Chapter 2

Exact Solutions of Heat Conduction and Diffusion Problems

1 Introduction

This chapter is devoted to the presentation and discussion of analytical solutions to selected heat conduction and substance diffusion problems. First, fundamental solutions are described. Fundamental solutions are solutions to selected fundamental problems in heat conduction and diffusion. They include steady as well as transient situations in the three most commonly used coordinate systems. The method of separation of variables is subsequently used to obtain solutions to more complicated problems under both steady state and transient conditions and for multidimensional systems in various coordinates.

2 Heat Conduction

Here we investigate solutions to special cases of the following form of the heat equation

\[ \frac{\partial T}{\partial t} = \alpha \nabla^2 T \]

subject to properly stated initial and boundary conditions.

Selected steady state problems will also be discussed. Recall that under steady state conditions with constant thermal properties the energy balance equation is

\[ \nabla^2 T = 0 \]

Finally, at steady state but in the presence of distributed internal heat generation the energy equation is

\[ \nabla \cdot (k \nabla T) = -g(r) \]

proper formulation requires the statement of boundary conditions.

Exact solutions to selected special cases of the above equations are presented below.
2.1 Fundamental Solutions to Steady State Problems

Solutions to steady state problems in one dimensional systems exhibiting symmetry are easily obtained as solutions of ordinary differential equations by direct integration.

Consider a solid slab whose thickness $L$ is much smaller than its width and its height. In cartesian coordinates the steady state heat balance equation becomes

$$\frac{d^2 T}{dx^2} = 0$$

the general solution of which is

$$T(x) = Ax + B$$

where the constants $A$ and $B$ must be determined from the specific boundary conditions involved. This represents the steady state loss of heat through a flat wall.

Similarly, consider the infinite hollow cylinder with inner and outer radii $a$ and $b$, respectively. At steady state the heat equation in cylindrical coordinates with azimuthal symmetry becomes

$$\frac{d}{dr} (r \frac{dT}{dr}) = 0$$

the general solution of which is

$$T(r) = A \ln r + B$$

where the constants $A$ and $B$ must be determined from the specific boundary conditions involved. This represents the steady state loss of heat through a cylindrical wall.

Finally, consider the hollow sphere with inner and outer radii $a$ and $b$, respectively. At steady state the heat equation in spherical coordinates with azimuthal and poloidal symmetry becomes

$$\frac{d}{dr} \left( r^2 \frac{dT}{dr} \right) = 0$$

the general solution of which is

$$T(r) = \frac{A}{r} + B$$

where the constants $A$ and $B$ must be determined from the specific boundary conditions involved. This represents the steady state loss of heat through a spherical shell.
2.2 Fundamental Solutions to Transient Problems

Transient problems resulting from the effect of instantaneous point, line and planar sources of heat lead to useful fundamental solutions of the heat equation. By considering media of infinite or semi-infinite extent one can conveniently ignore the effect of boundary conditions on the resulting solutions.

Let a fixed amount of energy $Q \rho C_p$ be released at time $t = 0$ at the origin of the three dimensional solid of infinite extent, initially at $T = 0$ everywhere. The heat equation is

$$\frac{1}{\alpha} \frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}$$

and this must be solved subject to

$$T(x, y, z, 0) = 0$$

for all $x, y, z$ and energy $Q \rho C_p$ released instantaneously at $t = 0$ at the origin.

The fundamental solution of this problem is

$$T(x, y, z, t) = \frac{Q}{(4\pi \alpha t)^{3/2}} e^{-\frac{x^2+y^2+z^2}{4\alpha t}}$$

This solution is useful in the study of thermal explosions where a buried explosive load located at $r = 0$ is suddenly released at $t = 0$ and the subsequent distribution of temperature at various distances from the explosion is measured as a function of time. A slight modification of the solution produced by the method of reflexion constitutes an approximation to the problem of surface heating of bulk samples by short duration pulses of high energy beams.

