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A Variational Calculation of Diffusive Flux in a Mixed Boundary Value Problem

Calcul variationnel du flux diffusif dans un problème de valeurs limites mixtes

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Abstract. A variational solution to the transient heat flow measure above a closed conductive region of arbitrary perimeter aspect, held at constant temperature, and which is embedded in an otherwise insulating boundary plane, is presented. Upon developing the general variational formulation, a full range solution for the circular disk conductor is considered as an example when implementing a two term trial function that comprises a general form based on known physical solutions to the problem at long and short times. The particular combination of the Lagrange density for the total transient diffusive flux and of the form of the trial functions are evidently effective in dealing with the difficulties often experienced when dealing with mixed boundary value heat transfer problems of the parabolic type which have a non-periodic time variable.

Résumé. Une solution variationnelle à la mesure du flux thermique transitoire au-dessus d'une région conductrice fermée d'aspect de périmètre arbitraire, maintenue à température constante, et qui est encadrée dans un plan limite autrement isolant, est présentée. Après avoir développé la formulation variationnelle générale, une solution complète pour le conducteur en forme de disque circulaire est considérée comme un exemple lors de la mise en œuvre d'une fonction d'essai à deux termes qui comprend une forme générale basée sur des solutions physiques connues du problème à des temps longs et courts. La combinaison particulière de la densité de Lagrange pour le flux diffusif transitoire total et de la forme des fonctions d'essai est évidemment efficace pour traiter les difficultés souvent rencontrées lors du traitement des problèmes de transfert de chaleur à valeur limite mixte de type parabolique qui ont une variable temporelle non périodique.

Keywords. Variational solution, Embedded conductor, Mixed boundary condition, Heat equation, Circular Disk.

Mots-clés. Solution variationnelle, conducteur incorporé, condition limite mixte, équation de la chaleur, disque circulaire.

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1. Introduction

This work concerns the development of a variational solution e.g. see [1] to a mixed boundary value heat transfer equation problem, in terms of a single monotonic expression across the full range of the system dimensionless time and distance variable. The result, in terms of the total transient diffusive heat flux, is appropriate to describe a smooth, two dimensional thermal conductor of arbitrary perimeter aspect, that is embedded in an otherwise insulating plane, e.g. $z = 0$. The inhomogeneous boundary value specification considered comprises a zero thermal flux condition over the insulated portion of the plane, and a constant temperature condition on the surface of the conductor, which are maintained at times $t > 0$. Initially, a constant temperature measure is specified throughout the entire half-space domain above the $z = 0$ plane. Diagrams of the Cartesian and circular coordinate systems used herein for analysis of the problem are shown in Figure 1.

At the outset, it is pointed out that generally, variational methods are most valuable in evaluating the relative efficacy of different physical models that describe conservative processes (and many conditioned dissipative processes) as they progress along specified system coordinates between two defined states. On the other hand, when no full analytic solution is known, the method may often be used effectively to obtain very accurate estimations (and sometimes analytic [2] solutions) to the problem.

Attention here is paid to the implementation and evaluation of a variational framework for solving mixed boundary heat transfer value problems (i.e. Zaremba type [3] comprising arbitrary shaped planar thermal sources. The variational solution for the present mixed boundary problem evidently has heretofore not been amenable to resolution to a single solution across the full range of a dimensionless system variable. To do so requires finding a symmetric operator on the trial function comprising the surface sources specified by the mixed boundary conditions, and a representation of same that can be made stationary with respect to first order changes in the path variables. The framework described uses a Fourier representation of the thermal source as a symmetric operator. Operationally, the mixed boundary parabolic heat transfer equation system is Laplace transformed, effectively moving the time dependency to a frequency one, exposing an elliptic modified Helmholtz equation system. A stationary form of a functional describing the transformed surface flux can be written as an integral equation solution of the new system. Using a symmetric Fourier representation of the boundary source functions, the equation system then contains a linear variational principle needed to assure a stationary form leading to the relevant solution. After integration of the result in Laplace space, the transient components of the inverse transform are assembled to obtain the total transient heat flux measure over the conductor.

The framework may be used to test trial functions for the total transient heat flow over any planar, arbitrary perimeter thermal source. The efficacy of the framework is demonstrated in this work by analysis of various example trial functions pertaining to flow over the inlaid circular disk source; this example is chosen since in this rare case, the analytical result is known (*vide infra*). Good estimates for the flux may be obtained for the flux at either short, or long, or all times with selected single term trial functions. Herein, a considered but simple two term trial function gives an accurate interpolation for the full range variable space.

As regards the specific example of the embedded circular disk thermal source conductor being applied to the present problem, only recently has the analytic solution been resolved. Bieniasz [4] has provided the analytic solution to the parabolic diffusion equation applied to electrochemical mass transport for the subject circular disk problem. It is usually found that mixed, non-harmonic time dependent flux and constant temperature boundary conditions on the same plane often complicate matters; e.g. the structure of several discontinuous integrals normally effective in the solution of many parabolic non-linear homogeneous heat transport problems

is destroyed. The approach taken by Bieniasz avoids these difficulties. After Laplace transformation of the parabolic equation system for the circular disk problem in cylindrical coordinates, conversion of the transformed differential equations to oblate spherical coordinates, which represent orthogonal profiles of constant temperature and flux profiles over the circular disk, the so-

