**The Stefan Problem with Internal Heat Generation in Spherical Coordinates**

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**Abstract**

A weakly time-dependent equation for the evolution of the solid-liquid interface in spherical coordinates, driven by internal heat generation, is derived for constant surface temperature boundary conditions. The derivation comes by making an assumption that the interface moves slowly compared to the changes in the temperature so that the technique of separation of variables may be applied. Under this approximation, we can separate the nonhomogeneous heat diffusion equation into transient and steady-state terms, then integrate to get the temperature relations. With the temperature equations in hand, the derivative can be taken and inserted into the interface equation to get a first-order differential equation for the location of the solid-liquid interface as a function of time. The results are compared to a previously derived quasi-static solution and a numerical simulation generated using the method of catching of the front into a space grid node. This method allows for direct tracking of a moving boundary via the calculation of the time it takes to move from node to node in a discretized grid characteristic of classical finite difference methods. Plots of the interface evolution show excellent agreement between the three methods, especially for lower Stefan numbers. For the Stefan numbers *St* = 1.0 and 10.0, the weakly time-dependent solutions are in better agreement with the numerical results than the quasi-static solutions.

**Keywords**

Stefan problem

Internal heat generation

Sharp interface model

**Nomenclature**

An, Bn – series constants

C1, C2 – integration constants

cp – specific heat [J/kgK]

D – sphere diameter [m]

f,g – separation functions

g – gravitational constant [m/s2]

j0, n0 – spherical Bessel functions

k – thermal conductivity [W/mK]

– internal heat generation [W/m3]

r – radial variable

r0 – radius of sphere [m]

s – distance to interface [m]

t – time [sec]

T – temperature function [K]

Tm – melting temperature [K]

T0 – temperature at surface [K]

Greek

a – thermal diffusivity [m2/sec]

b – coefficient of thermal expansion [K-1]

Dhf – latent heat [J/kg]

h – nondimensional radius

f – initial temperature distribution

F – nondimensional temperature distribution

 – eigenvalues

n – kinematic viscosity [m2/s]

q – nondimensional temperature

t – nondimensional time

z – nondimensional distance to interface

Dimensionless Groups

 – internal heat generation, constant surface temperature conditions

St – Stefan number

Gr\* – modified Grashof number

Subscripts

liq – liquid phase

sol – solid phase

ss – quasi steady-state

tr – quasi transient

1. **Introduction**

The solid-liquid moving boundary problem was first studied by Lamé and Clapeyron [1] and Neumann (as described in Weber [2]), but widely published by Stefan [3], for whom the problem is now named. Since then, the problem has been well-analyzed and Rubenstein [4] assembled a number of solutions. Gupta [5] supplements the work of Rubenstein by including thermodynamical and metallurgical aspects of Stefan problems, phase change with supercooling, and superheating due to volumetric heat sources.

Stefan-like phase change in spherical coordinates has been extensively studied. Chutia [6] used Laplace transforms to find temperature profiles in perfectly insulated spheres melting under the influence of a point source within the material. Solutions of inward and outward solidification of saturated liquid in spherical containers were found by Huang and Shih [7] who used Landau’s transformation to immobilize the moving boundary, which normalized the position of the moving interface, replacing the time variable, the solution was then found by applying regular parameter perturbation techniques. Mori and Araki [8] presented a review of a number of methods to study heat conduction of moving boundaries. In the paper, integral methods, variational techniques, and quasi-static analyses, among others, were discussed. The quasi-static method was used to solve several spherical geometry phase change problems. Stewartson and Waechter [9] used asymptotic theory for small Stefan numbers to determine the temperature profiles of inward solidification of a sphere with initially molten material at the fusion temperature. Their results were compared with numerical studies. Later, Soward [10] provided a unified solution to the same problem discussed by Stewartson and Waechter. He found uniformly valid approximations up to the instant the material was completely frozen. Moore and Bayazitoglu [11] studied melting of a phase change material within a spherical enclosure. They determined interface positions and temperature profiles over a range of Stefan and Fourier numbers, and their mathematical model was confirmed by experimental results. Caldwell and Chan [12] studied spherical solidification using the enthalpy method and compared their results to the heat balance integral method, which is a front-tracking technique. They showed that the results compared very well except for small Stefan numbers. McCue, et al. [13], solved the classical Stefan problem for spheres using the method of matched asymptotic expansions in both the solid and liquid phases. They showed that the temperature in both phases depended algebraically on the inverse Stefan number on the first time scale, but at later times the two phases decoupled with the inner core only contributing exponentially small terms to the location of the solid-liquid interface. Reddy, et al. [14], employed a two-dimensional differential transform method to solve the one-dimensional problem for a solid sphere with time-dependent boundary temperature. A series solution was found for the temperature profiles in the melting or solidifying sphere.

