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Mathematical modelling of phase change with a flowing thin film

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Summary. This paper concerns the practical applications and modelling of Stefan problems with a flowing thin liquid layer. The modelling will be discussed in the context of two practically important scenarios, Leidenfrost (when a liquid droplet floats above a hot surface) and contact melting. The governing equations will be derived and then reduced to a more tractable system. Along the way we will introduce an accurate variant of the Heat Balance Integral Method, which allows us to approximate the solution to the Stefan problem on a finite domain. In both cases excellent agreement between the model results and experimental data will be demonstrated.

1 Introduction

Phase change in the presence of a flowing liquid layer occurs in a multitude of situations. For example, ice growth from a thin moving water layer has been studied in the context of aircraft icing and ice accretion on wind turbines and power transmission equipment. Analogous problems also arise in the modelling of lava flow, atherosclerosis (plaque build-up on artery walls) and wax deposition in oil pipelines, see [5, 10, 11] for example.

In this paper we focus on two particular, related problems, namely Leidenfrost and contact melting. Leidenfrost occurs when a liquid is placed on a surface which is above the phase change temperature. The heat flux from the surface causes the fluid to evaporate and so the fluid floats on a vapour layer. The vapour layer is constantly being renewed through continued evaporation whilst it is also being squeezed out due to the fluids weight. Contact melting is a similar process in that it involves a melting solid on a hot surface. This process is exploited industrially as a means of energy storage.

The mathematical modelling of this class of problem involves solving the heat equation in solid, liquid or vapour layers, where the boundary position is determined through a Stefan condition and force balance. Since the Stefan problem only has an exact solution in highly idealised situations we begin our analysis by describing an approximate method for the one-dimensional Stefan problem. The accuracy of this method is then compared to the standard large Stefan number perturbation solution. It is then used in the solution of the contact melting problem. Finally, we employ a similar analysis on the Leidenfrost model.

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2 Heat balance integral method and Stefan problems

Consider

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \qquad 0 < x < s(t) \tag{1}$$

$$u(0,t) = 1, \qquad u(s,t) = 0, \qquad \beta \frac{ds}{dt} = -\left.\frac{\partial u}{\partial x}\right|_{x=s}, \qquad s(0) = 0. \tag{2}$$

This is scaled in such a way that the only remaining parameter is the Stefan number $\beta = L_m/(c_p\ \Delta u)$, where L_m is the latent heat of melting, c_p the specific heat capacity and Δu the temperature variation. The exact solution is

$$u = 1 - \operatorname{erfc}\left(\frac{x}{2\sqrt{t}}\right)(\operatorname{erf}(\alpha))^{-1}, \qquad s(t) = 2\alpha\sqrt{t}, \tag{3}$$

where α satisfies the transcendental equation $\sqrt{\pi}\beta\alpha\,\operatorname{erf}(\alpha)e^{\alpha^2} = 1$.

The large Stefan number ($\beta \gg 1$) solution may be obtained by carrying out a perturbation analysis after re-scaling time and using a boundary fixing transformation to give

$$s = \sqrt{\frac{2t}{\beta}}\left(1 - \frac{1}{6\beta} + \frac{23}{360\beta^2} + \cdots\right). \tag{4}$$

Of course this must coincide with the large β expansion of the exact solution. Further details may be found in [4] for example.

An alternative approach to find an approximate solution to this problem is via a Heat Balance Integral Method (HBIM). The basic HBIM involves approximating the temperature by a function of the form

$$u = a\left(1 - \frac{x}{s}\right) + (1-a)\left(1 - \frac{x}{s}\right)^m. \tag{5}$$

