Numerical solution of transient temperature for pulsed heating in a single spherical particle model

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I.V. Grozescu and M.M. Moksin
Applied Optics Group, Physics Department, Universiti Putra Malaysia, Selangor, Malaysia

Introduction

Recently, an addition of a microscope objective in the detection system of a photothermal technique (Moksin, 1995) has provided a means of measuring thermal radiation from a selected single isolated particle. In this technique, surface cooling rate is determined from the time-resolved measurement of blackbody radiation subsequent to a short pulse heating. The change in the emitted blackbody radiation is determined by the change in the surface temperature of the sample, which in turn is affected by absorption of the heating radiation and the interaction of heat waves with the sample.

Detection of infrared radiation emission from a single particle is important in those domains of science (e.g. high-tech products particle contaminants control, air pollution monitoring and forensic science) whereby only a limited number of particles can be available. The thermal properties and size of the particles, together with other properties available from other techniques can be used to identify the origin of the particles or source of the contaminants.

In this article a numerical solution for pulse-induced changes in theoretical thermal radiation emission from a single spherical particle on thermally bad conduction surface is derived, and this numerical result is compared with a corresponding analytical solution.

Heat conduction equation

We assume that the pulsed heating causes the temperature of a non-volatile spherical particle of radius, a, to increase rapidly and uniformly by θ_0. The temperature then declines as energy is lost to the surroundings by radiation, conduction and convection.

Thus, we can assume that inside the particle and at a sufficiently large distance from it:

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$$\frac{\partial \theta}{\partial r} = 0 \tag{1}$$

For a thermally bad conducting surface the heat conduction at the interface can be neglected and the transient behaviour is then defined by an energy balance over a differential spherical shell of surrounding air (Carslaw and Jaeger, 1989; Moksin, 1995) :

$$\frac{k}{r^2}\frac{\partial}{\partial r}\left[r^2 \frac{\partial \theta}{\partial r}\right] = \rho c \frac{\partial \theta}{\partial t} \tag{2}$$

where k, ρ and c are air thermal conductivity, density and specific heat capacity respectively.

For the case of small temperature difference, heat loss by thermal radiation and convection in the absence of air flow can be neglected. Thus, the remaining mechanism of heat transfer will be conduction to the surrounding air, as expressed below:

$$\frac{1}{3} a \rho_s c_s \frac{\partial \theta}{\partial t} = k \frac{\partial \theta}{\partial r} \tag{3}$$

where ρ_s and c_s are density and specific heat capacity of the particle respectively.

In order to find out the change in the surface temperature of the particle, equation (3) is solved with initial conditions at $t = 0$, i.e. $\theta = \theta_0$ for the particle and $\theta = 0$ for the surrounding air. Using dimensionless variables: $X = \frac{r}{a}$, $V = \frac{\theta}{\theta_0}$, $U = X\frac{\theta}{\theta_0}$, and $L = \frac{l}{a}$ (l = distance between particles centres) equations (1-3) can be rewritten as:

$$\frac{\partial V}{\partial X} = 0 \text{ at } X = L \tag{4}$$

$$\frac{\partial^2 U}{\partial X^2} = \frac{\partial U}{\partial \tau} \tag{5}$$

$$\Phi \frac{\partial V}{\partial t} = \frac{\partial V}{\partial X} \text{ at } X = 1 \tag{6}$$

where $\tau = kt/(3\rho c a^2)$ and $\Phi = \rho_s c_s/(3\rho c)$.