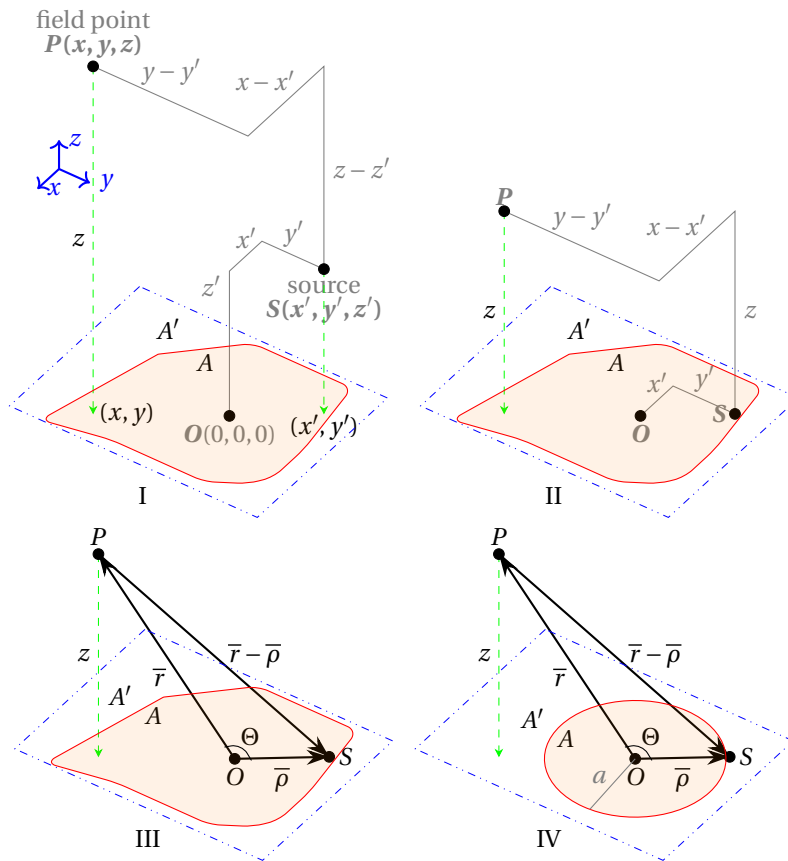


Figure 1. (I) A standard system of Cartesian coordinates for a general heat transfer problem posed in the half space above an infinite plane A' at $z = 0$. The system is referenced to $O(0,0,0) \in A$, which represents a conducting, closed region embedded in A' , which is otherwise everywhere insulating. A thermal point source $S(x', y', z')$ and an arbitrary diffusion field point $P(x, y, z)$ lie in the half space $z \geq 0$. (II) The present problem requires that all thermal sources $S(x', y', z')$ are present only on the surface of A , i.e., $S(x', y', 0) = S(x', y')$. (III) Variational functionals that arise for the surface flux under the conditions of (II) after Fourier transformation of the system of equations, are more conveniently reduced if the system is also expressed in terms of circular coordinates. Here are shown the 3 characteristic vectors required to specify the spatial aspect of the distances between the sources and field points for a conductive region of arbitrary perimeter aspect, and in (IV) the circular disk conductor that is discussed as an example in this work. In (III) and (IV), $\bar{\rho} = \bar{\rho}(x', y')$ is a two dimensional vector locating surface heat sources $S(x', y') \in A$ at $t \geq 0$. The vector $\bar{r} = \bar{r}(x, y, z)$ locates arbitrary points $P(x, y, z)$ in the half-space so specifying the magnitude of the difference vector $\bar{r} - \bar{\rho}$ as the distance between arbitrary field points and surface sources.

lution for the circular disk problem, after inverse transformation to the time domain, follows in terms of infinite series of spheroidal wave functions. Numerical evaluation of these series is not trivial, and requires significant computational resources. In subsequent work, Bieniasz [5] provides several selected approximation techniques to reduce the computational overhead, but at the cost of some reduction of accuracy, especially at short time scales. In any case, for research work, the full analytical solution is available for very high accuracies across the entire time range. Analytic solutions to other arbitrary perimeter planar sources under mixed boundary conditions of this type are rare.

2. Formulation of the variational inequality

Consider diffusive heat transport in the semi-infinite space region A' (the $z = 0$ plane); except for a finite section A thereon, which is conductive, the plane has an insulating boundary condition. If the temperature $u(x, y, z, 0) = U_0$ is constant throughout the domain $z > 0$ at the initial instant of time $t = 0$, and a value $u(x, y, 0, t) = U_1$ is maintained over the section A for all subsequent times, the relevant equations for $u(x, y, z, t)$ are

$$\begin{aligned}\nabla^2 u - \frac{1}{k} \frac{\partial u}{\partial t} &= 0, \quad z > 0 \\ u(x, y, z, 0) &= U_0, \quad z > 0 \\ u(x, y, 0, t) &= U_1, \quad (x, y) \in A \\ \frac{\partial}{\partial z} u|_{z=0} &= 0, \quad (x, y) \in A',\end{aligned}\tag{1}$$

wherein the region is characterized by isotropic constant thermal diffusivity $k = \kappa / \rho c_p$ (with density ρ , thermal conductivity κ , and specific heat c_p). A modified Helmholtz equation representation for the problem is evident after a Laplace integral transform of the system i.e.

$$\begin{aligned}\bar{u}(x, y, z, p) &= \int_0^\infty \exp(-pt) u(x, y, z, t) dt \\ \nabla^2 \bar{u} - \lambda^2 \bar{u} &= -\frac{U_0}{k}, \quad \lambda^2 = \frac{p}{k} \\ \bar{u} &= \frac{U_0}{p} + \bar{U}(x, y, z, p) \\ \nabla^2 \bar{U} - \lambda^2 \bar{U} &= 0 \\ \bar{U}(x, y, z, p) &= \frac{1}{2\pi} \int_A \frac{\exp(-\lambda |\vec{r} - \vec{\rho}'|)}{|\vec{r} - \vec{\rho}'|} \left(-\frac{\partial \bar{U}}{\partial z'} \right)_{z'=0} d\vec{\rho}',\end{aligned}\tag{2}$$

wherein the Fourier integral equation for $\bar{U}(x, y, z, p)$ in the last line of Equation (2) is admitted by Fourier transform of the modified Helmholtz equation.

An integral equation for the transformed normal magnitude of \bar{U} over surface of the bounding (x, y) plane,

$$-\frac{\partial \bar{U}}{\partial z'} \Big|_{z'=0} = \bar{F}(\vec{\rho}), \quad \vec{\rho} \in A\tag{3}$$

then is

$$\frac{U_1 - U_0}{p} = \frac{1}{2\pi} \int_A \frac{\exp(-\lambda |\vec{\rho} - \vec{\rho}'|)}{|\vec{\rho} - \vec{\rho}'|} \bar{F}(\vec{\rho}') d\vec{\rho}', \quad \vec{\rho} \in A,\tag{4}$$

From Equation (3) a total thermal ‘‘Laplace flux’’ auxiliary function over the surface of A , may be denoted as

$$\bar{Q}(p) = \kappa \int_A \bar{F}(\vec{\rho}) d\vec{\rho}, \quad \kappa = \rho c k\tag{5}$$

and it is desired to write a variational form considering a stationary value of the functional. Note that if $\Delta U = U_1 - U_0$ then with Equations (4) and (5)

$$\frac{\Delta U}{p} \kappa \int_A \bar{F}(\bar{\rho}) d\bar{\rho} = \frac{\kappa}{2\pi} \int_A \bar{F}(\bar{\rho}) \frac{\exp(-\lambda |\bar{\rho} - \bar{\rho}'|)}{|\bar{\rho} - \bar{\rho}'|} \bar{F}(\bar{\rho}') d\bar{\rho} d\bar{\rho}'. \quad (6)$$

Furthermore

$$2 \frac{\Delta U}{p} \kappa \int_A \bar{F}(\bar{\rho}) d\bar{\rho} - \frac{\kappa}{2\pi} \int_A \bar{F}(\bar{\rho}) \frac{\exp(-\lambda |\bar{\rho} - \bar{\rho}'|)}{|\bar{\rho} - \bar{\rho}'|} \bar{F}(\bar{\rho}') d\bar{\rho} d\bar{\rho}' = \frac{\Delta U}{p} \bar{Q}(p) \quad (7)$$

constitutes a stationary variational representation for $\bar{Q}(p)$. Let $\hat{\bar{F}} = \bar{F} + \delta\bar{F}$, where \bar{F} satisfies the integral equation Equation (4). Substituting into Equation (7) and employing the coordinate symmetry of the function

$$\bar{K}(\bar{\rho}, \bar{\rho}') = \frac{1}{2\pi} \frac{\exp(-\lambda |\bar{\rho} - \bar{\rho}'|)}{|\bar{\rho} - \bar{\rho}'|}, \quad (8)$$

it follows that

$$\begin{aligned} \frac{\Delta U}{p} \bar{Q}(p) &= \frac{\Delta U}{p} \kappa \int_A \bar{F}(\bar{\rho}) d\bar{\rho} - \kappa \int_A \delta\bar{F}(\bar{\rho}) \bar{K}(\bar{\rho}, \bar{\rho}') \delta\bar{F}(\bar{\rho}') d\bar{\rho} d\bar{\rho}' \\ &= \frac{\Delta U}{p} \kappa \int_A \bar{F}(\bar{\rho}) d\bar{\rho} - \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} \frac{d\xi d\eta}{\sqrt{\xi^2 + \eta^2 + \lambda^2}} \left| \int_A \delta\bar{F} \exp(i\xi x + i\eta y) dx dy \right|^2 \\ &< \frac{\Delta U}{p} \kappa \int_A \bar{F}(\bar{\rho}) d\bar{\rho}, \end{aligned} \quad (9)$$