One application of the spherical Stefan problem is in phase change materials (PCMs). Assis, et al.[15] numerically and experimentally studied melting of paraffin wax PCMs in spherical shells. Over a range of shell diameters and temperatures, they investigated convection, volumetric expansion of the fluid and close contact melting and found favorable agreement between the numerical and experimental results. Later, Assis, et al. [16] explored the solidification of PCMs in spherical shells and observed streamline patterns and void formations during the process. Experimental and numerical studies of n-octadecane were performed by Hosseinizadeh, et al. [17]. They found that the melting rate is high at the beginning of the melt process due to good contact between the hot shell and the PCM, then decreases as the PCM melts. Amin, et al. [18] demonstrated that determining an effective thermal conductivity can simplify the modeling process of spherical encapsulations of PCMs. The lattice Boltzmann method was shown by Lin, et al. [19] to be an advantageous method to simulate natural convection flow and heat transfer in encapsulated PCMs. Wang, et al. [20], use a lumped parameter analysis to study heat transfer in microparticles of phase change material. Their results were validated by both perturbation and finite-difference methods. Kenisarin, et al. [21], give a review of the latent heat storage method.

While the classical Stefan problem involves heat exchange with external sources, a variation of the problem arises when the phase change occurs due to volumetric heat generation within the material. This variation is not well explored, despite its many applications. Some of these applications are melting processes in both nuclear fuels [22,23] and planetary cores [24]. Among many sources, the internal heat generation can come from Joule heating and the by-product of nuclear reactions. Dhir, et al. [25] performed numerical studies of one-dimensional, non-homogeneous transient heat transfer in the liquid and solid regions of a volumetrically heated sphere with external cooling. They showed that depending on the relative magnitudes of the internally generated heat and external cooling, the molten fluid can solidify completely, solidify and remelt or have a solid crust with an inner molten core. Kumar, et al. [26], performed a computational fluid dynamics safety analysis of severe accidents in nuclear fast reactors, specifically molten fuel coolant interaction. They investigated the phase change problem in molten fuel droplets. One of the few relevant solutions to this problem is presented by Gibson who found that the non-homogenous spherical heat equation in an infinite spatial domain subject to a moving boundary may be solved exactly with separation of variables provided that the boundary moves as the square root of time [27].

When enforcing a finite domain, the Stefan problem can no longer be solved analytically through the classical technique of similarity solution. Therefore, it must be approached through approximation. As changing the dimensionless Stefan number modulates the speed of the interface, it is logical to use an approximation dependent on the rate of change of interface location. In classical electrodynamics, it is common to adopt a “quasi-static” approximation which states that one can use the equations for electrostatics when dealing with a system containing time-dependent charge and current densities, the primary condition of this approximation is that the system does not rapidly vary with time. Adapting this to the Stefan problem we introduce the weakly time-dependent approximation which, providing the interface is not moving too fast compared to the evolution of the temperature, the heat equation may be solved as if the interface is simply at a static location locally in time. With this treatment, the spherical non-homogenous heat equation is a linear partial differential equation. The portion of the equation affected by the change to spherical coordinates are the spatial derivatives which take the form a Laplacian in 3D space. The spherical Laplacian can be solved directly through separation of variables and has been analyzed thoroughly as such in both electrostatics [28], and atomic physics [29]. The Stefan problem in spherical coordinates with internal heat generation is a challenging problem with many important applications that cannot be solved directly through analytic techniques. The weakly time-dependent approximation affords the opportunity to recast this problem into a form easily analyzed with well understood classical techniques. The applications, the dearth of solutions, and the ability to recast the problem into a form which can be approached classically motivates our study of this problem.

1. **Problem Derivation**

We consider the problem of solid-liquid phase change in spherical coordinates with internal heat generation as shown in Figure 1. The outer surface of the sphere is held at a constant temperature, . We assume that there is no mushy zone and that at the solid-liquid interface, the melting temperature , remains constant. In addition, the internal heat generation is constant and remains the same in both phases. The material properties are assumed to be constant, uniform and equal in both phases. Finally, we neglect convection in the liquid phase since the homogeneity of physical properties between the phases yields zero velocity. This can be seen from the velocity expression for spherically symmetric systems given in Myers, et al. [30]. We provide an additional justification for this constraint in the results section. The solution technique outlined in this paper is similar to that of McCord, et al. [31], which was used to solve this problem in Cartesian coordinates. A related problem in cylindrical coordinates with fixed temperature and fixed heat flux at the outer boundary was studied by Barannyk, et al. [32,33], using similar methods.