In order to solve these equations the Laplace transform approach is used, i.e. instead of solving the given differential equation with initial and boundary condition directly, the original equation is transformed to an ordinary differential equation. Thus, the Laplace transform of equation (5), after inserting the initial conditions, is:

$$\frac{d^2U}{dX^2} = pU \tag{7}$$

which has a general solution:

$$U(X,p) = \gamma_1(p)\exp[\sqrt{p}X] + \gamma_2(p)\exp[-\sqrt{p}X] \tag{8}$$

where the functions $\gamma_1(p)$ and $\gamma_2(p)$ can be obtained from the boundary condition in equations (4) and (6). Therefore, the Laplace transform of the change in the surface temperature of the particle can be written as:

$$\mathcal{L}\left\{\frac{\theta}{\theta_o}\right\} = V = \frac{U(X,p)}{X} \tag{9}$$

The final form of the Laplace transform for normalised change in the surface temperature of the particle can be obtained substituting the general solution (8) into (9) for corresponding values of γ_1 and γ_2 and also inserting $X = 1$ as $L \rightarrow \infty$ (in the single particle model l, distance between the particles centres, $\rightarrow \infty$). Thus

$$\mathcal{L}\left\{\frac{\theta}{\theta_o}\right\} = \frac{1}{p + \alpha\sqrt{p} + \alpha} \tag{10}$$

where $\alpha = 1/\Phi$. With the help of the inversion of the Laplace transform, it is possible to find the change in the surface temperature from the image function (10). Consequently, normalised change in the temperature of the particle surface is:

$$\frac{\theta}{\theta_o}(\tau) = \mathcal{L}^{-1}\left\{\frac{1}{p + \alpha\sqrt{p} + \alpha}\right\} \tag{11}$$

Results and discussion

An analytical solution of (11) cannot be found in the literature even though the Laplace transforms are discussed extensively (Oberhettinger and Badii, 1973; Roberts and Kaufman, 1966). For the particles of interest the constant α is less than 0.005 (see Table I) and we found that function

$$T_{th}(p) = \frac{1}{p + a\sqrt{p} + a}$$

can be approximated with function $T_{ap}(p) = \frac{1}{p + \alpha}$ (Figure 1).

In this case, the normalised temperature of the particle surface can be expressed as:

$$\frac{\theta}{\theta_o} = \exp[-\alpha\tau] = \exp\left[-\frac{3kt}{\rho_s c_s a^2}\right] \tag{12}$$

Figure 1 shows that the approximation function, $T_{ap}(p)$, and theoretical function, $T_{th}(p)$, have the same behaviour, especially with a large value of p. We have deliberately plotted both functions for $\alpha = 0.02$ to be able to see the extent of deviation between the functions. In our case, when $\alpha < 0.005$, for $p > 0.2$ the difference between T_{th} and T_{ap} is less than 1 per cent and for $p > 100$ the difference is less than 0.05 per cent with an asymptotic behaviour to 0 in the neighbourhood of $p \rightarrow \infty$ (see Figure 2).

According to the Laplace transform theory (Doetsch and Herschel, 1971; Krylov and Skoblia, 1969) it is expected that the solution obtained from equation (11) will be identical to formula (12) at small values of time if the image functions are identical for large values of p. Nevertheless, it is necessary to

Table I.
Analytical and numerical decay time for pulsed induce change in thermal radiation from a single spherical particle for some materials of interest

Material	Density, ρ_s (kg/m^3)	Specific heat capacity, c_s J/(kg·K)	Φ	α	τ_a (ms)	τ_n (ms)
Coal	737	1,300	270	0.0037	2.723	2.696
Cement	1,500	700	296	0.0034	2.985	2.961
Sand	1,515	800	341	0.0029	3.445	3.421
Lead	11,373	130	416	0.0024	4.203	4.178
Limestone	2,500	900	633	0.0016	6.396	6.370
Clay	1,460	880	362	0.0028	3.653	3.627