in as much as

$$\begin{aligned} &\frac{\exp(-\lambda |\bar{r} - \bar{r}'|)}{2\pi |\bar{r} - \bar{r}'|} \\ &= \frac{2}{(2\pi)^3} \int_{-\infty}^{\infty} \frac{\exp(i\xi(x-x') + i\eta(y-y') + i\zeta(z-z'))}{\xi^2 + \eta^2 + \zeta^2 + \lambda^2} d\xi d\eta d\zeta \\ &= \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} \frac{\exp(i\xi(x-x') + i\eta(y-y'))}{\sqrt{\xi^2 + \eta^2 + \lambda^2}} \exp\left(-\sqrt{\xi^2 + \eta^2 + \lambda^2} |z-z'|\right) d\xi d\eta \\ &= \frac{1}{(2\pi)^2} \int_0^{\infty} \frac{\sigma d\sigma}{\sqrt{\sigma^2 + \lambda^2}} \exp\left(-\sqrt{\sigma^2 + \lambda^2} |z-z'|\right) \int_{\Theta}^{\Theta+2\pi} \exp(i\sigma R \cos(\Psi - \Theta)) d\Psi \\ &= \frac{1}{2\pi} \int_0^{\infty} \frac{\sigma J_0(\sigma R)}{\sqrt{\sigma^2 + \lambda^2}} \exp\left(-\sqrt{\sigma^2 + \lambda^2} |z-z'|\right) d\sigma \end{aligned} \quad (10)$$

using

$$R^2 = (x-x')^2 + (y-y')^2, \quad \cos\Theta = (x-x')/R, \quad \sin\Theta = (y-y')/R, \quad (11)$$

see Figure 1. Thus

$$\bar{Q}|_{\text{variational estimate}} < \bar{Q}|_{\text{true value}} \quad (12)$$

establishes that the use of increasingly accurate trial functions for $\bar{F}(\bar{\rho})$ in Equation (7) result in variational solutions to the total flux values that approach the true value from below.

3. Formulation and analysis using a two-term trial function

Write, using Equations (7) and (8),

$$\bar{Q}(p) = 2\kappa \int_A \bar{F}(\bar{\rho}) d\bar{\rho} - \frac{\kappa p}{\Delta U} \int_A \bar{F}(\bar{\rho}) \bar{K}(\bar{\rho}, \bar{\rho}') \bar{F}(\bar{\rho}') d\bar{\rho} d\bar{\rho}', \quad (13)$$

and adopt the two term trial function

$$\bar{F}(\bar{\rho}) = \frac{\alpha}{\lambda} + \frac{\beta f(\bar{\rho})}{\lambda^2} \quad (14)$$

with

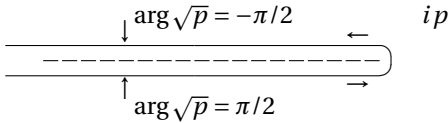
$$\int_A f(\bar{\rho}) K(\bar{\rho}, \bar{\rho}')|_{\lambda=0} d\bar{\rho}' = 1, \quad \rho \in A, \quad (15)$$

whose respective parts are suggested by approximate solutions of the integral equation Equation (4) in the limits $\lambda \rightarrow \infty$, $\lambda \rightarrow 0$.

Now

$$\begin{aligned} \bar{Q}(p) &= \frac{2\kappa\alpha}{\lambda} A + \frac{2\kappa\beta}{\lambda^2} \int_A f(\bar{\rho}) d\bar{\rho} - \frac{k\kappa\alpha^2}{\Delta U} \int_A \bar{K}(\bar{\rho}, \bar{\rho}') d\bar{\rho} d\bar{\rho}' \\ &\quad - 2\kappa \frac{k\alpha\beta}{\lambda\Delta U} \int_A \bar{K}(\bar{\rho}, \bar{\rho}') f(\bar{\rho}') d\bar{\rho} d\bar{\rho}' \\ &\quad - \frac{k\kappa\beta^2}{\lambda^2\Delta U} \int_A f(\bar{\rho}) \bar{K}(\bar{\rho}, \bar{\rho}') f(\bar{\rho}') d\bar{\rho} d\bar{\rho}' \end{aligned} \quad (16)$$

and inverse Laplace transformation is now appropriate:



$$\begin{aligned} P_1 &= \frac{1}{2\pi i} \int \exp(pt) \exp(-\sqrt{p}\mu) dp, \quad \mu > 0 \\ &= \frac{1}{2\pi i} \left[\int_{\infty}^0 \exp(-vt) \exp(i\mu\sqrt{v}) (-dv) + \int_0^{\infty} \exp(-vt) \exp(-i\mu\sqrt{v}) (-dv) \right] \\ &= \frac{1}{\pi} \int_0^{\infty} \exp(-vt) \sin \mu\sqrt{v} dv = \frac{2}{\pi} \int_0^{\infty} \exp(-x^2 t) \sin \mu x dx \\ &= \frac{1}{\pi} \int_0^{\infty} \sin \mu x d\left(\frac{\exp(-x^2 t)}{t}\right) = \frac{\mu}{\pi t} \int_0^{\infty} \exp(-x^2 t) \cos \mu x dx \\ &= \frac{\mu}{\pi t} \cdot \frac{1}{2} \sqrt{\frac{\kappa}{t}} \exp\left(-\frac{\mu^2}{4t}\right) = \frac{\mu}{2\sqrt{\pi}} \cdot \frac{1}{t^{3/2}} \exp\left(-\frac{\mu^2}{4t}\right) \end{aligned} \quad (17)$$

$$\begin{aligned} P_2 &= \frac{1}{2\pi i} \int \exp(pt) \frac{\exp(-\sqrt{p}\mu)}{\sqrt{p}} dp \\ &= \frac{1}{2\pi i} \left[\int_{\infty}^0 \exp(-vt) \exp(i\mu\sqrt{v}) \frac{(-dv)}{-i\sqrt{v}} + \int_0^{\infty} \exp(-vt) \exp(-i\mu\sqrt{v}) \frac{(-dv)}{i\sqrt{v}} \right] \\ &= \frac{1}{\pi} \int_0^{\infty} \exp(-vt) \frac{\cos \mu\sqrt{v}}{\sqrt{v}} dv = \frac{2}{\pi} \int_0^{\infty} \exp(-x^2 t) \cos \mu x dx \\ &= \frac{2}{\pi} \cdot \frac{1}{2} \sqrt{\frac{\kappa}{t}} \exp\left(-\frac{\mu^2}{4t}\right) = \frac{1}{\sqrt{\pi t}} \exp\left(-\frac{\mu^2}{4t}\right) \end{aligned} \quad (18)$$

$$\begin{aligned} P_3 &= \frac{1}{2\pi i} \int \exp(pt) \frac{\exp(-\sqrt{p}\mu)}{p} dp, \quad \frac{dP_3}{d\mu} = -P_2 = -\frac{1}{\sqrt{\pi t}} \exp(-\mu^2/4t) \\ &= \frac{1}{\sqrt{\pi t}} \int_0^{\mu} \exp(-v^2/4t) dv + \text{Constant} = \frac{2}{\sqrt{\pi}} \int_0^{\mu/2\sqrt{t}} \exp(-\xi^2) d\xi + 1 \\ &= 1 + \operatorname{erf}\left(\frac{\mu}{2\sqrt{t}}\right) \end{aligned} \quad (19)$$

