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<td>Citation</td>
<td>Vladimir, K., &amp; Kirill, V. P. (2012). A generalized relation between the local values of temperature and the corresponding heat flux in a one-dimensional semi-infinite domain with the moving boundary. International Journal of Heat and Mass Transfer, 55(23–24), 6595-6599.</td>
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<td><a href="http://hdl.handle.net/10220/8724">http://hdl.handle.net/10220/8724</a></td>
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A generalized relation between the local values of temperature and the corresponding heat flux in a one-dimensional semi-infinite domain with the moving boundary

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Keywords:
Ultra-fast heat transfer
Thermal waves
Thin films
Phase lagging

Abstract:
The paper presents generalized relation between the local values of temperature and the corresponding heat flux in a one-dimensional semi-infinite domain with the moving boundary. The generalized relation between the local values of temperature and the corresponding heat flux has been achieved by the use of a novel technique that involves generalized derivatives (in particular, derivatives of non-integer orders). Confluent hyper-geometric functions, known as Whittaker’s functions, appear in the course of the solution procedure, upon applying the Laplace transform to the original transport equation. The relation is written in the integral form and provides a relationship between the local values of the temperature and heat flux.
1. Introduction

Understanding ultra-fast heat transfer processes, induced by ultra-short laser pulses, is of great importance due to their wide applications in microelectronics [1], micro- and nano-electro mechanical devices, data storage devices [2,3], etc.

Mathematical description of such ultra-fast heat transfer processes is reduced to solving partial differential equations within a certain domain (see, for instance, [4–6]) that is a complex mathematical problem. Numerical simulations are often the only choice to obtain solutions.

However, an analytical solution of this problem can be obtained in the form of a Volterra-type integral equation that relates the local values of temperature and the corresponding heat flux within a semi-infinite domain. This methodology, based on fractional calculus, was shown by Lage and Kulish [7,8] to be extremely effective when applied to solving transient diffusion problems and then, it was generalized by Frankel for finite domains [9]. In papers [10,11], it was extended to solve analytically ultra-fast heat transfer problems described by the hyperbolic heat conduction equation without source term as well as the dual-phase-lag model proposed by Tzou [6].

This paper presents an integral solution of the generalized one-dimensional phase-lagging heat equation with the source and convective terms. Problems of ultra-fast heat transfer in domains with moving boundaries are commonly found in scientific and engineering applications [12–14].

The solution of the problem has been achieved by the use of a novel technique that involves generalized derivatives (in particular, derivatives of non-integer orders). Confluent hyper-geometric functions, known as Whittaker’s functions, appear in the course of the solution procedure, upon applying the Laplace transform to the original transport equation. The analytical solution of the problem is written in the integral form and provides a relationship between the local values of the temperature and heat
flux. The solution is valid everywhere within the domain, including the domain boundary.

2. Generalized equation of heat transfer

A generalized heat transfer equation with the convective term can be obtained from the conservation equation of thermal energy written in the differential form:

\[
C \frac{\partial T(r, t)}{\partial t} + \nabla \cdot \mathbf{q}''(r, t) = S(r, t).
\]  

(1)

In this study C is assumed to be constant. The conservation equation involves two unknown variables, \( T \) and \( \mathbf{q}'' \), and, hence, must be coupled with a constitutive equation that would relate these unknown quantities. In general, constitutive equations are but assumptions and, unlike the conservation equation, cannot be derived from fundamental principles. Therefore, the final form of the equation of heat transfer depends on the form of the constitutive equation used.
In the present model, the following constitutive equation is used:

\[ \frac{1}{c} \mathbf{q}''(\mathbf{r}, t + \tau) = -\alpha(\mathbf{r}, t) \nabla T(\mathbf{r}, t) + \mathbf{u}(\mathbf{r}, t) F(\mathbf{r}, t). \] (2)

It is considered that heat is transported by both diffusion (the first term in the right side of the constitutive equation) and convection (the second term in the right side). The parameter \( \tau \) represents the time lag between the onset of the gradient of the temperature and the occurrence of heat flux. Hence, unlike Fick’s or Fourier’s constitutive equations, Eq. (2) accounts for a finite speed of the transport process and is more general than the latter.