The heat diffusion equation in spherical coordinates neglecting the polar and azimuthal angles and assuming that the thermal conductivity, *k*, is constant, is given by [34],



where the initial and boundary conditions in the liquid phase are,



and the initial and boundary conditions in the solid phase are given by,



Applying an energy balance between the solid and liquid phases yields the interface equation [35],



To reduce the number of parameters we nondimensionalize the governing equations with the following variables,



Inserting these variables into Eq. yields,



and the nondimensional initial and boundary conditions in the liquid phase become,



and in the solid phase,



Since the heat equation is nonhomogeneous for the temperature *q* in both phases, we wish to split each problem into transient and steady-state portions so that the transient part *q*tr will satisfy the homogeneous heat equation and homogeneous boundary conditions while the steady-state solution *q*ss will satisfy the nonhomogeneous steady-state heat equation and will absorb the nonhomogeneous boundary conditions. While this is a standard approach for solving nonhomogeneous partial differential equations on a given fixed domain [36], we note that the front, i.e., the right or left boundary of the liquid or solid phases, respectively, depends on time. To make this approach applicable for our problem, we assume that the interface position depends on time on a weaker time scale than the temperature in both phases. We call the interface weakly time-dependent. We start with,



Equation holds for both the liquid and solid phases. While we expect the transient solution to decay with time, the steady-state solution would still implicitly depend on time since the domain weakly depends on time. Strictly speaking we should use the term “pseudo steady-state” but for simplicity we will drop the term “pseudo” and use “steady-state” instead throughout the paper. Inserting Eq. into Eq. and splitting the terms gives the quasi steady-state heat equation in both phases,



On the liquid side, the boundary conditions are,



After integrating twice and applying the boundary conditions we find the quasi steady-state temperature profile in the liquid phase,



For the transient solution, we begin with,



The boundary conditions for the liquid phase are,



and in the solid phase,



To solve the homogeneous boundary value problem Eqs.- in the liquid phase, we can use separation of variables since the equations are linear, homogeneous [34,35], and the interface has been assumed to be nearly static,



Note that the boundary *z*(*t*) of the domain for *f* depends on *t*. Assuming that the interface *z*(*t*) varies slowly with time when compared to the temperature variations in either phase enables us to use the method of separation of variables to find the transient solution. After inserting and separating we find,



where *l*2 is a separation constant. The boundary conditions for *f* are,



Solving the eigenvalue problem in the liquid phase, we find, *f* in the form of spherical Bessel functions,



Abramowitz and Stegun [37] show some analytic properties that spherical Bessel functions possess, and *Mathematica* documentation [38] compiles these properties in the following form,



Using Eq. and the derivative boundary condition and the fact that  and  diverges, we find that . From there we use the second boundary condition for the liquid phase to obtain,



Since  gives a trivial solution, we use Eq. and see that for integers ,  equals zero for , which are eigenvalues of the problem. With this information we can use Eq. and the principle of linear superposition to find  in terms of the infinite series, and hence,



Here, the Fourier coefficients,  are found by taking advantage of  natural orthogonality,



as the spherical Bessel functions are orthogonal with respect to the weight function *h*2, according to Sturm-Liouville theory. Using the same methods as described above but applied to the solid phase, we find,



Knowing the temperature profiles, we can take the corresponding derivatives, evaluate them at the interface and insert into the dimensionless interface equation,



to get the first-order differential equation governing the motion of the interface, *z*,



1. **Numerical Technique: Method of Catching of the Front into a Space Grid Node**

The numerical method used to validate our weakly time-dependent solutions is the method of catching of the front into a space grid node as described by Samarskii and Vabishchevich [39]. This method uses a uniformly discretized spatial grid with the step size D*h* and a variable time step D*t*. The time step D*t* is determined in such a way that the interface shifts exactly by one spatial step D*h* during the time D*t*. The heat equation is solved by using an implicit four-point stencil finite difference scheme that is first-order in time and second-order in space accurate. Discretization of partial derivatives results in a tridiagonal system that is solved iteratively by the Thomas algorithm described in section 7.3.3 in Anderson, et al. [40]. The method terminates when the interface reaches steady-state. At the beginning of the simulations when there is only one phase, for example, solid, the heat equation is solved by a fixed time step D*t* =10-4. Once the temperature reaches the melting temperature and the interface is formed, the method of catching of the front into a space grid node defines the time step D*t*. A similar approach is used during the solidification process. As the Stefan number increases, the time step decreases as a result of a more intensive melting process. Crepeau, et al.[41], have utilized this method to solve the related problem in cylindrical coordinates.