With the identification $\mu = R/\sqrt{k}$, it follows from Equation (16) that

$$\begin{aligned}
 Q(t) = & \frac{2\kappa\alpha Ak}{\sqrt{\pi kt}} + 2\kappa k\beta \int_A f(\vec{\rho}) d\vec{\rho} \\
 & - \frac{k^2\kappa\alpha^2}{\Delta U} \frac{1}{4(\pi kt)^{3/2}} \int_A d\vec{\rho} d\vec{\rho}' \exp(-R^2/4kt) \\
 & - \frac{2\kappa\alpha\beta k^2}{\sqrt{\pi t}\Delta U} \int_A \frac{d\vec{\rho} d\vec{\rho}'}{2\pi R} \exp(-R^2/4kt) f(\vec{\rho}') \\
 & - \frac{\kappa\beta^2 k^2}{\Delta U} \int_A \frac{d\vec{\rho} d\vec{\rho}'}{2\pi R} f(\vec{\rho}) f(\vec{\rho}') \left[1 + \operatorname{erf}\left(\frac{R}{2\sqrt{kt}}\right) \right].
 \end{aligned} \tag{20}$$

In the limit $R/\sqrt{kt} \rightarrow 0$,

$$Q(t) \doteq 2\kappa k\beta \int_A f(\vec{\rho}) d\vec{\rho} - \frac{\kappa\beta^2 k^2}{\Delta U} \int_A f(\vec{\rho}) d\vec{\rho}, \tag{21}$$

and the condition $\partial Q/\partial\beta = 0$ leads to the specification

$$k\beta = \Delta U. \tag{22}$$

Given that

$$\frac{1}{4\pi kt} \exp\left[-\frac{(x-x')^2 + (y-y')^2}{4kt}\right] \rightarrow \delta(x-x') \delta(y-y'), \tag{23}$$

the representation Equation (20) implies that

$$Q(t) \rightarrow \frac{2\kappa\alpha Ak}{\sqrt{\pi kt}} - \frac{k^2\kappa\alpha^2}{\Delta U\sqrt{\pi kt}} + O(1), \quad t \rightarrow 0 \tag{24}$$

and the condition $\partial Q/\partial\alpha = 0$ provides the specification

$$k\alpha = \Delta U \tag{25}$$

whence Equation (20) acquires the definite form

$$\begin{aligned}
 Q(t) = & \frac{2A\Delta U\kappa}{\sqrt{\pi kt}} + 2\kappa\Delta U \int_A f(\vec{\rho}) d\vec{\rho} \\
 & - \frac{\kappa\Delta U}{4(\pi kt)^{3/2}} \int_A d\vec{\rho} d\vec{\rho}' \exp(-R^2/4kt) \\
 & - \frac{2\kappa\Delta U}{\sqrt{\pi t}} \int_A \frac{d\vec{\rho} d\vec{\rho}'}{2\pi R} \exp(-R^2/4kt) f(\vec{\rho}') \\
 & - \kappa\Delta U \int_A \frac{d\vec{\rho} d\vec{\rho}'}{2\pi R} f(\vec{\rho}) f(\vec{\rho}') \left[1 + \operatorname{erf}\left(\frac{R}{2\sqrt{kt}}\right) \right],
 \end{aligned} \tag{26}$$

which assumes the proper limiting values when $t \rightarrow 0$ and $t \rightarrow \infty$.

4. Application of a specific trial function appropriate to the circular disk

Consider now that the domain A has a circular aspect of radius a , and return to Equation (5) with the above specifications for α, β , i.e.:

$$\begin{aligned}
 \bar{Q}(p) = & \frac{2\kappa\Delta UA}{k\lambda} + \frac{2\kappa\Delta U}{k\lambda^2} \int_A f(\vec{\rho}) d\vec{\rho} - \frac{\kappa\Delta U}{k} \int_A \bar{K}(\vec{\rho}, \vec{\rho}') d\vec{\rho} d\vec{\rho}' \\
 & - 2\kappa \frac{\Delta U}{k\lambda} \int_A \bar{K}(\vec{\rho}, \vec{\rho}') f(\vec{\rho}') d\vec{\rho} d\vec{\rho}' - \frac{\kappa\Delta U}{\kappa\lambda^2} \int_A f(\vec{\rho}) \bar{K}(\vec{\rho}, \vec{\rho}') f(\vec{\rho}') d\vec{\rho} d\vec{\rho}'
 \end{aligned} \tag{27}$$

and

$$f(p) = \frac{2}{\pi} \frac{1}{\sqrt{a^2 - \rho^2}}. \tag{28}$$

Thus

$$\int_A f(\bar{\rho}) d\bar{\rho} = \frac{2}{\pi} \cdot 2\pi \int_0^a \frac{\rho d\rho}{\sqrt{a^2 - \rho^2}} = 4a, \quad (29)$$

$$\int_A \bar{K}(\bar{\rho}, \bar{\rho}') d\bar{\rho} d\bar{\rho}' = \frac{1}{2\pi} \int_0^\infty \frac{d\sigma}{\sqrt{\sigma^2 + \lambda^2}} \int_A J_0(\sigma R) d\bar{\rho} d\bar{\rho}' \quad (30)$$

$$= 2\pi \int_0^\infty \frac{\sigma d\sigma}{\sqrt{\sigma^2 + \lambda^2}} \left(\int_0^a \rho J_0(\sigma \rho) d\rho \right)^2 = 2\pi a^2 \int_0^\infty \frac{J_1^2(\sigma a)}{\sigma \sqrt{\sigma^2 + \lambda^2}} d\sigma, \quad (31)$$

$$\int_A \bar{K}(\bar{\rho}, \bar{\rho}') f(\bar{\rho}') d\bar{\rho} d\bar{\rho}' = \frac{1}{2\pi} \int_0^\infty \frac{\sigma d\sigma}{\sqrt{\sigma^2 + \lambda^2}} (2\pi)^2 \frac{2}{\pi} \int_0^a \rho J_0(\sigma \rho) d\rho \int_0^a \frac{\rho' J_0^2(\sigma \rho')}{\sqrt{a^2 - \rho'^2}} d\rho' \quad (32)$$

$$= 4a \int_0^\infty \frac{J_1(\sigma a)}{\sqrt{\sigma^2 + \lambda^2}} \frac{\sin \sigma a}{\sigma} d\sigma, \quad (33)$$

$$\int_A f(\bar{\rho}) \bar{K}(\bar{\rho}, \bar{\rho}') f(\bar{\rho}') d\bar{\rho} d\bar{\rho}' = \frac{1}{2\pi} \left(\frac{2}{\pi} \right)^2 (2\pi)^2 \int_0^a \frac{\sigma d\sigma}{\sqrt{\sigma^2 + \lambda^2}} \left(\int_0^a \frac{\rho J_0(\sigma \rho) d\rho}{\sqrt{a^2 - \rho^2}} \right)^2 \quad (34)$$

$$= \frac{8}{\pi} \int_0^\infty \frac{\sin^2 \sigma a}{\sqrt{\sigma^2 + \lambda^2}} \frac{d\sigma}{\sigma}. \quad (35)$$

Accordingly

$$\begin{aligned} \bar{Q}(p) &= \frac{2\kappa \Delta U A}{k\lambda} + \frac{2\kappa \Delta U}{k\lambda^2} \cdot 4a - \frac{\kappa \Delta U}{k} \cdot 2\pi a^2 \int_0^\infty \frac{J_1^2(\sigma a)}{\sigma \sqrt{\sigma^2 + \lambda^2}} d\sigma \\ &\quad - 2\kappa \frac{\Delta U}{k\lambda} \cdot 4a \int_0^\infty \frac{J_1(\sigma a)}{\sqrt{\sigma^2 + \lambda^2}} \frac{\sin \sigma a}{\sigma} d\sigma \\ &\quad - \frac{\kappa \Delta U}{k\lambda^2} \cdot \frac{8}{\pi} \int_0^\infty \frac{\sin^2 \sigma a}{\sqrt{\sigma^2 + \lambda^2}} \frac{d\sigma}{\sigma}. \end{aligned} \quad (36)$$