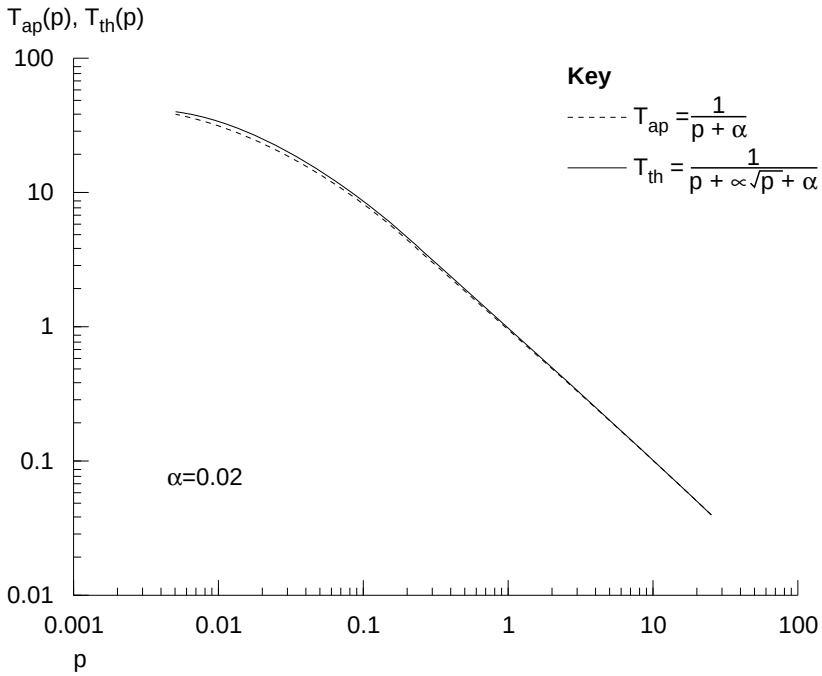

Figure 1.
Behaviour of the functions $T_{ap}(p)$ and $T_{th}(p)$, especially for large values of p parameter, $\alpha = 0.02$ in logarithmic presentation for both axes

compare the exact solution of equation (11) with the approximation (12). This requires the inverse Laplace transform to be performed numerically (see Appendix). Instead of applying this procedure directly to the function T_{th} it is more preferable to evaluate the inverse Laplace transform of function T_{th}-T_{ap}. By assuming:

$$f_1(\tau) = \mathcal{L}^{-1}\{T_{th}-T_{ap}\} \quad (13)$$

the normalised change in surface temperature can be expressed as (Oberhettinger and Badii, 1973)

$$\frac{\theta}{\theta_o}(\tau) = \exp[-\alpha\tau] + f_1(\tau) \quad (14)$$

This allows the finding of straightforward deviation between the numerical solution and the approximation (12).

Figure 3 shows the plot of the computed deviation $f_1(\tau)$ for a coal particle. The analytical and numerical solutions are identical to within less than 1 per cent. This is also obvious in Figure 4 where the numerical and analytical solutions are shown in a logarithmic presentation.

The decay times, τ_a (for analytical solution) and τ_n (for numerical solution) are shown in Table I. For particles which satisfy the condition $\alpha < 0.005$ ($\Phi > 270$) the decay time measurement error is less than 1 per cent. For a fictitious particle with $\alpha = 0.02$ ($\Phi = 50$) the error is less than 5 per cent.