This satisfies the boundary conditions at $x = 0, s$. The HBIM then proceeds by integrating the heat equation over $x \in [0,s]$, with u specified by the above polynomial. This leads to and ODE for s. The value of a is also unknown and so the Stefan condition is invoked to provide a second equation. The simple one-phase analysis is described in [6]. In the original HBIM of Goodman [3] the exponent m was set to 2 or 3. However, recently Myers [14] has developed a method whereby m is chosen through minimising the error

$$E_n = \int_0^s (u_t - u_{xx})^2\, dx. \tag{6}$$

This method ensures that the HBIM approach is accurate and, for certain situations such as a constant flux boundary condition, it can reduce the error by orders of magnitude from the $n = 2$ solution [13,14]. An alternative to the HBIM is the RIM [7] (or integral method by integration [4]) which simply involves integrating the heat equation twice. Mitchell & Myers [8] propose a different method to reduce the error by employing both the HBIM and RIM to provide a further equation to determine m. This is then termed the Combined Integral Method (CIM). Following the HBIM or RIM, with a minimised error, or the CIM, we may easily determine an analytical expression for $s \propto \sqrt{t}$, which may then be compared to the exact solution. For large Stefan number we may also expand the result and compare with the perturbation solution. For example, with the CIM we obtain

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$$s = \sqrt{\frac{2t}{\beta}}\left(1 - \frac{1}{6\beta} + \frac{149}{2520\beta^2} + \cdots\right). \tag{7}$$

This differs from the perturbation solution at 2nd order by 7.4%. However, unlike the perturbation solution the HBIM solution is not only valid at large β and so can provide a wider range for the validity of the approximate solution. In [8] it is shown that the CIM result is more accurate than the 2nd order perturbation for $\beta < 7$. For water and paraffin wax typically $\beta \in [1,10]$, so for physically realistic problems the heat balance methods are more accurate.

3 Contact Melting

Contact melting is a process frequently exploited as a method of latent heat storage in the construction industry. However, perhaps the most familiar example occurs when a block of ice is placed on a warm surface. The ice melts to form a layer of water between the ice and surface. This water is squeezed out due to the weight of the ice, however as the ice approaches the surface the melting process speeds up and so a balance forms between melting and squeezing.

Now consider a two-dimensional phase change problem, where a block of initial thickness H and width $2L$ is placed on a warm substrate. The mathematical model must deal with (at least) two distinct stages. When the phase change material is placed on the warm surface there is an initial stage where the PCM heats up to the melt temperature. Subsequently melting occurs and heat propagates into the solid. The most general description is given by

$$\eta \frac{\partial^2 u}{\partial z^2} = \frac{\partial p}{\partial x}, \qquad \frac{\partial p}{\partial z} = 0, \qquad \frac{\partial u}{\partial x} + \frac{\partial w}{\partial z} = 0, \tag{8}$$

$$\frac{\partial^2 T}{\partial z^2} = 0, \qquad \frac{\partial \theta}{\partial t} = \kappa_s \frac{\partial^2 \theta}{\partial z^2}, \tag{9}$$

$$\rho_s L_m \frac{\mathrm{d}h_m}{\mathrm{d}t} = k_s \frac{\partial \theta}{\partial z}\bigg|_{z=h} - k_l \frac{\partial T}{\partial z}\bigg|_{z=h}, \qquad 2\rho_s L\left[H_0 - h_m(t)\right] g = \int_{-L}^{L} p \, \mathrm{d}x. \tag{10}$$

This system represents: equation (8) fluid flow in the melt layer, subject to the lubrication approximation; equation (9) heat flow in the liquid and solid (where only the T_{zz} term remains since the liquid layer is thin); equation (10a) the Stefan condition; equation (10b) a mass balance, where the weight of the block is balanced by the fluid pressure. An important point to note is that the observed film thickness of the liquid layer, h, is different to the height of melted liquid, h_m, due to the squeeze effect, hence the Stefan condition involves h_m but the derivatives are evaluated at h. Further details may be found in [12].

In the pre-melt stage the temperature profile in the solid can be found exactly, or approximated using the HBIM. In the melt stage the temperature in the liquid layer is obviously approximately linear, whilst in the solid we must solve the Stefan problem over a finite domain and so require the HBIM. The problem reduces to solving 3 equations of the form

$$3\frac{\mathrm{d}h}{\mathrm{d}t} + \frac{\mathrm{d}\delta}{\mathrm{d}t} = \frac{c_0}{\delta - h} \qquad \frac{\mathrm{d}h_m}{\mathrm{d}t} = \frac{c_1}{\delta - h} + \frac{c_2}{1 + c_3 h} \tag{11}$$

together with the mass balance (10) to determine the unknowns h, h_m, δ. The terms c_i are constants that depend on the thermal properties of the materials. The term δ is key to HBIM analyses. It is termed the heat penetration depth and represents a notional distance over which the heat penetrates into the solid.