Inverse Laplace transform is now in order, and the appropriate results i.e.

$$\begin{aligned} \Phi_1 &= \frac{1}{2\pi i} \int \exp(pt) \frac{dp}{\sqrt{\sigma^2 + p/k}} \\ &= \frac{\sqrt{k}}{2\pi i} \left\{ \int_\infty^{k\sigma^2} \exp(-\xi t) \frac{(-d\xi)}{-i\sqrt{\xi - k\sigma^2}} + \int_{k\sigma^2}^\infty \exp(-\xi t) \frac{(-d\xi)}{i\sqrt{\xi - k\sigma^2}} \right\} \\ &= \frac{\sqrt{k}}{\pi} \int_{k\sigma^2}^\infty \exp(-\xi t) \frac{d\xi}{\sqrt{\xi - k\sigma^2}} = 2 \frac{\sqrt{k}}{\pi} \int_0^\infty \exp(-(k\sigma^2 + v^2)t) dv \\ &= 2 \frac{\sqrt{k}}{\pi} \exp(-k\sigma^2 t) \cdot \frac{1}{2} \sqrt{\frac{\pi}{t}} = \sqrt{\frac{k}{\pi t}} \exp(-k\sigma^2 t), \end{aligned} \quad (37)$$

$$\begin{aligned} \Phi_2 &= \frac{1}{2\pi i} \int \exp(pt) \frac{dp}{p\sqrt{\sigma^2 + p/k}}, \quad \frac{d\Phi_2}{dt} = \Phi_1 = \sqrt{\frac{k}{\pi t}} \exp(-k\sigma^2 t) \\ &= \frac{1}{\sigma} - \frac{2}{\pi} \sqrt{k} \exp(-k\sigma^2 t) \int_0^\infty \exp(-v t) \frac{dv}{v^2 + k\sigma^2} \rightarrow 0, t \rightarrow 0 \end{aligned} \quad (38)$$

$$\therefore \Phi_2 = \sqrt{\frac{k}{\pi}} \int_0^t \frac{1}{\sqrt{\tau}} \exp(-k\sigma^2 \tau) d\tau = \frac{2}{\sqrt{\pi \sigma}} \int_0^{\sqrt{\pi t \sigma}} \exp(-\xi^2) d\xi = \frac{1}{\sigma} \operatorname{erf}(\sqrt{k t \sigma}),$$

and the third inverse transform follows, when considering the path

$$-p\sigma^2 \overbrace{\hspace{10em}}^{\leftarrow} \underset{\rightarrow}{\hspace{10em}} 0 ,$$

i.e.

$$\begin{aligned} \Phi_3 &= \frac{1}{2\pi i} \int \exp(pt) \frac{dp}{\sqrt{p}\sqrt{\sigma^2 + p/k}} \\ &= \frac{\sqrt{k}}{\pi} \int_0^{k\sigma^2} \exp(-\xi t) \frac{d\xi}{\sqrt{\xi}\sqrt{k\sigma^2 - \xi}} = \frac{\sqrt{k}}{\pi} \int_0^1 \frac{\exp(-k\sigma^2 t \lambda)}{\sqrt{\lambda(1-\lambda)}} d\lambda \\ &= \frac{\sqrt{k}}{\pi} \exp(-k\sigma^2 t/2) \int_{-1}^1 \frac{\exp(-k\sigma^2 t \mu/2)}{\sqrt{(1-\mu^2)}} d\mu = \sqrt{k} \exp(-k\sigma^2 t/2) I_0\left(\frac{k t \sigma^2}{2}\right) . \end{aligned} \tag{39}$$

Assembling the inverse transforms Φ_1, Φ_2, Φ_3 in Equation (36) the result

$$\begin{aligned} \frac{Q(t)}{\kappa \Delta U} &= \frac{2A}{\sqrt{\pi k t}} + 8a - \frac{2A}{\sqrt{\pi k t}} \int_0^\infty \frac{J_1^2(x)}{x} \exp(-k t x^2/a^2) dx \\ &\quad - 8a \int_0^\infty J_1(x) \exp(-k t x^2/2a^2) I_0\left(\frac{k t x^2}{2a^2}\right) \frac{\sin x}{x} dx \\ &\quad - \frac{8a}{\pi} \int_0^\infty \frac{\sin^2 x}{x^2} \operatorname{erf}\left(\frac{\sqrt{k t}}{a} x\right) dx \end{aligned} \tag{40}$$

expresses an unreduced variational calculation of the total transient flux. The first integral therein can be reduced (see the Appendix) to

$$\int_0^\infty \frac{J_1^2(\alpha x)}{x} \exp(-(\beta x)^2) dx = \frac{1}{2} - \frac{1}{2} \exp(-\alpha^2/2\beta^2) \left(I_0\left(\frac{\alpha^2}{2\beta^2}\right) + I_1\left(\frac{\alpha^2}{2\beta^2}\right) \right), \tag{41}$$

and after a change of variables therein ($\alpha \rightarrow 1; \beta \rightarrow \sqrt{k t}/a$) and substitution of the resulting form into Equation (40), and rearrangement, note that

$$\frac{Q(t)}{\kappa a \Delta U} = \sqrt{\pi} \frac{a}{\sqrt{k t}} \left[1 + \exp\left(-\frac{a^2}{2k t}\right) \left(I_0\left(\frac{a^2}{2k t}\right) + I_1\left(\frac{a^2}{2k t}\right) \right) \right] dx \tag{42a}$$

$$- 8 \int_0^\infty J_1(x) \exp\left(-\frac{k t x^2}{2a^2}\right) I_0\left(\frac{k t x^2}{2a^2}\right) \frac{\sin x}{x} dx \tag{42b}$$

$$+ 8 \left(\frac{1}{2} + \frac{1}{\pi} \int_0^\infty \frac{\sin^2 x}{x^2} \operatorname{erfc}\left(\frac{\sqrt{k t}}{a} x\right) dx \right) \tag{42c}$$

provides a full range dimensionless representation of of the total variational flux measure.

Noting that the calculation asymptotically approaches the known limiting values at long and short times, i.e. $\sqrt{k t} \gg a$ and $\sqrt{k t} \ll a$:

$$\begin{aligned} \frac{Q(t)}{\kappa \Delta U} &\doteq \frac{A}{\sqrt{\pi k t}}, & \sqrt{k t} \ll a \\ &\doteq 4a, & \sqrt{k t} \gg a, \end{aligned} \tag{43}$$

and provides a continuous, non-patched and strictly monotonic (i.e. with no resonance perturbations, discontinuities, etc.) representation of the integrated flux between the known limits, Equation (42) must provide an accurate interpolation of the integrated flux over the range of the relevant system variable $\sqrt{k t}/a$.

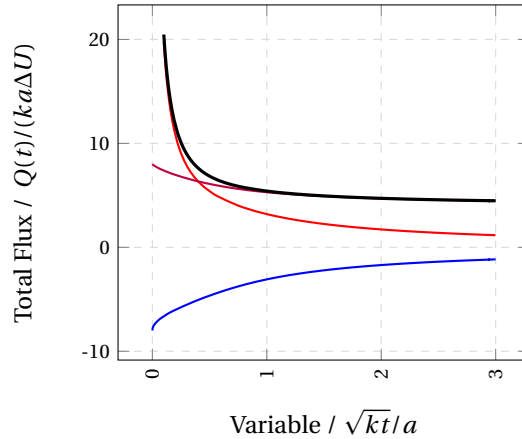


Figure 2. The variational solution for the total flux as a function of the dimensionless variable \sqrt{kt}/a in the transition range $\sqrt{kt}/a \leq 3$. The upper (black) trace is the variational result for the total flux, as given by Equation (42). The red trace represents values of Equation (42a), and is the primary short-time contributor to the total flux. The magenta trace represents values of Equation (42b) and is the primary long-time contributor to the total flux. The blue trace represents values of Equation (42c), and enters as the interpolation corrector to the sum of Equation (42a) and Equation (42b) components.