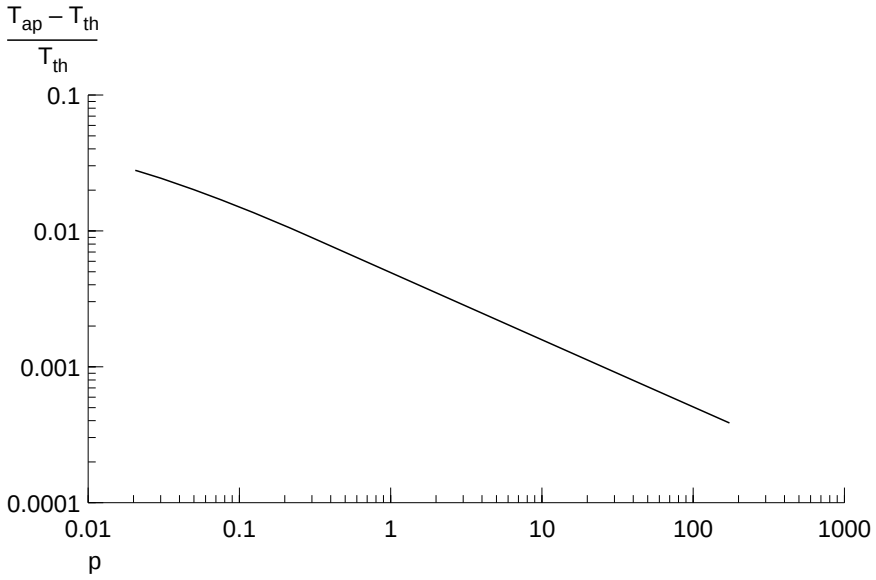

Figure 2. Relative difference of $T_{ap}(p)$ and $T_{th}(p)$ for $\alpha = 0.005$, logarithmic presentation. For large values of p difference between the image functions $T_{ap}(p)$ and $T_{th}(p)$ has an asymptotic behaviour to zero. According to Laplace transform theory, the approximation (12) and exact solution of equation (11) should be identical for small values of time

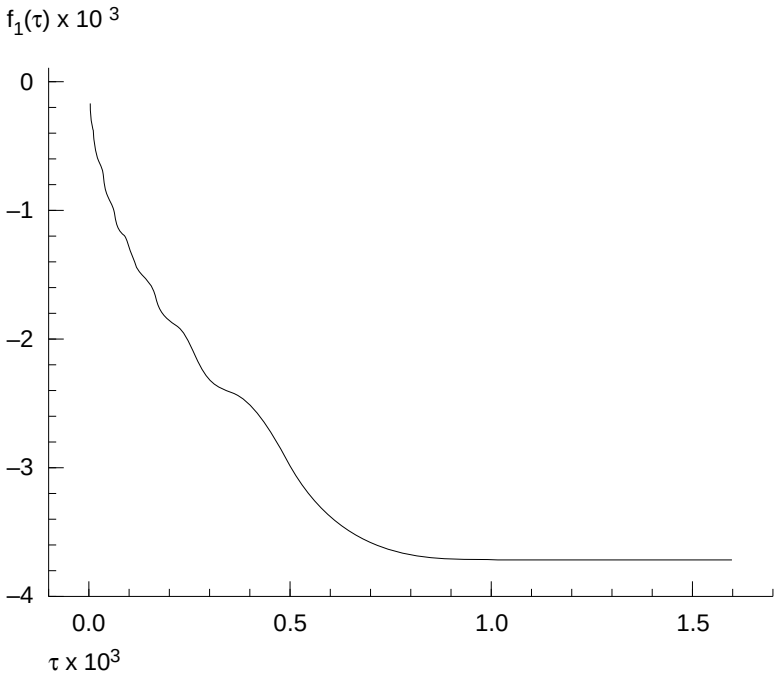

Figure 3.
Numerical inverse Laplace transform of the function T_{ap}-T_{th} versus relative time τ, for coal particle α = 0.0037

