

NOTE

Parameterized Solution of One-Dimensional Thermal Diffusion with a Heat Source and a Moving Boundary*

In this note we show how to construct a simple and accurate ordinary differential equation (ODE) approximation to a one-dimensional, partial differential, thermal diffusion equation (PDE), where there is both a heat source and a moving boundary. The physical problem we use to illustrate the method is that of thermal diffusion and evaporation of a water drop irradiated by laser light that it absorbs, in this case the 10.6 μm emission of a CO_2 laser. The water drop heats internally and evaporates at the surface. The problem is to determine the internal drop temperature profile $T(r, t)$ and radius $r_d(t)$ as time evolves, where r is the radial coordinate in spherical geometry. The problem is spherically symmetric, since we assume that the water drop absorbs laser power independently of spatial position within the drop (so-called volumetric absorption). This is a good approximation if the drop radius is less than the wavelength of the laser light as is the case for most cloud water drops with respect to the CO_2 laser wavelength. Although we consider spherical geometry, the ideas apply to other geometries, for example, cylindrical geometry. We begin by describing the model and show how it can be solved by a conventional finite difference method. Then a parameterized form of the model is presented that is much simpler. It is the construction and solution of this model that is the main subject of this paper.

The equations defining the problem are thermal diffusion within the drop given as

$$\rho_w c_w \frac{\partial T}{\partial t} = p_l + \frac{\kappa_w}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial T}{\partial r}, \quad (1)$$

and conservation of energy at the drop surface

$$\begin{aligned} \frac{4\pi}{3} \rho_w L \frac{dr_d^3}{dt} - 4\pi \kappa_a r_d [T(r_d) - T_a] \\ = 4\pi \kappa_w r_d^2 \left. \frac{\partial T}{\partial r} \right|_{r_d}, \end{aligned} \quad (2)$$

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where this energy is partitioned between vaporization and thermal conductivity to the air exterior to the drop: the first and second terms on the l.h.s. of Eq. (2), respectively. The quantities ρ_w , c_w , L , and κ_w are the mass density, specific heat at constant volume, latent heat of vaporization, and the thermal conductivity of water, respectively; κ_a is the thermal conductivity of air, T_a is the ambient air temperature far from the drop, and p_l is an energy source term that depends on the laser power, the absorption efficiency, and is determined from Mie theory [1].¹ We take p_l to be a positive constant. The water drop radius, r_d , is a function of time whose evolution is determined by Eq. (2), which expresses energy flow balance at the drop surface. To complete the system a boundary condition must be specified for Eq. (1) at radius r_d . We choose the simple constraint $T(r_d) = T_b$, where T_b is the boiling point of water and is a constant. (Much more complicated boundary conditions can be constructed by considering the detailed kinetics of water vapor at the drop surface [2, 3]. This will not fundamentally change the following discussion.) Since the domain of Eq. (1) is $0 \leq r \leq r_d(t)$, we perform a variable transformation to a fixed coordinate x defined by $x \equiv r/r_d(t)$ so that $0 \leq x \leq 1$ independent of time [4]. To this end we use

$$\frac{\partial}{\partial r} = \frac{1}{r_d} \frac{\partial}{\partial x}, \quad (3a)$$

$$\left. \frac{\partial}{\partial t} \right|_r = \left. \frac{\partial}{\partial t} \right|_x - \frac{x}{r_d} \frac{dr_d}{dt} \frac{\partial}{\partial x}, \quad (3b)$$

to transform Eqs. (1, 2). These become

$$\begin{aligned} \rho_w c_w \frac{\partial T}{\partial t} = p_l + \rho_w c_w \left(\frac{1}{r_d} \frac{dr_d}{dt} \right) x \frac{\partial T}{\partial x} \\ + \frac{\kappa_w}{r_d^2 x^2} \frac{\partial}{\partial x} x^2 \frac{\partial T}{\partial x}, \end{aligned} \quad (4)$$

$$\rho_w L \frac{dr_d^2}{dt} = 2 \left[\kappa_a (T_b - T_a) + \kappa_w \left. \frac{\partial T}{\partial x} \right|_{x=1} \right], \quad (5)$$

¹ The values of these parameters are: $\rho_w = 1 \text{ g/cm}^3$, $c_w = 1 \text{ cal/(g-K)}$, $L = 540 \text{ cal/g}$, $\kappa_w = 6.0 \times 10^4 \text{ erg/(s-cm-K)}$, $\kappa_a = 2.39 \times 10^3 \text{ erg/(s-cm-K)}$.

where henceforth it is understood that the partial derivatives with respect to time are taken at constant values of x . Because of the moving boundary Eqs. (4), (5) are, when considered together, nonlinear in both T and r_d . When transformed to the fixed coordinate x an advective term is added, given by the second term on the r.h.s. of Eq. (4), to what was otherwise a diffusion equation.

