;1)$ and $s(t;1)$ and the respective approximations of each; however, confirmation of this by an examination of the range of values for $c_j$ for which both Taylor series converge has been left as a topic for further research.

Concluding Remarks

This paper analyses the one phase superheated Stefan problem, where the Stefan number, $\alpha$, is greater than $1$ using, as far as the author is aware, a novel application of homotopy analysis. In particular, an explicit approximate solution has been developed and the relationship between this approximation and the corresponding exact solution presented. Subject to the comments in the previous section regarding the convergence control parameter, $c_0$, the approximation may be made arbitrarily accurate by adding extra terms to the approximation to produce an exact, albeit complicated, analytic solution.

References