Similarly, if the heat is released instantaneously at $t = 0$ but along the $z-$axis, the corresponding fundamental solution is

$$T(x, y, z, t) = \frac{Q}{4\pi \alpha t} e^{-\frac{x^2+y^2}{4\alpha t}}$$

where $Q \rho C_p$ is now the amount of heat released per unit length.

Finally, if the heat is instantaneously released at $t = 0$ but on the entire the $y-z$ plane at $x = 0$ the corresponding fundamental solution is

$$T(x, y, z, t) = \frac{Q}{(4\pi \alpha t)^{1/2}} e^{-\frac{z^2}{4\alpha t}}$$

where $Q \rho C_p$ is now the amount of heat released per unit area.

Another important solution is obtained for the case of a semi-infinite solid ($x \geq 0$) initially at $T = T_0$ everywhere and suddenly exposed to a fixed temperature $T = 0$ at $x = 0$. The statement of the problem is

$$\frac{1}{\alpha} \frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2}$$
subject to

\[ T(x,0) = T_0 \]

and

\[ T(0,t) = 0 \]

The solution is easily obtained introducing the \textit{Laplace transform}. Multiply the heat equation by \( \exp(-st) \), where \( s \) is the parameter of the transform, and integrate with respect to \( t \) from 0 to \( \infty \), i.e.

\[
\frac{1}{\alpha} \int_0^\infty \exp(-st) \frac{\partial T}{\partial t} \, dt = \int_0^\infty \exp(-st) \frac{\partial^2 T}{\partial x^2} \, dt
\]

introducing the notation \( L[T] = T^* = \int_0^\infty \exp(-st)T \, dt \) the transformed heat equation becomes

\[
\frac{d^2 T^*}{dx^2} = \frac{s}{\alpha} T^*
\]

an ordinary differential equation which is readily solved for \( T^* \). The desired result \( T(x,t) \) is finally obtained from \( T \) by inverting the transform and is

\[
T(x,t) = T_0 \text{erf} \left( \frac{x}{2\sqrt{\alpha t}} \right)
\]

where the \textit{error function}, \( \text{erf} \) is defined as

\[
\text{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z \exp(-\xi^2) \, d\xi
\]

The above solution is an appropriate mathematical approximation of the problem of quenching hot bulk metal samples.

\textbf{2.3 Solution to Steady State Problems in Finite Media by Separation of Variables}

At steady state \( \partial T/\partial t = 0 \) so that, in two dimensional systems, the temperature satisfies Laplace’s equation

\[
\nabla^2 T = 0
\]

From Green’s theorem, Laplace’s equation requires that

\[
\iint \frac{\partial T}{\partial n} \, d\sigma = 0
\]
which states that under steady state conditions the boundary heat flux cannot be chosen arbitrarily but must average zero.

Also, from Green’s theorem, if $T_1$ and $T_2$ are two solutions of a steady state problem whose values coincide at the boundary

$$\int \int \int_V [\nabla (T_2 - T_1)]^2 d\tau = 0$$

so that $T_2 - T_1 = $ constant. The constant is zero when the problem involves only prescribed temperatures at the boundary (Dirichlet problem) and can be nonzero when normal derivatives of $T$ at the boundary are specified (Neumann problem).

Consider steady state heat conduction in a thin rectangular plate of width $l$ and height $d$. The edges $x = 0$, $x = l$ and $y = 0$ are maintained at $T = 0$ while at the edge $y = d$ $T(x, d) = f(x)$. No heat flow along the $z$ direction perpendicular to the plate. The required temperature $T(x, y)$ satisfies

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$

To find $T$ by separation of variables we assume the a particular solution can be represented as a product of two functions each depending on a single coordinate, i.e.

$$T_p(x, y) = X(x)Y(y)$$

substituting into Laplace’s equation gives

$$-\frac{1}{X} \frac{d^2 X}{dx^2} = \frac{1}{Y} \frac{d^2 Y}{dy^2} = k^2$$

where $k^2$ is a constant and this is true since the LHS is a function of $x$ alone while the RHS a function of $y$ alone. The constant is selected as $k^2$ in order to obtain a proper Sturm-Liouville problem for $X$ (with real eigenvalues). With the above the original PDE problem has been transformed into a system of two ODE’s, i.e.

$$X'' + k^2 X = 0$$

subject to $X(0) = X(l) = 0$ and

$$Y'' - k^2 Y = 0$$

subject to $Y(0) = 0$.

