



# On the one-phase reduction of the Stefan problem with a variable phase change temperature<sup>☆</sup>



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## ABSTRACT

The one-phase reduction of the Stefan problem, where the phase change temperature is a variable, is analysed. It is shown that problems encountered in previous analyses may be traced back to an incorrectly formulated Stefan condition. Energy conserving reductions for Cartesian, cylindrically and spherically symmetric problems are presented and compared with solutions to the two-phase problem.

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## 1. Introduction

The Stefan problem where the phase change temperature is fixed is a classical example of a moving boundary problem and has been well-studied for more than 100 years. However, with the advent of a number of new technologies, the situation where a material's phase change temperature differs from the standard value is becoming increasingly important. For example, materials made from supercooled liquids are currently used in medicine, defence and aerospace equipment, electronics and sports [8,15]. The phase change temperature of supercooled liquids can vary because the liquid molecules have lower energy than when solidifying under normal circumstances and this affects their ability to move to the solid interface. Nanoparticles have a vast array of applications in medicine, environmental remediation, materials and energy [7]. A key factor in understanding the melting of nanoparticles is the large decrease in melt temperature with decreasing size, for example a 2 nm radius gold nanoparticle will melt at approximately 500 K below the bulk melt temperature [3]. In this case the high curvature of the melt interface leads to a large value for the surface tension induced stress which then reduces the melt temperature.

In order to simplify the mathematical description of the phase change process it is common to neglect one of the material phases, to produce the *one-phase Stefan problem*. When the melt temperature is the standard (or homogeneous) phase change temperature, here denoted  $T_m^*$ , then the one-phase problem is usually well-defined. However, when the phase change temperature is variable then difficulties arise (for example, energy may not be conserved) [6,13,19]. The issue with the one-phase formulation has been investigated by looking at

asymptotic limits of low thermal conductivity in the solid (compared to that in the liquid) [6] and large conductivity in the solid [13].

In this paper we will demonstrate that problems with the one-phase reduction may arise due to inconsistent assumptions concerning the temperature in the neglected phase. If the reduction is carried out consistently then there is no problem with the energy conservation. The one-phase reduction is invoked to simplify the analysis, and another standard simplification involves assuming constant thermal properties throughout the process. If we consider the ratio of the thermal conductivity of water to ice  $k = k_s/k_l \approx 4$  and the specific heat ratio  $c = c_s/c_l \approx 0.5$  then it is clear that this assumption can lead to significant errors. Consequently in the following we will work with different (constant) values in each phase. The density also varies, usually to a lesser extent than conductivity and specific heat [1]. If we include density change in our analysis then the governing equations become more complex, with the addition of advection and kinetic energy, see [9]. Consequently, to keep down the number of terms in the equations and so simplify the arguments we will focus on the situation where the density,  $\rho$ , is constant throughout the process. However, the arguments may be easily adapted to include it using the equations described in [9].

## 2. Governing equations for phase change

We will now derive the Stefan condition and heat equations for a one-dimensional Cartesian problem via an energy balance. For simplicity we examine the case of fixed density and so avoid the velocity terms caused by the shrinkage or expansion of the material.

The governing equations for the Stefan problem may be obtained from the energy conservation equation

$$\frac{\partial}{\partial t} [\rho l^*] = -\nabla \cdot \mathbf{q}^*, \quad (1)$$

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where  $\rho$  is the density,  $I^*$  the internal energy and the conductive heat flux  $\mathbf{q}^* = -k\nabla T^*$ . This simply states that internal energy varies with time due to heat movement through the boundary. The star superscript indicates dimensional variables. The internal energy/unit mass is

$$I_s^* = c_s(\theta^* - T_m^*) \quad I_l^* = c_l(T^* - T_m^*) + L_f, \quad (2)$$

where subscripts  $s$  and  $l$  denote solid and liquid, and  $\theta^*$  and  $T^*$  denote the respective temperatures. The heat equations may be obtained from the energy balance by simply substituting for  $I^*$  and  $\mathbf{q}^*$  in Eq. (1)

$$\frac{\partial}{\partial t^*} [\rho c_s(\theta^* - T_m^*)] = \frac{\partial}{\partial x} \left( k_s \frac{\partial \theta^*}{\partial x^*} \right) \quad (3)$$

$$\frac{\partial}{\partial t^*} [\rho c_l(T^* - T_m^*) + L_f] = \frac{\partial}{\partial x} \left( k_l \frac{\partial T^*}{\partial x^*} \right). \quad (4)$$