The left and right sides of the constitutive relation are written for two different time moments. In order to overcome this difficulty, the left side of Eq. (2) is expanded into the Taylor series because \( \tau \ll 1 \text{ s} \) (for most of media, \( \tau \) is of the order \( 10^{-12} \) to \( 10^{-10} \text{ s} \)).
Neglecting the second-order infinitesimal terms of the series, the constitutive equation becomes

$$\frac{1}{C} \left\{ q''(r, t) + \tau \frac{\partial q''(r, t)}{\partial t} \right\} = -\alpha(r, t) \nabla T(r, t) + u(r, t) T(r, t).$$  \hspace{1cm} (3)

Upon applying the divergence operator to both parts of Eq. (3), the latter becomes

$$\frac{1}{C} \left\{ \nabla \cdot q''(r, t) + \tau \frac{\partial \nabla \cdot q''(r, t)}{\partial t} \right\}$$
$$= -\nabla \cdot [\alpha(r, t) \nabla T(r, t)] + \nabla \cdot [u(r, t) T(r, t)].$$  \hspace{1cm} (4)

Expressing term $\nabla \cdot q''(r, t)$ from Eq. (1) and substituting it into Eq. (4), the equation becomes

$$\frac{\partial T(r, t)}{\partial t} + \tau \frac{\partial^2 T(r, t)}{\partial t^2} + \nabla \cdot [u(r, t) T(r, t)]$$
$$= \nabla \cdot [\alpha(r, t) \nabla T(r, t)] + \frac{1}{C} \left\{ S(r, t) + \tau \frac{\partial S(r, t)}{\partial t} \right\}. \hspace{1cm} (5)$$

Eq. (5) is the generalized equation of heat transfer. It reduces to the classical diffusion heat equation if $\tau = 0$ and $u(r, t) = 0$. If only $u(r, t) = 0$, the generalized equation of heat transfer reduces to the classical heat wave equation [15]. Note the presence of the apparent energy source $\frac{\partial S(r, t)}{\partial t}$ in (5); it appears due to the finite time lag between the excitation and the response to it.

Further, it is assumed that the diffusion coefficient and velocity are both constant, hence Eq. (5) can be rewritten as

$$\frac{\partial T(r, t)}{\partial t} + \tau \frac{\partial^2 T(r, t)}{\partial t^2} + u \nabla T(r, t) = \alpha \nabla^2 T(r, t) + \frac{1}{C} \left\{ S(r, t) + \tau \frac{\partial S(r, t)}{\partial t} \right\}. \hspace{1cm} (6)$$
3. Problem formulation

Consider a heat transfer process that occurs in a homogeneous (no preferred direction), one-dimensional semi-infinite domain whose boundary moves with a constant speed $u$ and whose diffusion coefficient depends neither on spatial variable nor on time. In view of different domain geometries, the generalized equation of heat transfer (6) becomes

$$
\frac{\partial T(r, t)}{\partial t} + \tau \frac{\partial^2 T(r, t)}{\partial t^2} + u \frac{\partial T(r, t)}{\partial r} = \kappa \left\{ \frac{\partial^2 T(r, t)}{\partial r^2} + \frac{2\gamma}{r} \frac{\partial T(r, t)}{\partial r} \right\} + \frac{1}{c} \left\{ S(r, t) + \tau \frac{\partial S(r, t)}{\partial t} \right\}. \tag{7}
$$

In Eq. (7), the parameter $\gamma$ characterizes the domain geometry. Thus, $\gamma = 0$ corresponds to the domain with the flat boundary (no curvature); $\gamma = \pm 1$ represents the spherical case with the convex and concave boundary, respectively; whereas $\gamma = \pm 1/2$ describes the cylinder whose boundary is either convex ($\gamma = 1/2$) or concave ($\gamma = -1/2$) [16,17].

The spatial variable $r = x \pm R$, where $x$ is the actual distance from the origin and $R$ is the initial radius of curvature. Note that the sign of $R$ must be the same as the sign of $\gamma$.

Initially, at $t = 0$, the domain is in equilibrium with a constant value of the temperature, $T_0$, throughout the domain, $0 \ll r < +\infty$.