The solution for $X(x)$ is

$$X = X_n = A_n \sin\left(\frac{n\pi x}{l}\right)$$
with eigenvalues

\[ k_n = \frac{n\pi}{l} \]

for \( n = 1, 2, 3, \ldots \).

The solution of \( Y(y) \) is

\[ Y_n = B_n \sinh\left(\frac{n\pi y}{l}\right) \]

The principle of superposition allows the creation of a more general solution from individual particular solutions by simple linear combination. Therefore the final form of the particular solution is

\[ T_n = \sum_{n=1}^{\infty} a_n \sin\left(\frac{n\pi x}{l}\right) \sinh\left(\frac{n\pi y}{l}\right) \]

The \( a_n \)'s are determined by making the above satisfy the nonhomogeneous condition at \( y = d \), i.e.

\[ f(x) = \sum_{n=1}^{\infty} [a_n \sinh\left(\frac{n\pi d}{l}\right)] \sin\left(\frac{n\pi x}{l}\right) \]

which is the Fourier sine series representation of \( f(x) \) with coefficients

\[ c_n = a_n \sinh\left(\frac{n\pi d}{l}\right) = \frac{2}{l} \int_0^l f(x) \sin\left(\frac{n\pi x}{l}\right) dx \]

so that the final solution is

\[ T(x,y) = \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi x}{l}\right) \frac{\sinh\left(\frac{n\pi y}{l}\right)}{\sinh\left(\frac{n\pi d}{l}\right)} \]

Therefore, as long as \( f(x) \) is representable in terms of Fourier series, the obtained solution converges to the desired solution. Note also that the presence of homogeneous conditions at \( x = 0, x = l \) made feasible the determination of the required eigenvalues.

2.4 Solution to Transient Problems in Finite Media by Separation of Variables

A simple but important conduction heat transfer problem consists of determining the temperature history inside a solid body which is quenched from a high temperature. More specifically, consider the homogeneous problem of finding the one-dimensional temperature distribution inside a slab of thickness \( L \) and thermal diffusivity \( \alpha \) undergoing transient heat conduction. The initial temperature distribution of the slab is \( T(x,0) = f(x) \). The slab is
quenched by forcing the temperature at its two surfaces \( x = 0 \) and \( x = L \) to become equal to zero (i.e. \( T(0,t) = T(L,t) = 0 \); Dirichlet conditions) for \( t > 0 \).

The zero values at the boundaries make the problem homogeneous and easier to deal with. The mathematical statement of the heat equation for this problem is:

\[
\frac{\partial^2 T(x,t)}{\partial x^2} = \frac{1}{\alpha} \frac{\partial T(x,t)}{\partial t}
\]

subject to

\[
T(0,t) = T(L,t) = 0
\]

and

\[
T(x,0) = f(x)
\]

for all \( x \) when \( t = 0 \).

The method of separation of variables starts by assuming the solution to this problem has the following particular form

\[
T(x,t) = X(x)\Theta(t)
\]

If the assumption is wrong, one discovers soon enough, but if it is correct then we may just find a solution to the problem! The latter turns out to be the case for this and many other similar problems.

Introducing the above assumption into the heat equation and rearranging yields

\[
\frac{1}{X} \frac{d^2X}{dx^2} = \frac{1}{\alpha \Theta} \frac{d\Theta}{dt}
\]

However since \( X(x) \) and \( \Theta(t) \), the left hand side of this equation is only a function of \( x \) while the right hand side is a function only of \( t \). For this to avoid being a contradiction (for arbitrary values of \( x \) and \( t \)) both sides must be equal to a constant. For physical reasons the required constant must be negative; let us call it \(-\omega^2\).