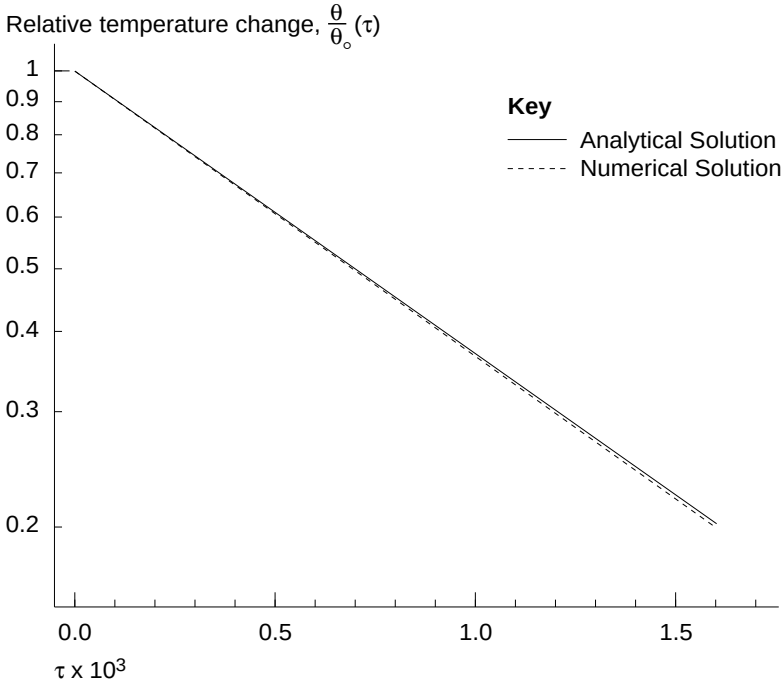

Figure 4.
Comparison between analytical and numerical change of the surface temperature for a coal particle

Summary
The transient temperature for pulsed heating in a single spherical model has been derived using the Laplace transform algorithm based on Fourier series. We assumed that the substrate is a thermally bad conducting surface and then head conduction at the interface can be neglected. The computation for the transient surface temperature of the particle was performed in such a way as to obtain a straightforward deviation of the analytical solution (12) from the numerical result. It has been proved that for some particles ($\alpha < 0.005$) the analytical solution provided a reasonably accurate description of the model, otherwise the numerical solution should be used in the general case.

References

Carslaw, H.S. and Jaeger, J.C. (1989), *Conduction of Heat in Solids*, Oxford University Press, London.

Doetsch, G. and Herschel, R. (1971), *Guide to the Applications of the Laplace and B-Transforms*, Van Nostrand Reinhold, London.

Krylov, V.I. and Skoblia, N.S. (1969), *Handbook of Numerical Inversion of Laplace Transforms* (Translated from Russian), Israel Program for Scientific Translations, Jerusalem.

Moksin, M.M. (1995), "Optothermal study of small single particles", *Review of Scientific Instruments*, Vol. 66 No. 9, pp. 4716-17.

Oberhettinger, F. and Badii, L. (1973), *Tables of Laplace Transforms*, Springer-Verlag, Berlin.

Roberts, G.E. and Kaufman, H. (1966), *Table of Laplace Transforms*, W.B. Saunders Company, Philadelphia.

Appendix

The main idea of inverse Laplace transform using Fourier series is to obtain the original function, $g(t)$ from a finite number of values of its image function, $G(t)$. Only the values of the image function, $G(p)$, at the equidistant points $p = (2n + 1)\sigma$ (σ is an arbitrary number greater than 0, $n = 0, 1, 2 \ldots$) are used. The algorithm is based on two assumptions, which do not, however, limit its generality. First, the function to be transformed, $G(p)$ must exist for $p > 0$. Second we assume that $g(t)$, ($g(t) = L^{-1}\{G(p)\}$) satisfies the condition $g(0) = 0$. Both conditions are fulfilled by the function $(T_{th} - T_{ap})(p)$. Then, the expression of deviation between the exact solution and approximate solution can be expressed as:

$$f_1(\beta) = \sum_{k=0}^{\infty} C_k \sin(2k + 1)\beta \tag{15}$$

where, $\beta = \arccos[\exp(-\sigma\tau)]$ while C_k has to be computed. The value of σ is chosen according to the interval in which $f_1(t)$ is to be found. For small τ, large σ is chosen and on the other hand for large τ, small σ is chosen because $t \to \infty$ corresponds to $p \to \infty$ (Doetsch, 1971). In our computation, we have used 17 terms into expression (15) which is more than enough for Fourier series to converge.