Noting that all thermal properties and  $T_m^*$  are constant within each phase leads to the familiar form

$$\rho c_s \frac{\partial \theta^*}{\partial t^*} = k_s \frac{\partial^2 \theta^*}{\partial x^{*2}} \quad \rho c_l \frac{\partial T^*}{\partial t^*} = k_l \frac{\partial^2 T^*}{\partial x^{*2}}. \quad (5)$$

The Stefan condition may also be obtained from the conservation Eq. (1) via the Rankine–Hugoniot condition

$$\frac{\partial f}{\partial t} + \nabla \cdot \mathbf{g} = 0 \quad \Rightarrow \quad [f]^\pm s_t = [\mathbf{g} \cdot \mathbf{n}]^\pm, \quad (6)$$

where  $\mathbf{n}$  is the unit normal (in this case it is simply  $\hat{\mathbf{x}}$ ) and  $f$  and  $\mathbf{g}$  are functions evaluated on either side of the discontinuity,  $x^* = s^*(t^*)$ . For the case where a fluid initially occupying  $x^* \geq 0$  is solidified from the boundary  $x^* = 0$  we take the  $+$  superscript to indicate fluid,  $x^* > s^*$ , and  $-$  to indicate solid,  $x^* < s^*$ . Comparing the energy balance (Eq. (1)) to the Rankine–Hugoniot condition shows that  $f = \rho I^*$ ,  $\mathbf{g} = \mathbf{q}^*$ , and the Stefan condition follows from the second of Eq. (6)

$$\rho \left[ c_l(T^*(s^*, t^*) - T_m^*) + L_f \right] - c_s(\theta^*(s^*, t^*) - T_m^*) s_t^* = -k_l \frac{\partial T^*}{\partial x^*} \Big|_{x^*=s^*} + k_s \frac{\partial \theta^*}{\partial x^*} \Big|_{x^*=s^*}. \quad (7)$$

The spherically and cylindrically symmetric versions are obtained from

$$\frac{\partial}{\partial t^*} [\rho c_s(\theta^* - T_m^*)] = \nabla \cdot (k_s \nabla \theta^*) \quad \frac{\partial}{\partial t^*} [\rho c_l(T^* - T_m^*) + L_f] = \nabla \cdot (k_l \nabla T^*) \quad (8)$$

$$\rho \left[ c_l(T^*(s^*, t^*) - T_m^*) + L_f \right] - c_s(\theta^*(s^*, t^*) - T_m^*) s_t^* = -k_l \frac{\partial T^*}{\partial r^*} \Big|_{r^*=R^*} + k_s \frac{\partial \theta^*}{\partial r^*} \Big|_{r^*=R^*}, \quad (9)$$

where the phase change front is now located at  $r^* = R^*$  and temperatures depend on  $r^*$ ,  $t^*$ .

### 3. Stefan problem with melting point depression

The standard two-phase, one-dimensional Cartesian Stefan problem with melting point depression is typically specified by heat equations in the solid and liquid phases and the following Stefan condition

$$\rho \left[ (c_l - c_s)(T_l^*(t) - T_m^*) + L_f \right] s_t^* = -k_l \frac{\partial T^*}{\partial x^*} \Big|_{x^*=s^*} + k_s \frac{\partial \theta^*}{\partial x^*} \Big|_{x^*=s^*}, \quad (10)$$

where  $T_l^*(t)$  is the interface temperature, see [1,4,6,7,20,13,18,19]. The variation of  $T_l^*(t)$  may be described by a number of relations. For

supercooling models an exponential relation between  $T_l^*$  and  $s_t^*$  holds. This is frequently linearised for small departures from the bulk phase change temperature so  $T_l^* - T_m^* \propto s_t^*$  [5,8]. With high curvature some form of Gibbs–Thomson relation is typically used [7,8].