For the parameters in Eqs. (1), (2) that are physically relevant to water and for significantly fast heating rates we find that the drop temperature can increase much faster than the radius shrinks due to evaporation, at least until a slowly evolving near steady state temperature profile is established that changes only in response to changes in r_d . So for a small timestep, determined by following $T(x, t)$ accurately in Eq. (4), r_d is very nearly constant. This makes the numerical solution of Eqs. (4), (5) quite straightforward. We simply difference Eq. (4) for $T(x, t)$ fully implicit in time and use second-order accurate centered spatial differencing in x . This gives a tridiagonal matrix that is easily inverted by elimination. We assume known values for the coefficients r_d and dr_d/dt at the beginning of each timestep. These are iterated to convergence for each timestep by using Eq. (5), given a new estimated value for $T(x, t)$. This works well because $r_d(t)$ is slowly changing. The solution of Eqs. (4), (5) shows three evolution regimes. First there is a rapid rise in $T(x, t)$ with r_d changing by only a small amount. Next $T(x, t)$ and $r_d(t)$ evolve slowly on the same timescale. Finally, a true steady state is achieved when r_d becomes small enough that thermal conduction to the air balances absorbed laser power so that the r.h.s. of Eq. (5) equals zero.

The purpose of this note is to show how a simple ODE approximation to Eqs. (4), (5) can be constructed. The point is that, although for a single water drop these equations are simple enough to solve, for a cloud where a distribution of drop sizes exists that may vary with spatial location the solution of Eqs. (4), (5) for a large set of drop types becomes computationally intensive. We need an approximation that follows all stages of evolution of the drop accurately. Particularly important is the fast initial temperature rise in the center, since if the drop heats to about 305°C a spontaneous phase transition to vapor occurs and the drop explodes [5]. We wish to accurately predict this onset for a distribution of initial drop sizes typical of a given cloud. It is natural to choose a parametrized form for $T(x, t)$ that includes the steady state solution of Eqs. (4), (5) and also allows for representation of the transient boundary layer associated with uniform heating. Thus we choose

$$T(x, t) = T_0(t) + (T_b - T_0(t)) x^{n(t)} \quad (6)$$

which automatically satisfies the boundary condition at $r = r_d$. There are two parameters, $T_0(t)$ and $n(t)$, the tem-

perature on the axis and the exponent, to determine. This is a trial function approximation to the solution of Eqs. (4), (5). It has three desirable features. First, it allows for the correct steady state solution of the diffusion equation to be achieved; second, it allows for transient diffusion in an approximate way; and finally, it is simple to integrate analytically. With this form, Eq. (5) becomes

$$\rho_w L \frac{dr_d^2}{dt} = 2 \left[\kappa_a (T_b - T_a) - \kappa_w n (T_0 - T_b) \right]. \quad (7)$$

Obviously the approximate solution, Eq. (6), can satisfy Eqs. (4), (5) only in some integral sense. For accomplishing this integral we use as a weighting function the monomial x^j , where j is any positive integer. This simple choice is made because there is no characteristic spatial scale length, relative to x , in this problem. We define for a given x^j the quantity e_j as

$$e_j \equiv (j+1) \int_0^1 T x^j dx - T_b = \frac{n(T_0 - T_b)}{(n+j+1)}, \quad (8)$$

where the second part of this expression results from using Eq. (6). In defining e_j we have chosen the $(j+1)$ factor as a convenient normalization and have subtracted T_b so that if T is constant at the boundary value $e_j = 0$. With this definition of e_j , Eq. (4) can be transformed, with the help of Eq. (7) to eliminate dr_d/dt , to obtain

$$\rho_w c_w \frac{de_j}{dt} = p_l - \frac{(j+1) c_w}{L r_d^2} \left[\kappa_a (T_b - T_a) - (n+j+1) \kappa_w e_j \right] e_j - \frac{(j+1)(n+1)(n+j+1) \kappa_w}{(n+j-1) r_d^2} e_j. \quad (9)$$

Since there are only two parameters to determine, T_0 and n , only two values of j need to be chosen.² Thus Eq. (9) is used twice for the moments e_1 and e_2 , whence

$$e_1 = \frac{n}{(n+2)} (T_0 - T_b), \quad (10a)$$

$$e_2 = \frac{n}{(n+3)} (T_0 - T_b). \quad (10b)$$

² The best choice has been found to be $j=1$ and $j=2$, although the results are not overly sensitive to this. Obviously, two large values of j lead to poorer results since the two monomials are then not very independent.