As the heat transfer process goes on, the condition $\lim_{r \to \infty} T(r, t) = T_0$ must be imposed in order to comply with the principle of energy conservation. At this point, the second boundary condition is deliberately not imposed. This issue will be clarified in the following section.
4. Solution procedure

Upon introducing the new variable, \( \eta = r / \sqrt{\alpha} \), and the excess of the temperature \( \hat{T} = T - T_0 \), the heat Eq. (7) can be rewritten as

\[
\frac{\partial \hat{T}(\eta,t)}{\partial t} + \tau \frac{\partial^2 \hat{T}(\eta,t)}{\partial t^2} = \frac{\partial^2 \hat{T}(\eta,t)}{\partial \eta^2} + 2 \left( \frac{\eta}{\eta} - \omega \right) \frac{\partial \hat{T}(\eta,t)}{\partial \eta} + \hat{S}(\eta,t) + \tau \frac{\partial \hat{S}(\eta,t)}{\partial t},
\]

(8)

where \( \omega = u(2\sqrt{\alpha}) \) and \( \hat{S}(\eta,t) / C \).

The initial condition becomes \( \hat{T}(\eta,0) = 0 \), and the boundary condition is now \( \lim_{\eta \to \infty} \hat{T}(\eta, t) = 0 \).

The Laplace transform of Eq. (8) is

\[
\frac{d^2 \Phi(\eta;s)}{d\eta^2} + 2 \left( \frac{\eta}{\eta} - \omega \right) \frac{d \Phi(\eta;s)}{d \eta} - s(1 + \tau s) \Phi(\eta;s) = -(1 + \tau s) Q(\eta;s),
\]

(9)

where \( \Phi(\eta;s) \) is the Laplace transform of the excess of the temperature \( \hat{T}(\eta,t) \) and \( Q(\eta;s) \) represents the Laplace transform of the source function \( \hat{S}(\eta,t) \), provided that this Laplace transform exists.

The general solution of Eq. (9) is

\[
\Phi(\eta;s) = \left\{ C_1(s) M_{\kappa,\mu}[2\eta f(s)] + C_2(s) W_{\kappa,\mu}[2\eta f(s)] \right\} \frac{e^{\omega \eta}}{\eta} + P(\eta;s),
\]

(10)

where \( f(s) = \sqrt{s(1 + \tau s)} + \omega \), \( P(\eta;s) \) is a particular solution of (9), \( C_1(s) \) and \( C_2(s) \) are two arbitrary functions of \( s \), \( M_{\kappa,\mu}(z) \) and \( W_{\kappa,\mu}(z) \) are Whittaker’s functions, defined as

\[
M_{\kappa,\mu}(z) = e^{-z/2} z^{\mu+1/2} M(1/2 + \mu - \kappa, 1 + 2\mu, z)
\]

(11)
and

\[ W_{\kappa,\mu}(z) = e^{-z/2}z^{\mu+1/2}U(1/2 + \mu - \kappa, 1 + 2\mu, z), \]  

(12)

where \( z = 2\eta f(s), \kappa = \gamma \omega/f(s) \) and \( \mu = \gamma - 1/2 \). Functions \( M \) and \( U \) in (11) and (12), respectively, are Kummer’s confluent hyper-geometric functions, defined as

\[ M(a, b, z) = 1 + \frac{az}{b} + \frac{(a)_{2}z^{2}}{(b)_{2}2!} + \cdots + \frac{(a)_{n}z^{n}}{(b)_{n}n!} + \cdots; \]  

(13)

\[ U(a, b, z) = \frac{\pi}{\sin(\pi b)} \left[ \frac{M(a, b, z)}{\Gamma(1 + a - b)\Gamma(b)} - z^{1-b}M(1+a-b, 2-b, z) \right]; \]  

(14)

where \((a)_{n} = a(a + 1)(a + 2) \ldots (a + n - 1), (b)_{n} = b(b + 1)(b + 2) \ldots (b + n - 1)\), and \((a)_{0} = (b)_{0} = 1 \) [18, page 504].

Writing in terms of Kummer’s functions, Eq. (10) becomes

\[ \Phi(\eta; s) = \{C_{1}(s)M(a, b, 2\eta f(s)) + C_{2}(s)U(a, b, 2\eta f(s))\} \times \left[ 2f(s)^{\eta}e^{\eta(\omega-f(s))} + P(\eta; s) \right], \]  

(15)

where \( a = \gamma(1 - \omega/f(s)) \) and \( b = 2\gamma \).

