Journal of Computational and Applied Mathematics 276 (2015) 98–109

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

On the numerical solution of a Stefan problem with finite extinction time

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ARTICLE INFO

Article history:
Received 16 April 2014
Received in revised form 13 August 2014

Keywords:
Evaporation
Stefan problem
Keller box scheme
Extinction time

ABSTRACT

In many phase-change problems of practical interest, it is important to know when a phase is depleted, a quantity referred to as the extinction time; however, there are no numerical schemes that are able to compute this with any degree of rigour or formal accuracy. In this paper, we develop such a scheme for the one-dimensional time-dependent problem of an evaporating spherical droplet. The Keller box finite-difference scheme is used, in tandem with the so-called boundary immobilization method. An important component of the work is the careful use of variable transformations that must be built into the numerical algorithm in order to preserve second-order accuracy in both time and space, in particular as regards resolving a square-root singularity in the droplet radius as the extinction time is approached.

1. Introduction

The problem of the transient heating of an evaporating spherical droplet, as considered recently in [1], constitutes a phase-change (Stefan) problem that is posed on a domain initially of finite extent which vanishes after a finite time, termed hereafter as the extinction time. Whilst this situation is prevalent for evaporating drops [2], it is not the only practical situation in which this occurs: other examples are the melting or freezing of spheres [3–8], the solidification of metal in continuous casting processes [9–13], the region containing oxygen in biological tissue [14–17], and in the course of drug diffusion through polymeric spheres [18].

Whilst there exist many numerical methods for solving Stefan problems in general, there are none which are able to compute the extinction time with any level of rigour or accuracy. Indeed, whilst Mitchell et al. [1] went as far as to determine analytically that the radius of the droplet, R, would decrease with time, t, as

$$R(t) \sim (t_e - t)^{1/2}, \tag{1}$$

where t_e is the extinction time, they stopped their computations before R actually reached zero; this is also typically the case elsewhere [8,19].

Thus, the purpose of this paper is to devise a numerical scheme that is not only able to solve the Stefan problem accurately for $t < t_e$, but is also able to calculate t_e and to recover extinction behaviour of the moving boundary; in line with our recent

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http://dx.doi.org/10.1016/j.cam.2014.08.023
0377-0427/

work on the use of the boundary immobilization method in tandem with the Keller box scheme for the numerical solution of Stefan problems [20–23], we once again seek to ensure that the temperature, its spatial derivative, $R(t)$ and t_e are all second-order accurate. To illustrate the idea, we will use the problem considered in [1] as an example.

The layout of this paper is as follows. In Section 2, we briefly describe the relevant equations given in [1], whereas in Section 3 we provide the auxiliary analysis that is necessary to improve the earlier numerical scheme. In Section 4, we present and discuss the new results, and conclusions are drawn in Section 5.

2. Mathematical formulation

2.1. Governing equations

A liquid fuel droplet, initially of radius R_0 and at temperature T_0, is immersed into a homogeneous hot gas at constant temperature, T_g, that is greater than T_0. Heat transfer within the droplet is assumed to occur by conduction alone; the effects of thermal radiation are ignored here, an assumption justified and discussed in more detail in [2]. At the surface of the droplet, evaporation and convection are assumed respectively to be the dominant cooling and heating mechanisms, and the radius of the droplet, $R(t)$, is expected to decrease with time t, if the effects of thermal swelling are ignored.

More details of the derivation are given in [1] but, for completeness, we summarize them now. The droplet temperature, $T(r, t)$, is governed by the heat conduction equation in spherical coordinates,

$$\rho_l c_l \frac{\partial T}{\partial t} = \frac{k_l}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial T}{\partial r}\right), \quad 0 \le r < R(t),\ 0 \le t \le t_e, \tag{2}$$

where r is the distance from the centre of the droplet, c_l is the specific heat capacity of the liquid, k_l is its thermal conductivity and ρ_l its density. At this stage we introduce $\kappa = k_l/\rho_l c_l$ as the thermal diffusivity of the liquid fuel, for brevity. In addition, t_e is the time taken for the droplet to evaporate completely.

For boundary conditions, we have, at $r = 0$,

$$\frac{\partial T}{\partial r} = 0, \tag{3}$$

which expresses spherical symmetry and ensures that the temperature is bounded at $r = 0$.

At $r = R(t)$, we equate the conductive heat flux to the heat lost due to convective and evaporative cooling. This gives

$$k_l \frac{\partial T}{\partial r} + h(T - T_g) = \rho_l L \dot{R}(t), \tag{4}$$

where L is the specific heat of evaporation, and $h(t)$ is the convection heat transfer coefficient, defined by $h(t) = k_g/R(t)$, with k_g as the thermal conductivity of the gas. Note that the dot denotes differentiation with respect to t.

The moving boundary at $r = R(t)$ is controlled by fuel vapour diffusion from the droplet surface, and satisfies [24]

$$\dot{R} = -\frac{k_g \ln(1 + B_M)}{\rho_l c_g R}, \tag{5}$$

where c_g is the specific heat capacity of the gas, $B_M = \mathcal{Y}_{fs}/(1 - \mathcal{Y}_{fs})$ is the Spalding mass transfer number, and $\mathcal{Y}_{fs}$ is the mass fraction of fuel vapour near the droplet surface:

$$\mathcal{Y}_{fs} = \left[1 + \left(\frac{P_g}{P_{fs}} - 1\right)\frac{M_g}{M_f}\right]^{-1}. \tag{6}$$

Here, P_g and P_{fs} are the ambient gas pressure and the pressure of saturated fuel vapour near the surface of the droplet, respectively, and M_g and M_f are the molar masses of the gas, here assumed to be air and fuel. The variable P_{fs} is calculated from the Clasius–Clapeyron equation as

$$P_{fs} = \exp\left[a - \frac{b}{T_s - 43}\right], \tag{7}$$

where a and b are constants to be given for specific fuels and $T_s = T(R(t), t)$ is the surface temperature of the fuel droplet.

Finally, the initial conditions are

$$T(r, 0) = T_0, \qquad R(0) = R_0, \tag{8}$$

where T_0 and R_0 are constant.

We must solve the coupled equations (2) and (5) to determine $T(r, t)$ and $R(t)$, using the initial and boundary conditions specified above, noting that P_{fs} involves the unknown surface temperature T_s.