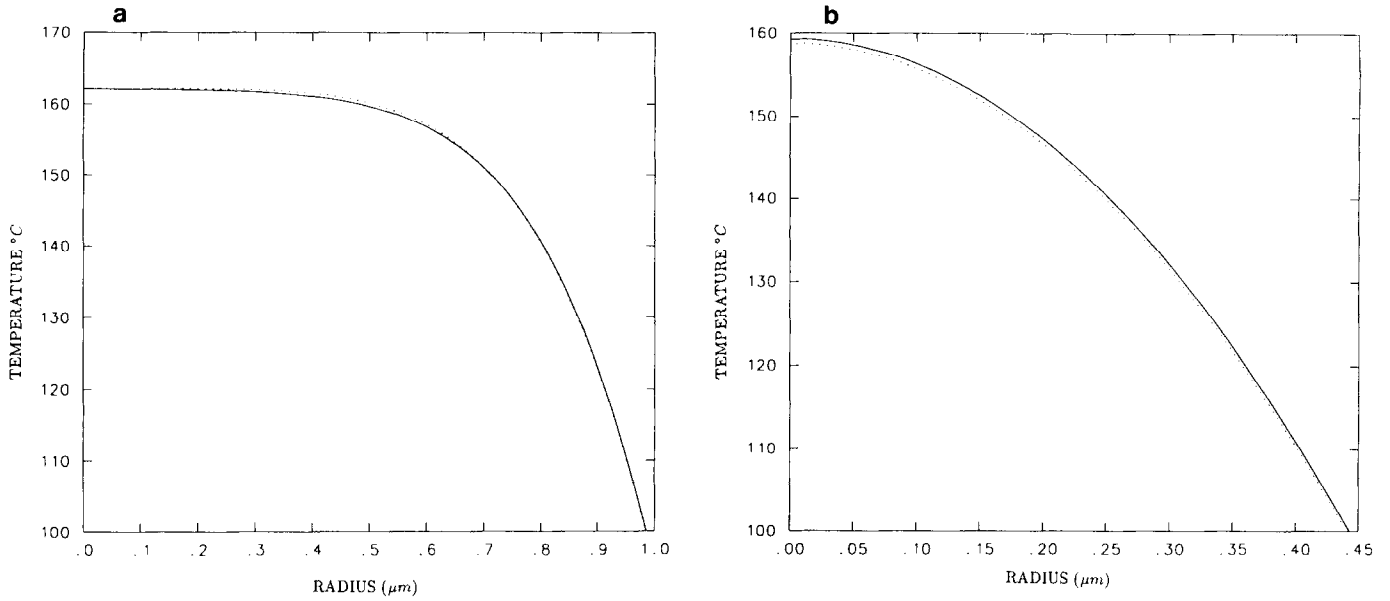


FIG. 1. Temperature (°C) vs radius (microns)—solid curve, PDE system; dashed curve, ODE system: (a) at 0.25 μs; (b) at 5.0 μs.

Inverting Eqs. (10) gives

$$n = \frac{(2e_1 - 3e_2)}{(e_2 - e_1)}, \quad T_0 = T_b + \frac{(n + 2)}{n} e_1. \quad (11a), (11b)$$

We thus have three ODEs to solve, Eq. (7) and Eq. (9) for ($j=1$) and ($j=2$), where Eqs. (10) and (11) serve as constitutive expressions relating (e_1, e_2), to (T_0, n) and vice versa. These equations may be conveniently solved by any numerical scheme. We require as initial conditions some value of $n \geq 2$ and $T_0 > T_b$. Use of a time dependent boundary condition, $T_b(t)$ say, in place of a constant T_b in Eq. (4) will simply introduce terms involving $\partial T_b / \partial t$ and $T_b(t)$ that can be evaluated given an additional expression for determining the time evolution of $T_b(t)$ (see Ref. [2]).