5. Other trial functions

It is instructive to consider other simple trial functions that have properties that might be considered as components for more sophisticated models for a specified problem. The exercise also demonstrates the framework’s efficacy in testing the range of applicability as a possible trial function. It is usually the case that proposed trial functions are first checked for their applicability in reproducing (or at least approaching) initial and/or final (steady state) conditions for a problem that are already known (or required).

Below are the evaluations of two trial functions that are known to provide the correct (limiting) thermal fluxes at at least one of the limits of the dimensionless variable for the mixed boundary system for the circular disk source.

5.1. A short time trial function

One might consider, for example, using the single term trial function

$$\bar{F}(\vec{\rho}) = \alpha$$

as suggested when $a^2/kt \gg 1$, so that then Equation (13) becomes

$$\bar{Q}(p) = 2\alpha\kappa A - \frac{\kappa\alpha^2 p}{\Delta U} \int_A \bar{K}(\vec{\rho}, \vec{\rho}') d\vec{\rho} d\vec{\rho}', \tag{44}$$

and the condition

$$\frac{\partial \bar{Q}}{\partial \alpha} = 0 \tag{45}$$

implies that

$$\alpha = \frac{A\Delta U}{p \int_A \bar{K}(\vec{\rho}, \vec{\rho}') d\vec{\rho} d\vec{\rho}'} \tag{46}$$

whence the variational estimate has the form

$$\bar{Q}(p) = \frac{\kappa A^2 \Delta U}{p \int_A \bar{K}(\vec{\rho}, \vec{\rho}') d\vec{\rho} d\vec{\rho}'} = \frac{\kappa A \Delta U / 2}{p \int_0^\infty (J_1^2(\sigma a) / (\sigma \sqrt{\sigma^2 + \lambda^2})) d\sigma}. \quad (47)$$

Thus

$$\bar{Q}(p) = \frac{\kappa A \Delta U / 2}{\sqrt{k p} \int_0^\infty (J_1^2(x) / x) dx} = \frac{\kappa \Delta U A}{\sqrt{k p}}, \quad p \rightarrow \infty \quad (48)$$

and therefore

$$Q(t) = \kappa \Delta U \frac{A}{\sqrt{\pi k t}}, \quad a / \sqrt{k t} \gg 1 \quad (49)$$

which comprises the known short-time limiting value of the total flux in the infinite half space above a circular conducting region with area A . On the other hand,

$$\bar{Q}(p) = \frac{\kappa A \Delta U / 2}{p \int_0^\infty (J_1^2(\sigma a) / \sigma^2) d\sigma} = \frac{\kappa A \Delta U / 2}{p a \int_0^\infty (J_1^2(x) / x^2) dx}, \quad p \rightarrow 0 \quad (50)$$

which yields

$$\begin{aligned} Q(t) &= \frac{\kappa \Delta U / 2 \cdot \pi a^2}{4a / (3\pi)} = \kappa \Delta U a \cdot \frac{3\pi^2}{8}, \quad a / \sqrt{k t} \rightarrow 0 \\ &= 3.7 \cdot \kappa \Delta U a \\ &< 4 \cdot \kappa \Delta U a, \end{aligned} \quad (51)$$

i.e. the variational estimate provides a lower bound, as expected, at long times.

5.2. A long time trial function

Next, employing another single term trial function

$$\bar{F}(\vec{\rho}) = \beta \bar{f}(\vec{\rho}), \quad f = \frac{2}{\pi} \frac{1}{\sqrt{a^2 - \rho^2}}, \quad \int_A f d\vec{\rho} = 4a \quad (52)$$

as is an appropriate form when $a^2 / k t \ll 1$,

$$\bar{Q}(p) = 2\kappa\beta \cdot 4a - \frac{\kappa p \beta^2}{\Delta U} \int_A f(\rho) \bar{K}(\vec{\rho}, \vec{\rho}') f(\rho') d\vec{\rho} d\vec{\rho}' \quad (53)$$

and the condition

$$\frac{\partial \bar{Q}}{\partial \beta} = 0 \quad (54)$$

implies that

$$\beta = \frac{4a \cdot \Delta U}{p \int_A f(\rho) \bar{K}(\vec{\rho}, \vec{\rho}') f(\rho') d\vec{\rho} d\vec{\rho}'}. \quad (55)$$

Accordingly, the corresponding variational estimate becomes

$$\begin{aligned} \bar{Q}(p) &= \kappa (4a)^2 \Delta U \frac{1}{p \int_A f(\rho) \bar{K}(\vec{\rho}, \vec{\rho}') f(\rho') d\vec{\rho} d\vec{\rho}'} \\ &= \frac{2\pi \kappa a^2 \Delta U}{p \int_0^\infty (\sin^2(\sigma a) / (\sigma \sqrt{\sigma^2 + p/k})) d\sigma} = \frac{2\pi \kappa a^2 \Delta U}{\sqrt{k p} \int_0^\infty (\sin^2(\sqrt{p/k} ax) / (x \sqrt{x^2 + 1})) dx} \\ &= \frac{2\pi \kappa a^2 \Delta U}{p \int_0^\infty \sin^2(\sigma a) / \sigma^2 d\sigma} = \frac{2\pi \kappa a \Delta U}{p \int_0^\infty \sin^2(x) / x^2 dx} \\ &= \frac{\kappa \Delta U \cdot 4a}{p}, \quad p \rightarrow 0 \end{aligned} \quad (56)$$

and

$$Q(t) = 4a \cdot \kappa \cdot \Delta U, \quad a^2 / k t \rightarrow 0, \quad (57)$$

the anticipated limit.

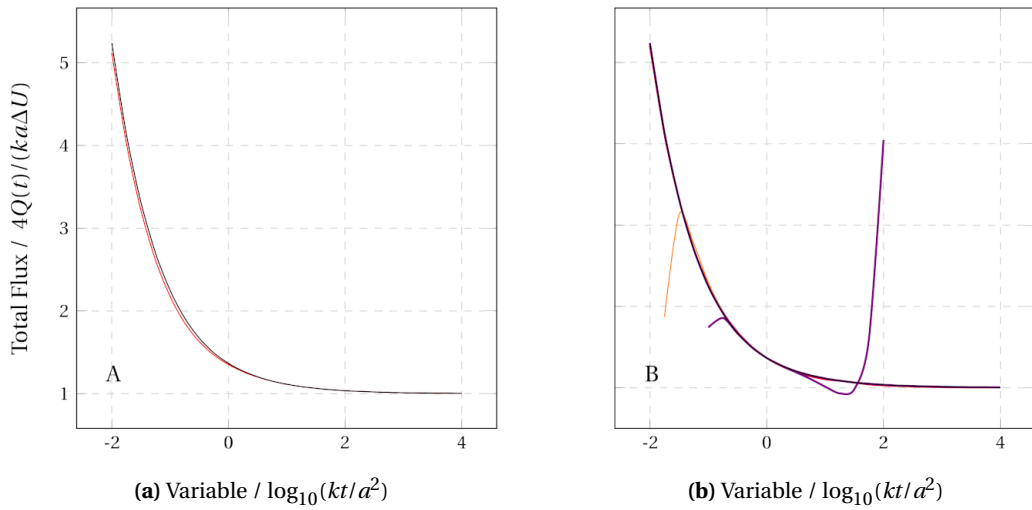


Figure 3. (a) The variational solution (red) from Equation (42) and the analytic solution (black) [4] for the transient heat flux over the circular disk as a function of the dimensionless variable $\log_{10}(kt/a^2)$ over a variable range of six orders of magnitude. (b) Examples of existing long and short time estimations: (black) [4] analytic result; (violet) Mahon [6] short and long time estimates; (orange) Aoki [7] long time estimate. Information on Shoup [8] and Rajendran and Sangaranarayanan [9–11] data is given in the text.