Since \( \lim_{\eta \to \infty} M(a, b, 2\eta f(s)) = \frac{\Gamma(b)}{\Gamma(a)}e^{2\eta f(s)}(2\eta f(s))^{a-b} \) [18, page 504], the first term in (15) becomes unbounded for large values of \( \eta \). Hence, for the solution to be bounded, the arbitrary function \( C_{1}(s) \) must be identically zero. On the other hand, \( \lim_{\eta \to \infty} U(a, b, 2\eta f(s)) = (2\eta f(s))^{-a} \) [18, page 504]. Therefore, provided that \( Re(s) > 0 \) (this is really the case, because the Laplace transform variable corresponds to time and is always positive), the second term in Eq. (15) decreases as \( \eta \) increases and vanishes as \( \eta \) becomes infinitely large. Consequently, the solution becomes
Differentiating Eq. (16) with respect to $\eta$, and noting that

$$\frac{dU(a, b, 2\eta f(s))}{d\eta} = -2af(s)U(a + 1, b + 1, 2\eta f(s)), \tag{17}$$

the equation becomes

$$\frac{d\Xi(\eta; s)}{d\eta} = C(s)(2f(s))^{\gamma} e^{\eta(\omega - f(s))} \times \{U(a, b, 2\eta f(s))(\omega - f(s)) - 2af(s)U(a + 1, b + 1, 2\eta f(s))\}, \tag{18}$$

where $\Xi(\eta; s) = \Phi(\eta; s) - P(\eta; s)$.

Furthermore, it follows from Eq. (16) that

$$C(s) = \frac{\Xi(\eta; s)}{U(a, b, 2\eta f(s))(2f(s))^{\gamma} e^{\eta(\omega - f(s))}}. \tag{19}$$

Substituting Eq. (19) into (18), the equation can be written as

$$\frac{d\Xi(\eta; s)}{d\eta} = \Xi(\eta; s) \left\{ (\omega - f(s)) + 2\gamma(\omega - f(s)) \frac{U(a + 1, b + 1, 2\eta f(s))}{U(a, b, 2\eta f(s))} \right\}. \tag{20}$$

Dividing both the left and right parts of Eq. (20) by $f(s)$, the last one can be rewritten as follow

$$- \frac{1}{f(s)} \frac{d\Xi(\eta; s)}{d\eta} = \Xi(\eta; s) \left\{ \left( 1 - \frac{\omega}{f(s)} \right) + 2\gamma \left( 1 - \frac{\omega}{f(s)} \right) \frac{U(\gamma(1 - \omega/f(s)) + 1, 2\gamma + 1, 2\eta f(s))}{U(\gamma(1 - \omega/f(s)), 2\gamma, 2\eta f(s))} \right\}. \tag{21}$$

Due to $\frac{U(\gamma(1 - \omega/f(s)) + 1, 2\gamma + 1, 2\eta f(s))}{U(\gamma(1 - \omega/f(s)), 2\gamma, 2\eta f(s))} = \frac{1}{2\eta f(s)}$, Eq. (21) can be simplified into
The inverse Laplace transform of \(1/f(s)\) is \([18, \text{page 1025}]\)

\[
L^{-1}\left\{ \frac{1}{\sqrt{s(1 + \tau s) + \omega^2}} \right\} = \frac{e^{-t/(2\tau)}}{\sqrt{\tau}} I_0\left( \frac{t}{2\tau} \sqrt{1 - 4\tau \omega^2} \right), \tag{23}
\]

where \(I_0\) is the modified Bessel function \([18, \text{page 1022}]\). The inverse Laplace transform of \(1/f(s)^2\) is

\[
L^{-1}\left\{ \frac{1}{s(1 + \tau s) + \omega^2} \right\} = \frac{2e^{-t/(2\tau)}}{\sqrt{1 - 4\tau \omega^2}} \times \sinh\left( \frac{t}{2\tau} \sqrt{1 - 4\tau \omega^2} \right). \tag{24}
\]

In view of Eqs. (23) and (24), taking the inverse Laplace transform of Eq. (22) and restoring the original variables, the solution of Eq. (7) corresponding to the problem formulation becomes

\[
T(r, t) = T_0 - \frac{1}{\sqrt{\tau}} \int_0^t e^{-t/(2\tau)} I_0\left( \frac{t - \zeta}{2\tau} \sqrt{1 - \frac{u^2}{c^2}} \right) \frac{\partial[T(r, \zeta) - p(r, \zeta)]}{\partial r} d\zeta

+ \left( \frac{u}{2\tau c} - \frac{\gamma c}{r} \right) \int_0^t e^{-t/(2\tau)} I_0\left( \frac{t - \zeta}{2\tau} \sqrt{1 - \frac{u^2}{c^2}} \right) [T(r, \zeta) - T_0]