In Figs. (1) and (2) we show a comparison of solutions of Eqs. (4), (5) and Eqs. (7), (9) for an initial water drop radius of 1.0 μm, an initial temperature of 25°C, and a constant laser flux of 1.0 MW/cm². We choose $T_a = 25^\circ\text{C}$ and $T_b = 100^\circ\text{C}$. Equations (4), (5) are solved by implicit time differencing as described previously; Eqs. (7), (9) are solved by the common fourth-order Runge-Kutta scheme [6], where $T_0 = 100.1^\circ\text{C}$ and $n = 2$ initially. A fixed timestep $\Delta t = 0.01 \mu\text{s}$ is used. Figure 1 shows the temperature versus radius across the drop. Part (a) is at 0.25 μs, an early time where the temperature profile is still developing and is relatively flat in the drop center; part (b) is at 5.0 μs, where a parabolic temperature profile which changes only in response to the shrinking drop radius has been established. The solid curve is the solution to the PDE system, Eqs. (4), (5); the dotted curve shows the solution to the ODE

approximation, Eqs. (7), (9). Note that the drop radius has changed very little in part (a). Figure 2 shows the temperature versus time at the drop center for the two sets of equations. As seen, the approximation of the solution of the ODE system to the primitive PDE is extremely good.

An explicit solution of Eqs. (7) and (9) leads to a stability constraint that is exactly analogous to that obtained in explicitly solving Eq. (4) for thermal diffusion except that the drop radius in the ODE replaces the grid spacing in the PDE. This is readily seen from the last term on the r.h.s. of

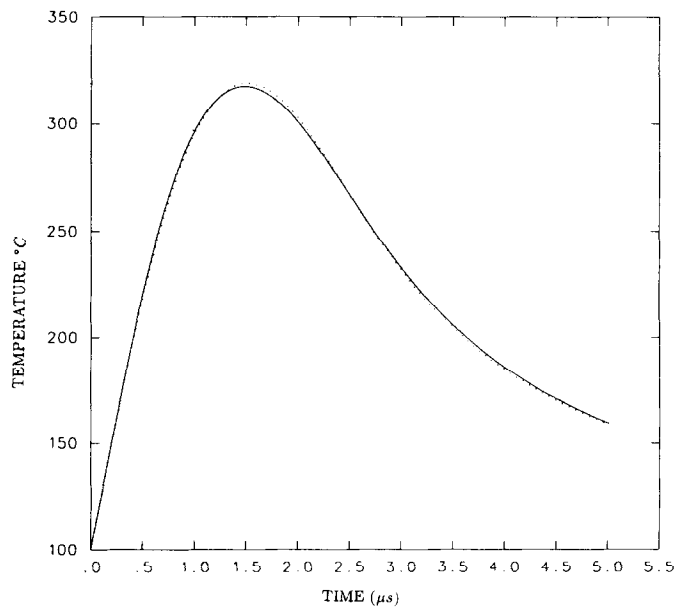


FIG. 2. Temperature (°C) vs time (μs) at the drop center: solid curve, PDE system; dashed curve, ODE system.