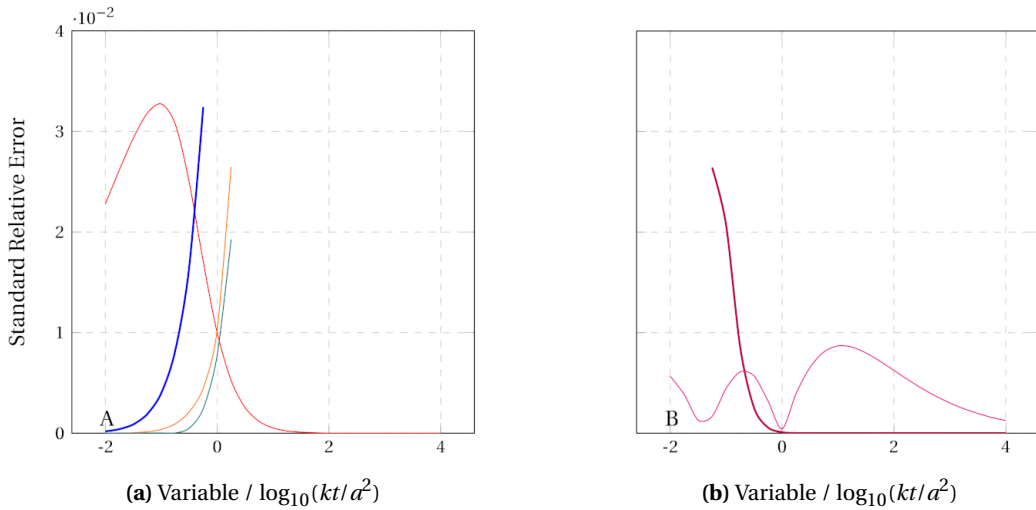


Figure 4. (a) Standard error plots of a number of analyses relative to the analytic solution [4] as a function of the dimensionless variable $\log_{10}(kt/a^2)$. By color: (red) the variational solution Equation (42); (blue) Phillips and Jansons [12] three term transient diffusion analysis; (orange) Jansons four term transient diffusion analysis; (teal) five term transient diffusion analysis based on [12]. (b) Standard error plots for other heuristic approximations: (purple) Aoki [7] long time estimate; (magenta) Laraqi [13].

6. Discussion

Results for the total transient flux measures for the circular disk case provided by the variational result Equation (42) are shown in Figures 3 and 4, along with prior estimates by other workers [4, 6–13]. The latter are primarily results derived for the analogous mass transport case. All of the prior approximations comprise either (a) independently derived series solutions for either or both of short and long time responses, or, (b) curve fitting estimates based on accepted phenomenological or simulated results. Most of these results provide good estimations to the analytic solution, as well as to established simulations, e.g. [14].

The selected two term trial function with terms $1/\lambda$ and $1/\lambda^2$ (Equation (14)) used for the circular disk gives a full representation of the total transient flux across the surface and between the limits of the system dimensionless variable. The solution represents as well a useful lower bound to the exact representation.

Figure 3a is a plot of the results of the variational solution for the total transient flux over the circular disk source (Equation (42)) over 6 orders of magnitude of the system dimensionless variable compared to that given in the recently resolved analytic solution, [4, Equation (44)].

Figure 3b is a similar plot of the results of the analytic solution, [4, Equation (44)], along with results from Aoki [7], and two plots of the results of Mahon [6] over extended regions. Approximations of Shoup [8] and three different ordered Pade approximations from Rajendran and Sangaranarayanan [9–11] are sufficiently accurate so as not to be distinguishable from the analytic plot at this resolution, and are therefore not shown.

Figure 4a shows the standard relative error plots for Equation (42) and for the three and four term asymptotic Jansons' series e.g. Jansons [12] short time transient stochastic model, and a five term one based on same. The Jansons series was developed in a mathematically rigorous manner, and consists of elements in increasing powers of \sqrt{t} elements.

It is noted that the two term trial function used in the variational framework herein can only address effects of the first two terms of the Jansons series, which in turn represent the initially high (surface area dependent) normal flux component at the conductor surface that decays as $1/\sqrt{t}$, and the effect of the total source perimeter (time independent) on the total transient flux. However, for the circular disk example, Equation (42) with this two term trial function, the interpolation already gives a maximum standard relative error at very short times of 0.03 against the analytic solution. The comparisons in Figure 4a show that

- (a) The region of highest error in the variational solution coincides with the regions of maximum pertinence of the effect of the various terms of the Jansons series. The two term variational solution does not contain any component in powers of \sqrt{t} or higher. Stochastic theory reveals that is those specific terms that apply to the transient effects on the flux due to the edges; specifically, these terms directly relate to the effect of degree of curvature of the conductor perimeter. Since this is the only region with significant relative error in the analysis, it is clear that a trial function with reference to at least a first term of the edge curvature would increase the accuracy of the interpolation.
- (b) The relative error of the variational solution falls at very short times. In the region of $a/\sqrt{kt} \gg 1$ the transient flux response asymptotically represents the known value $A/\sqrt{\pi kt}$, as does the analytic response. This is in line with the observations in Figure 4a since the lack of trial function reference to the curvature in the transition region is expected to occur at intermediate times between the known high accuracy regions at long and short times; more specifically, approximately when the thermal diffusion layer thickness effects have reached distances on the order of $\sqrt{kt}/a \approx 1$.
- (c) The four term Jansons series markedly increases the zone of high accuracy when compared to the analytic solution, with respect to the three term series. However, it is clear

from the structure of the Jansons series that the increasing powers of \sqrt{t} therein can only continue to extend the useful variable range a finite amount before it diverges. This is evident from:

- (d) The five term Jansons based series only slightly increases the useful variable range with respect to the fourth before diverging. Effects of the series is near the short time system variable limit.
- (e) The error in the variational solution decreases monotonically after dimensionless variable values ≈ 0.01 . The variational interpolation is becoming more effective in increasing the accuracy in the region where the effects of the short time Jansons series is less relevant. It is evident that the variational interpolation (always a lower bound solution) now is depending more on the total efficacy of the complete two term trial function. The solution continues to monotonically approach the correct long term analytic solution from below with continuous decrease in relative error, for all further increases in the system dimensionless variable.

Regarding the development of higher accuracy variational interpolations, applicable to all planar conductor geometries, it is clear from Figure 3a that an inclusion of a third term in \sqrt{t} in the trial solution certainly merits attention. Inspection of the Jansons series indicates that modification of the present trial function to incorporate a representation of such a term can be a relatively straightforward exercise. Again, such a term applies to the transient effects on the flux due to the curvatures of the conductor perimeter, and in fact, is needed to distinguish between various planar conductors aspects. In the Jansons series, the \sqrt{t} term comprises, for a given conductor geometry, a simple function of the number of disjoint sections and the number of holes in the aspect of the conductor. In essence, this is a representation of the difference of the average and total curvatures of the conductor surface aspect. Addition of this term to the trial function seems to be a logical first step in continued development, e.g. for starting investigations of models for more fundamental properties of surface heat transfer mechanisms.