- p(r, \zeta) d\zeta + \frac{\gamma u}{r \sqrt{1 - \frac{u^2}{c^2}}} \int_0^t e^{-t/(2\tau)} \sinh\left( \frac{t - \zeta}{2\tau} \sqrt{1 - \frac{u^2}{c^2}} \right)

\times [T(r, \zeta) - T_0 - p(r, \zeta)] d\zeta + p(r, t), \tag{25}
\]

where \(c = \sqrt{\frac{\alpha}{\tau}}\) is the speed of thermal waves propagation \([15]\), \(p(r, t)\) is the inverse Laplace transform of the particular solution \(P(r, s)\).

Finally, substituting constitutive Eq. (3) relating the temperature \(T\) with the heat flux \(q''\) and rewritten for one dimensional case with constant \(u\) and \(\alpha\), namely
into Eq. (25), the solution can be rewritten as follows

\[
-
\frac{\partial T(r,t)}{\partial r} = \frac{1}{\alpha} \left[ \frac{1}{C} \left\{ q''(r,t) + \tau \frac{\partial q''(r,t)}{\partial t} \right\} - uT(r,t) \right],
\]

(26)

where \( q'' \) denotes the effective flux due to the presence of the source function in the original equation, \( R \) represents the radius of curvature of the surface. The sign of \( R \) must be the same as the sign of the parameter \( \gamma \).

Eq. (27) is an generalized relation between the local values of temperature and the corresponding heat flux of heat transfer modeled by Eq. (7). It provides a relationship between the local values of the temperature \( T \) and the corresponding heat flux \( q'' \) and is valid everywhere within the domain, including the domain boundary.

5. Some special cases of the solution

In some special cases, the solution given by Eq. (27) must reduce to some known solutions of heat transport problems. In this section, it is shown that this is really the case.
Note that $I_0(z) \sim \frac{e^z}{\sqrt{2\pi z}}$ is large [18, page 377]. Hence, in the case $\tau = 0$ and $u = 0$, Eq. (27) reduces to

$$
T(x, t) = T_0 + \frac{1}{\Gamma(-\rho)} \int_0^t \frac{f(\zeta)}{(t - \zeta)^{\rho+1}} d\zeta,
$$

where derivatives of a negative fractional order $\rho$ are defined as

$$
\left\{ \frac{d^\rho}{dt^\rho} f(t) = \frac{1}{\Gamma(-\rho)} \int_0^t \frac{f(\zeta)}{(t - \zeta)^{\rho+1}} d\zeta \right\}
$$

where $f(t)$ is the function for which the above integral exists.

The solution given by (28) was reported for the case of no source function in [16,17].

Furthermore, if $\gamma = 0$ in Eq. (28) - which corresponds to the planar geometry – the solution becomes identical to the solution reported in [8]. If the source function is absent in the original equation, then Eq. (28) with $\gamma = 0$ becomes the case reported in [7].

Finally, in the case of $u = 0$, the solution given by Eq. (27) becomes

$$
T(x, t) = T_0 + \frac{1}{l} \int_0^t e^{\frac{t-\zeta}{2\tau}} I_0 \left( \frac{t - \zeta}{2\tau} \right) \left[ \frac{1}{C} \left\{ q''(x, \zeta) + t \frac{\partial q''(x, \zeta)}{\partial \zeta} \right\} \right.

$$

$$
+ \beta(x, \zeta) \bigg] d\zeta - \frac{\gamma c}{x \pm R} \int_0^t e^{\frac{t-\zeta}{2\tau}} I_0 \left( \frac{t - \zeta}{2\tau} \right)

$$

$$
\times \left[ T(x, \zeta) - T_0 - p(x, \zeta) \right] d\zeta + p(x, t),
$$

In the case of $\gamma = 0$ and no source function, Eq. (30) becomes identical with the integral equation which was reported in [10].
6. Model validation

To validate the model, Eq. (27) has been numerically solved for various sets of parameters. The physical properties of the domain were set as follows: \( c = 10^3 \text{ m s}^{-1} \) and \( \alpha = 10^{-8} \text{ m}^2 \text{ s}^{-1} \). Such a choice was made in order to be consistent with the results obtained in [10].