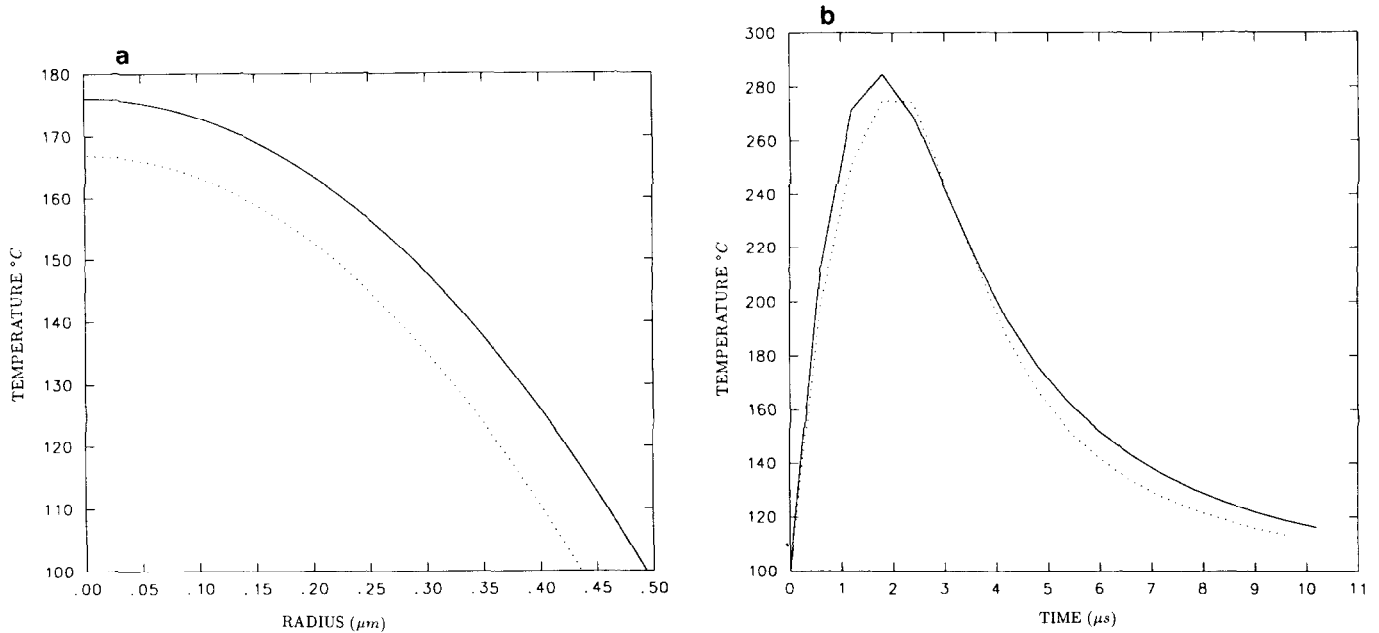


FIG. 3. Implicit time differencing—solid curve, PDE system; dashed curve, ODE system: (a) temperature (°C) vs radius (μm) at 4.8 μs, Δt = 0.6 μs; (b) temperature (°C) vs time (μs) at the center of the drop.

Eq. (9). We find for the explicit scheme the usual stability restriction

$$\frac{2(n+1)(n+2)}{n} \frac{\kappa_w \Delta t}{\rho_w c_w r_d^2} \leq C, \quad (12)$$

where for the steady state value of $n=2$ the constant C is found empirically to be about 0.9. Since the drop radius is much greater than any reasonable grid spacing across that radius this may not be a problem. However, if due to evaporation the drop radius becomes small implicit time differencing on terms linear in e_j in Eq. (9) is desirable.³

In Fig. 3 we show results using implicit time differencing of the ODE system in the simple manner just described for the same parameters as before except that now the timestep Δt is 0.6 μs, a factor of more than 10 above the explicit stability threshold. To enhance nonlinear stability we require that $n \geq 2$ at the end of each timestep by setting it equal to two if it goes below it. We also require $n \leq 20$ to ensure that e_1 and e_2 are sufficiently independent. In Fig. 3 the solid curve is the PDE solution while the dashed curve is the result of solving Eqs. (7), (9). Part (a) shows temperature versus radius at 4.8 μs; part (b) gives the temperature at the center of the drop versus time. It is seen that stability has been achieved and that both curves agree fairly well with each other. However, by comparison to Figs. 1 and 2, accuracy has been substantially degraded. This is to be expected since there are only 12 timesteps in 6 μs over

³ The steady state solution of Eqs. (1), (2) or Eqs. (7), (9) is $n=2$, $T_0 = T_b + (\kappa_a/2\kappa_w)(T_b - T_a)$, and $r_d = [(3\kappa_a/p_l)(T_b - T_a)]^{1/2}$ so that this restriction on Δt is readily evaluated.

which the temperature profile changes significantly. Thus, a variable timestep set to allow no more than some minimum change in T_0 and r_d on a given integration step should be implemented. A fixed timestep has been used here for clarity in quantifying the numerical results. It is found that the implicit differenced ODE approximation described above reproduces the exact steady state solution with no restriction on timestep, as expected.

We wish to note that the slow parametric change of the temperature profile after the initial fast transient as seen in Fig. 2 after 2 μs can be followed directly by setting $de_j/dt = 0$ in Eq. (9) and determining $T_0(t)$ and $n(t)$ algebraically, given r_d . Then from Eq. (7) dr_d/dt is known and r_d can be evolved with time and updated values of T_0 and n can be obtained. That is, given a monotone decreasing sequence of numbers for r_d , Eq. (9) determines a corresponding sequence of numbers for T_0 and n . Then Eq. (7) determines a set of time labels to associate with these sequences.

In summary, we have shown how a simple and very accurate ODE approximation to a one-dimensional PDE may be constructed by utilizing a generalization of the PDE's analytically known steady state solution. Appropriate moments of this solution were then taken to achieve an ODE model. Thus the correct steady state solution is automatically obtained by the approximation. Although the PDE considered, a thermal diffusion equation with a heat source and constant coefficients, is linear if the moving boundary is fixed, the ODE representation is highly nonlinear. The ODE representation exhibits the same linear stability restriction when solved by an explicit method as

the original PDE, with the characteristic physical system dimension playing the role of a spatial grid size. However, this is readily overcome by implicit differencing. Although we have considered spherical geometry the procedure described will carry over directly to cylindrical geometry. The basic ideas should be relevant to many physical problems where an accurate, simple, and fast approximation to a more complicated physical system is required.

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