In order to follow previous asymptotic reductions we will now formulate the non-dimensional version of the problem via the following scales,

$$\theta = \frac{\theta^* - T_m^*}{\Delta T^*} \quad T = \frac{T^* - T_m^*}{\Delta T^*} \quad x = \frac{x^*}{L} \quad t = \frac{t^*}{\tau} \quad (11)$$

where  $\Delta T^*$  is a temperature scale and  $\tau$  the time-scale. In the Stefan problem without melting point depression the length-scale  $L$  may be unknown. With melting point depression  $L$  may be specified according to the equation governing the phase change temperature. Choosing the time-scale for heat flow in the liquid,  $\tau = \rho c_l L^2 / k_l$ , the heat equations now reduce to

$$\frac{\partial \theta}{\partial t} = \frac{k}{c} \frac{\partial^2 \theta}{\partial x^2} \quad \frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2}. \quad (12)$$

The Stefan condition becomes

$$[(1-c)T_l(t) + \beta]s_t = -\frac{\partial T}{\partial x} \Big|_{x=s(t)} + k \frac{\partial \theta}{\partial x} \Big|_{x=s(t)}, \quad (13)$$

where  $\beta = L_f / (c_l \Delta T)$ ,  $k = k_s / k_l$ ,  $c = c_s / c_l$ .

These equations are often simplified via a one-phase approximation. Say, for example we neglect the solid phase, then we only need to solve the heat equation in the liquid while the Stefan condition becomes

$$[(1-c)T_l(t) + \beta]s_t = -\frac{\partial T}{\partial x} \Big|_{x=s}. \quad (14)$$

The most familiar form of the Stefan condition may be obtained by neglecting melting point depression, so setting  $T_l = 0$  ( $T_l^* = T_m^*$ ) in Eq. (14). Eq. (14) may also be obtained by choosing  $\theta(x, t)$  to be constant or a function of time. Wu et al. [19] discuss papers where the solid phase is simply ignored, see [17,21]. Many authors assume  $\theta(x, t) = T_l(t)$  [4,5, 10] or alternatively  $\theta(x, t) = 0$  [11]. The first choice has the problem that it does not satisfy the heat equation, while the second does not satisfy the interface boundary condition. A more formal way to reduce the system is to let  $k = 0$ , so the liquid conducts heat infinitely faster than the solid. Then the solid temperature is removed from the Stefan condition while the heat equation in the solid becomes  $\theta_t = 0$  and so  $\theta$  may be set as a function of  $x$ : in practice it is usually taken as 0 or the initial temperature  $\theta(x, 0) = \theta_0$ .

Evans and King [6] discuss a number of papers where the Stefan problem is incorrectly formulated and discuss in detail the approximation where Eq. (14) with  $T_l = 0$  is used in conjunction with melting point depression. They point out that this form is popular since it arises in the case without supercooling and is accurate in the limit of large Stefan number. It may also be derived from Eq. (13) with the common assumption that  $c = 1$  and then choosing  $k = 0$  to remove the contribution of the solid phase. Wu et al. [19] discuss similar reductions in the context of spherical nanoparticle melting. They state that when the initial temperature is different to the phase change temperature then the one-phase limit may only be derived under the assumption  $k \ll 0$ .

In [6] it is stated that the supercooled Stefan problem using Eq. (14) with  $T_l = 0$  does not conserve energy. To understand this statement consider the total internal energy in the system

$$E = \int_0^s c\theta \, dx + \int_s^\infty (T + \beta) dx, \quad (15)$$

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