To derive the relation for the time step, we begin with the interface relation, Eq. and rewrite it as,



Let *q*i,j be the temperature at the location *h*j and time *t*i. The dimensionless temperatures can then be expanded in a Taylor’s series centered at the interface location *h*i,



Here, *qi,j* is the temperature at the interface or the melting temperature, *qi,j+1* is the temperature in the solid phase, and *qi,j-1* is the temperature in the liquid phase. In order to maintain second-order accuracy, we use the nonhomogeneous form of the heat diffusion equation to solve for the second-order spatial derivative,



Evaluating the second-order partial derivative in Eq. at the interface and inserting into Eq. yields,



These results can then be inserted back into Eq. giving,



The numerical scheme was tested for convergence with a Stefan number of 1 and several levels of spatial and initial temporal discretization. The number of spatial nodes tested were 100, 400, and 1400 while the initial time step for solving the heat equation in one phase were 10-1, 10-3, 10-4, 10-6. The initial time step value did not have an observable effect on convergence. Figure 2 shows convergence results for spatial discretization. It can be seen that convergence is achieved at 700 nodes. The dashed black curve with 700 nodes is almost indistinguishable from the solid red curve obtained with 1400 nodes. The spatial resolution with 1400 nodes was used to generate the remaining figures.

1. **Results**

4.1 Convection Approximation

In this section we investigate whether it is reasonable to neglect convection by analyzing a modified Grashof number. Kee, et al. [42] defined the modified Grashof number, one that can be used for a heat generating fluid, as,



and showed that in a spherical shell, the critical value, when convection becomes important was,. He stated that these profiles were not too far from the conduction solutions. The relation between the modified Grashof number and the Stefan number is,



Using uranium oxide as the phase change material, the thermophysical properties can be found in [43]. For spheres with *D* = 2mm and , Table 1 gives the values of the modified Grashof number for various values of the Stefan number. For *St* = 0.01 and 0.1, the modified Grashof number is less than the critical value, and it is above the values for *St* = 1.0 and 10.0. However, at those higher values, the transient time required to reach steady-state is much smaller than for the smaller values. For *St* = 1 the system reaches steady-state in 1.75 seconds and for *St* = 10, steady-state is obtained in 0.64 seconds. Thus, for the values of the Stefan number and the internal heat generation considered in this paper, the effects of convection may be neglected.

4.2 Quasi-Static Results

A quasi-static approach used by Crepeau and Siahpush [44] assumed that the front depended on time but the temperature in each phase satisfied the steady-state heat equation. In comparison, the temperature in the weakly time-dependent case explicitly depends on time but decays exponentially. The approach described in [44] showed that the governing equations could be significantly simplified, and for a spherical geometry the motion of the phase change front is,



From Eq. the steady-state distance to the phase change front as a function of the non-dimensional heat generation is given by,



This relation shows that when , no melting occurs. It illustrates the balance the amount of heat generated internally and the heat transfer due to the constant temperature condition at the surface.

4.3 Series Solutions and Comparisons

We can now take the weakly time-dependent results of both solidification and melting obtained by solving Eq. and compare the curves to the numerical solutions generated by the method of catching of the front into a space grid node. The series terms in Eq. are truncated to 10-20 terms since the exponential terms decay quickly.

Equation is numerically integrated with the initial and boundary conditions given by,



The numerical integration of the initial condition begins at *z*0 = 0.99, since the result is undefined at *z*0 = 1. Figure 3 shows the time evolution of the interface position during solidification. The results are given for a nondimensional heat generation of  = 7, and Stefan numbers, *St* = 0.01, 0.1, 1.0 and 10.0. The value of  = 7 is chosen to ensure that there are both liquid and solid phases initially. The range of small to large values of the Stefan number represent the differences between the melting temperature and the fixed temperature at the outer boundary. For the two lowest Stefan numbers we see excellent agreement between the weakly time-dependent approximation, the quasi-static results of Eq. and the numerical solutions. However, as *St* increases, we observe a larger discrepancy between the three solutions. To better observe these differences, Fig. 4 gives an expanded view of Fig. 3 for values of *t* between 0 and 0.6. In Fig. 4 we see clearly that the weakly time-dependent approximation derived in this paper matches better the numerical results than the quasi-static solution for *St* = 1.0 and 10.0.