7. Summary

The work provides a variational framework for the testing of solutions to heat transfer problems described by an inhomogeneous differential equation system comprising mixed temperature and thermal flux boundary conditions. The thermal source is assumed to comprise a planar, closed, and arbitrary perimeter aspect, that is embedded in an otherwise insulating and infinite (in terms of the time frame of the experiment) plane.

Use of the framework requires a trial function that represents a model of the system that can provide a representation of the value of the initial and/or final states of the problem. The evaluation of the resulting variational integral and inverse Laplace transformation then provides the full transient interpolation between those states for all times. Any trial function for the problem e.g. the circular disk case, that provides a solution that everywhere retains Equation (42) as a lower bound, indicates that the new trial function is a representation closer to the exact solution than Equation (42), and approaches it from below.

8. Symbols used

a	Circular disk radius
c_p	Specific heat
erf	Error function
\bar{F}	Laplace space local source flux
$\delta\bar{F}$	Variation in \bar{F}
I_x	Modified Bessel functions of the first kind
J_x	Bessel functions of the first kind
k	Thermal diffusivity
\bar{K}	Symmetric Fourier space Green's function definition for the field of a point source
\mathcal{L}	Laplace transform
p	Laplace complex variable
P	Arbitrary field point
Q	Heat flux
r	Radial distance coordinate
\bar{r}	Three dimensional vector locating an arbitrary field point
t	Time
P	Arbitrary field point
S	Source point
u	General field variable
U	Constant field values for boundaries
x, y, z	Cartesian coordinates
Y	Plasma dispersion function
α, β	Trial function coefficients
λ	$\sqrt{p/\kappa}$
κ	Thermal conductivity
ρ	Density
$\bar{\rho}$	Two dimensional vector locating heat sources
$\alpha - \omega$	In Appendix, various integration variables.

Conflicts of interest

The authors have no conflict of interest to declare.

Acknowledgements

This paper is dedicated to the memory of Emeritus Professor Harold Levine, Department of Mathematics, Stanford University.

Appendix A. Reduction of Integrals

A.1. Reduction of the first integral in Equation (40)

Reduction follows from recent work [15] considering

$$\begin{aligned}
 F_1 &= \int_0^\infty \frac{J_1^2(\alpha x)}{x} \exp(-(\beta x)^2) dx \\
 \frac{dF_1}{b\beta} &= -\frac{1}{\beta} \exp\left(-\frac{\alpha^2}{2\beta^2}\right) I_1\left(\frac{\alpha^2}{2\beta^2}\right) \\
 \therefore F_1 &= \frac{1}{2} \int_\beta^{a^2/(2\beta^2)} \exp(-y) I_1(y) \frac{dy}{y} \\
 \text{Now } \int_0^\sigma \exp(-\sigma) I_1(y) \frac{dy}{y} &= \int_0^\sigma \exp(-y) I_1(y) y d\left(-\frac{1}{y}\right) \\
 &= -I_1(\sigma) \exp(-\sigma) + \int_0^\sigma \frac{1}{y} \exp(-y) [yI_0(y) - yI_1(y)] y dy \\
 &= 1 - \exp(-\sigma) [I_0(\sigma) - I_1(\sigma)] \\
 \therefore F_1 &= \frac{1}{2} - \frac{1}{2} \exp(-\alpha^2/2\beta^2) \left(I_0\left(\frac{\alpha^2}{2\beta^2}\right) + I_1\left(\frac{\alpha^2}{2\beta^2}\right) \right)
 \end{aligned} \tag{58}$$

A.2. Towards reduction of the third integral in Equation (40)

Consider the last integral in Equation (40) *viz.*

$$\begin{aligned}
 I &= \int_0^\infty \frac{\sin^2 x}{x^2} \operatorname{erf}(\alpha x) dx = \int_0^\infty \frac{\sin^2 x}{x^2} \operatorname{erf}(\alpha x) d\left(-\frac{1}{x}\right) \\
 &= \int_0^\infty \frac{1}{x} \left\{ \sin 2x \operatorname{erf}(\alpha x) + \sin^2 x \cdot \frac{2}{\sqrt{\pi}} \alpha \exp(-\alpha^2 x^2) \right\} dx \\
 &= \int_0^\infty \frac{\sin 2x}{x^2} \operatorname{erf}(\alpha x) dx + \frac{2}{\sqrt{\pi}} \alpha \int_0^\infty \frac{\sin^2 x}{x} \exp(-\alpha^2 x^2) dx \\
 &= I_1 + \frac{2}{\sqrt{\pi}} \alpha I_2
 \end{aligned} \tag{59}$$

and note that

$$\frac{dI_1}{d\alpha} = \frac{2}{\sqrt{\pi}} \int_0^\infty \sin 2x \exp(-\alpha^2 x^2) dx = \frac{1}{\sqrt{\pi}} \int_0^\infty \sin x \exp\left(-\frac{\alpha^2 x^2}{4}\right) dx \tag{60}$$

and furthermore that

$$\begin{aligned}
 \frac{dI_2}{d\alpha} &= -2\alpha \int_0^\infty x \sin^2 x \exp(-\alpha^2 x^2) dx = \frac{1}{\alpha} \int_0^\infty \sin^2 x d(\exp(-\alpha^2 x^2)) \\
 &= -\frac{1}{\alpha} \int_0^\infty \sin 2x \exp(-\alpha^2 x^2) dx = -\frac{1}{2\alpha} \int_0^\infty \sin x \exp\left(-\frac{\alpha^2 x^2}{4}\right) dx
 \end{aligned} \tag{61}$$

Thus, the same integral appears in the expressions for $dI_1/d\alpha$ and $dI_2/d\alpha$; and this can be specified as follows:

$$\int_0^\infty \sin x \exp\left(\frac{-\alpha^2 x^2}{4}\right) dx = \frac{\sqrt{\pi}}{4i \cdot \alpha/2} \exp\left(\frac{-1}{\alpha^2}\right) \left[\operatorname{erf}\left(\frac{i}{\alpha}\right) - \operatorname{erf}\left(-\frac{i}{\alpha}\right) \right] \tag{62}$$

In fact,

$$\frac{\operatorname{erf}(ix)}{i} = \frac{2}{\sqrt{\pi}} \int_0^x \exp(\xi^2) d\xi, \quad \frac{\operatorname{erf}(-ix)}{-i} = \frac{2}{\sqrt{\pi}} \int_0^x \exp(\xi^2) d\xi \tag{63}$$

and so

$$\int_0^{\infty} \sin x \exp\left(\frac{-\alpha^2 x^2}{4}\right) dx = \frac{2}{\alpha} \mathbb{F}\left(\frac{1}{\alpha}\right) \quad (64)$$

where

$$\mathbb{F}(\xi) = \exp(-\xi^2) \int_0^{\xi} \exp(\xi^2) d\xi = \xi Y(\xi) \quad (65)$$

is related to the plasma dispersion function $Y(\xi)$

$$Z(\xi) = i\sqrt{\pi} \exp(-\xi^2) [i + \operatorname{erf}(i\xi)] \quad (66)$$

i.e., $Z(\xi) = i\sqrt{\pi} \exp(-\xi^2) - 2\xi Y(\xi)$, for real argument.

The known expansions for $Y(\xi)$, i.e. when its argument is either small or large, are [16]

$$Y(\xi) = \sum_{n=0}^{\infty} \left[\frac{(-2)^n \xi^{2n}}{(2n+1)(2n-1)\cdots 3 \cdot 1} \right], \quad \xi \ll 1 \quad (67)$$

and

$$Y(\xi) = \frac{1}{2\xi^2} \sum_{n=0}^{\infty} \left[\frac{(2n-1)!!}{(2\xi^2)^n} \right], \quad \xi \gg 1 \quad (68)$$

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