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The numerical solution of the three differential equations is straightforward. In Figure 1 we compare the results of the current theory with experiments from [9]. These experiments involved the melting of a wide (and so quasi-two-dimensional) block of n-octadecane, with initial height 5.5cm. The sides and top were insulated, hence the experiments are ideal for comparison with our theory. Our model uses a finite heat transfer coefficient, also shown are results with an infinite heat transfer coefficient, the analytical expression from [9] and a standard quasi-steady solution (see [1]). Obviously the current theory provides excellent agreement with experiment.

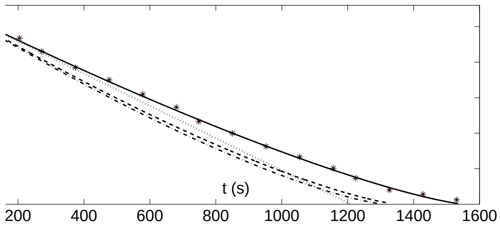

Fig. 1. Comparison of height $H(t)$ with experiment (asterisks) for the current theory with a) HTC = 7000 W/m^2 (solid line), b) infinite HTC (dashed line), c) theory of [9] (dash-dot line) and d) quasi-steady solution (dotted).

4 Leidenfrost

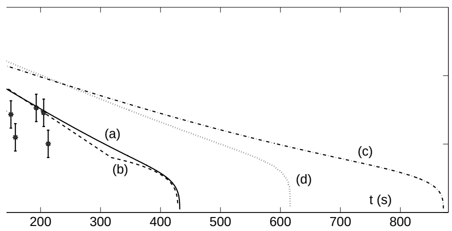

Fig. 2. Vapour layer thickness as a function of time and comparison with Biance [2] measurements, a) numerical solution and b) approximate solution with HTC 900W/m^{2}K, and evaporation at the top surface , c) numerical solution with HTC 900W/m^{2}K and no evaporation at the top, d) numerical solution with infinite HTC and no evaporation at the top

The Leidenfrost phenomenon occurs when a liquid drop is placed on a surface which is above the vaporisation temperature. This causes the droplet to float on a layer of vapour. Obviously this problem is analogous to the contact melting one, with the main differences being that the droplet shape constantly changes (large droplets are disk-like whilst small droplets are closer to hemispherical) and the temperature in the liquid is approximately constant.

The governing equations are similar to those of the contact melting problem, with two important differences. Firstly, since the liquid is free to circulate we assume it is everywhere at the liquidus and so do not solve a heat equation there. The vapour forms a thin film and so the temperature is approximately linear. Secondly, we must also incorporate the Young-Laplace equation, which balances gravity and surface tension, to describe the droplet shape.

In this case the numerical solution reduces to solving the Stefan condition coupled to the mass balance and the Young-Laplace equation. Comparison of numerical solutions showed that an important effect, neglected in previous studies, is evaporation from the upper surface of the droplet. Without this effect the droplet will never evaporate sufficiently rapidly, even if we take an infinite heat transfer coefficient at the base.

In Figure 2 we show a comparison of model solutions to experimental results for the height of the vapour layer thickness (taken from [2]). The curves represent the numerical solution of the governing equations, an approximate analytical solution and then solutions with different heat transfer and evaporation rates. In this case the experimental results are rather trickier to calculate due to the droplet motion and narrow gap width, however, it is clear that the current theory again provides excellent agreement.

5 Conclusion

Clearly for both problems the reduction of the full set of governing equations (Navier-Stokes, heat equations and a Stefan condition) to a set of three first order ordinary differential equations significantly simplified the problem. Comparison with experimental data clearly demonstrated the accuracy of the models. Although, when the Leidenfrost model was applied to very small droplets the agreement was not so good, presumably due to the fact that the vapour layer is no longer confined to a thin region.

Key to the solution of these problems is the HBIM. Previously this method could be quite inaccurate. However recent developments and variants have significantly improved the accuracy, to the extent that for physically realistic parameter values it provides more accurate solutions than the second order perturbation expansion.

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