In Fig. 5, we see the temperature profiles during solidification for  = 7 and *St* = 0.1. The dashed lines denote the temperatures determined using the weakly time-dependent model and the solid lines represent the solution using the method of catching of the front into a space grid node. Note that the earliest profile has a change in slope at the interface where *q* = 1. As *t* increases, the system adjusts to the sudden change in the temperature and settles into steady-state with a parabolic temperature profile. The temperature profiles shown in Fig. 4 are similar in shape and behavior for values of  greater than 6 and various Stefan numbers.

For the time-dependent behavior of the interface during melting, we see Fig. 6. The initial and boundary conditions for melting are,



As solidification solutions above, the numerical integration of Eq. is done with  = 7 and *St*= 0.01, 0.1, 1.0 and 10.0. The comparisons between the weakly time-dependent and the method of catching of the front into a space grid node again show excellent agreement for the lower Stefan numbers. At the higher Stefan numbers, the solutions to Eq. reach steady-state faster than the numerical solutions. Figure 7 illustrates the behavior of these curves over the range 0 ≤ *t* ≤ 0.6. As seen in the solidification curves of Fig. 4, the weakly time-dependent solutions more closely match the numerical results.

Figure 8 shows the change in the temperature profiles over time for  = 7 and *St* = 0.1. As before, the temperatures determined from the weakly time-dependent solutions are denoted by the dashed lines and solid lines represent the numerical solutions. For early times, a region of the solid phase is predicted to achieve temperatures above the melting temperature. Recent work by Paulus [45] on a similar problem in cylindrical coordinates suggests that this phenomenon may be the result of neglecting the mushy zone in the model. The amount of heat stored within the mushy zone was related to the area underneath the curve of the overheated region. As time passed, the size of the mushy zone decreased, and with it, the amount of stored energy. This coincided with the dissipation of the overheated region, similar to what is observed in the current problem with spherical coordinates.

1. **Conclusions**

Using a weakly time-dependent approximation for the interface, a solution to the nonhomogeneous heat diffusion equation in spherical coordinates subject to Stefan boundary conditions was found. Through substitution of these weakly time-dependent solutions into the interface condition, a first-order, time-dependent, nonlinear ordinary differential equation with infinite series terms has been derived which approximately models the movement of the solid-liquid phase change front for both melting and solidification in the presence of internal heat generation under a constant temperature boundary conditions at the surface of a sphere. These weakly time-dependent solutions closely match the results of numerical solutions generated using the method of catching of the front into a space grid node, illustrating the validity of this approximation for low Stefan numbers. The weakly time-dependent solutions contain two infinite series terms which both have exponentially decaying in time terms, which rarely appear in typical differential equations. The corresponding temperature profiles exhibit a progression towards steady-state, parabolic profiles, characteristic in materials with internal heat generation.

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Table 1. Relation between the Stefan number and the modified Grashof number for uranium oxide and .

|  |  |
| --- | --- |
| St | Gr\* |
| 0.01 | 9,974 |
| 0.1 | 99,742 |
| 1.0 | 997,420 |
| 10.0 | 9,974,420 |

![Diagram

Description automatically generated]()

**Fig. 1.** Schematic of the phase change problem in spherical coordinates.

Graphical user interface, chart

Description automatically generated

**Fig. 2.** Numerical convergence study of solidification curves at *St* = 1 for various spatial nodes, k.

Chart

Description automatically generated

**Fig 3.** Comparison of the movement of the interface during solidification with  using the weakly time-dependent solution, Eq., the quasi-static solution, Eq. and the catching the front method for four different Stefan numbers. Note that for the lower Stefan numbers the numerical solutions of the interface takes longer to reach steady-state.

Chart

Description automatically generated

**Fig 4.** This figure is similar to that shown in Fig. 3 except the non-dimensional time ranges only from 0 ≤ t ≤ 0.6. This view shows that the series solution better matches the numerical solution at the higher values of the Stefan number.

Chart, diagram

Description automatically generated

**Fig. 5.** Temperature profiles during solidification,  = 7, *St* = 0.1.

Chart

Description automatically generated

**Fig 6.** Comparison of the movement of the interface during melting with  = 7 with the weakly time-dependent solution, Eq., the quasi-static solution, Eq. and the catching the front method for four different Stefan numbers. Again, for the lower Stefan numbers, the numerical solution of the interface takes longer to reach steady-state.

Chart

Description automatically generated

**Fig 7.** This figure is similar to that shown in Fig. 6 except the non-dimensional time ranges only from 0 ≤ t ≤ 0.6. This view shows that the series solution better matches the numerical solution at the higher values of the Stefan number.

Chart, diagram

Description automatically generated

**Fig. 8.** Temperature profiles as time increases during melting,  = 7, *St* = 0.1.