Please note that in Eq. (27) all the terms \( p(x,t) \) and \( \beta(x,t) \), associated with the source term in Eq. (7) were set to zero. This was done, in order to see the effects of the domain geometry and boundary speed clearer. Several cases of solutions containing the source term were considered in [8,19]. Also, due to the linearity of Eq. (7), the effect from the source can be superimposed on the solutions presented in this section.

Fig. 1 shows the normalized value of the temperature, \( T/T_{max} \), on the moving planar boundary for different values of the boundary speed, when the flux is constant (\( q'' = 100 \text{ W m}^{-2} \)). The solution for the latter case is well-known, \( T/T_{max} \sim \sqrt{t} \). One can see from Fig. 1 that the solution grows slower the stronger the convective effect.

Fig. 2 presents the case of an expanding sphere \( (R = 4 \cdot 10^8 \text{ m}) \). The evolution of the normalized transported property is shown on the boundary of the sphere, provided the surface flux is constant \( (q'' = 100 \text{ W m}^{-2}) \). The parameters \( c \) and \( \alpha \) in the transport equation were set the same as in the previous case. The solution is further compared with the case of a stationary sphere \( (u = 0) \).

Fig. 3 shows the evolution of the normalized temperature on the moving boundary \( (u = 0.5c) \) in the case of a Gaussian flux. The heat flux was modeled as the surface flux \( q''_{surf}(t) = e^{-(t-b)^2} \) with \( b = 10 \) picoseconds and \( \sigma = 5 \) picoseconds, that mimics an almost instantaneous source of energy. Such a choice was made in order to provide a comparison with the results obtained previously for the laser pulse heating [10].

It is evident from Fig. 3 that, for the given set of conditions, the fastest heat transfer
takes place in the case of the spherical geometry. Yet all the solutions converge to each other as time increases. This is easily explained from the fact that the radius of the surface curvature increases as time goes on, \( \lim_{t \to \infty} R = \infty \), which corresponds to the planar geometry.

Finally, Fig. 4 shows the results obtained in the case of an expanding sphere \((R = 4 \cdot 10^{-8} \text{ m})\) with the Gaussian surface heat flux (the same as in the preceding case). The effect of convection is clearly seen in the figure.

7. Conclusions

The paper presents further development and generalization of the method that allows obtaining analytical solutions of various heat transfer problems. The method is based on a technique that involves the use of generalized derivatives (sometimes reducible to derivatives of non-integer orders, known as fractional differ-integrals). In this paper, the generalized equation of heat transfer has been derived by coupling the conservation equation with the constitutive equation that represented the heat flux as the superposition of the classical Fourier’s term and convective term. The constitutive equation also accounted for a possible finite time lag between the onset of the gradient of the temperature and the corresponding heat flux. The equation of heat transfer thus obtained was then solved in its one-dimensional form within a semi-infinite domain whose geometry was governed by one of the parameters in the equation. The solution has been written in the form of convolution (memory) integrals that relate the local values of the temperature and the corresponding heat flux. Such solutions are valid everywhere within the domain, including the domain boundary.

Furthermore, it has been shown that, in many special cases, the solution reduces to less general solutions that have been reported previously.

To validate the model, various solutions of the resulting integral equation have been numerically obtained. In the case of the planar geometry, all these solutions coincide
with the solutions obtained in previous works. Furthermore, it has been shown that the solutions obtained in the case of the spherical geometry converge to the corresponding planar solutions as the radius of the surface curvature increases.

In addition, the solution given by Eq. (27) provides some important cues of how heat transfer processes take place in general. Thus, for instance, it follows that a certain maximal speed of heat transfer should exist such that no process of heat transfer may occur with the speed larger than that maximum speed $c$. Furthermore, although allowed being very small, the time lag, $\tau$, in the solution is finite. This time lag may be viewed as the characteristic time, during which thermal waves exist. Moreover, the solution contains the characteristic length, $l$, which provides the order of the thermal wave propagation distance. Curiously enough, in the case of a non-zero value of the velocity $u$, the solution given by Eq. (27) becomes a mapping of the form $T_{n+1} = \mathcal{S}(T_n)$, where $\mathcal{S}$ denotes the integral operator in (27). Therefore, the integral relation (27) allows of chaotic or even biotic (self-organized) solutions [20]. This may become the topic of future studies.
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Fig. 4  Normalized value of the temperature in the case of an expanding sphere (Gaussian flux).
Fig. 1
Fig. 2
Fig. 3