Therefore, the original PDE is transformed into the following two ODE’s

\[
\frac{1}{X} \frac{d^2X}{dx^2} = -\omega^2
\]

and

\[
\frac{1}{\alpha \Theta} \frac{d\Theta}{dt} = -\omega^2
\]

General solutions to these equations are readily obtained by direct integration and are

\[
X(x) = A' \cos(\omega x) + B' \sin(\omega x)
\]
and

$$\Theta(t) = C \exp(-\omega^2 \alpha t)$$

and substituting back into our original assumption yields

$$T(x,t) = X(x)\Theta(t) = [A \cos(\omega x) + B \sin(\omega x)] \exp(-\omega^2 \alpha t)$$

where the constant $C$ has been combined with $A'$ and $B'$ to give $A$ and $B$ without losing any generality.

Now we introduce the boundary conditions. Since $T(0,t) = 0$, necessarily $A = 0$. Furthermore, since also $T(L,t) = 0$, then $\sin(\omega x) = 0$ (since $B = 0$ is an uninteresting trivial solution.) There is an infinite number of values of $\omega$ which satisfy this conditions, i.e.

$$\omega_n = \frac{n\pi}{L}$$

with $n = 1, 2, 3, ...$. The $\omega_n$'s are the eigenvalues and the associated functions $\sin(\omega_n x)$ are the eigenfunctions of this quenching problem. These eigenvalues and eigenfunctions play in heat conduction a role analogous to that of the deflection modes in structural dynamics, the vibration modes in vibration theory and the quantum states in wave mechanics.

Note that each value of $\omega$ yields an independent solution satisfying the heat equation as well as the two boundary conditions. Therefore we have now an infinite number of independent solutions $T_n(x,t)$ for $n = 1, 2, 3,...$ given by

$$T_n(x,t) = [B_n \sin(\omega_n x)] \exp(-\omega_n^2 \alpha t)$$

Using again the principle of superposition yields

$$T(x,t) = \sum_{n=1}^{\infty} T_n(x,t) = \sum_{n=1}^{\infty} [B_n \sin(\omega_n x)] \exp(-\omega_n^2 \alpha t) = \sum_{n=1}^{\infty} [B_n \sin(\frac{n\pi x}{L})] \exp(-\frac{n\pi}{L}^2 \alpha t)$$

The last step is to ensure the values of the constants $B_n$ are chosen so as to satisfy the initial condition, i.e.

$$T(x,0) = f(x) = \sum_{n=1}^{\infty} B_n \sin(\frac{n\pi x}{L}) = \sum_{n=1}^{\infty} B_n \sin(\frac{n\pi x}{L})$$

Note that this is the Fourier sine series representation of the function $f(x)$.

Recall that a key property of the eigenfunctions is the orthonormality property expressed in the case of the $\sin(\omega_n x)$ functions as

$$\int_{0}^{L} \sin(\frac{n\pi x}{L}) \sin(\frac{m\pi x}{L}) dx = \begin{cases} 0 & n \neq m \\ \frac{L}{2} & n = m \end{cases}$$
Using the orthonormality property one can multiply the Fourier sine series representation of \( f(x) \) by \( \sin(\frac{m\pi x}{L}) \) and integrate from \( x = 0 \) to \( x = L \) to produce the result

\[
B_n = \frac{2}{L} \int_0^L f(x) \sin(\frac{n\pi x}{L}) \, dx
\]

for \( n = 1, 2, 3, \ldots \).

Explicit expressions for the \( B_n \)'s can be obtained for simple \( f(x) \)'s, for instance if

\[
f(x) = \begin{cases} 
    x, & 0 \leq x \leq \frac{L}{2} \\
    L - x, & \frac{L}{2} \leq x \leq L 
\end{cases}
\]

then

\[
B_n = \begin{cases} 
    \frac{4L}{n^2\pi^2}, & n = 1, 5, 9, \ldots \\
    -\frac{4L}{n^2\pi^2}, & n = 3, 7, 11, \ldots \\
    0, & n = 2, 4, 6, \ldots 
\end{cases}
\]

Finally, the resulting \( B_n \)'s can be substituted into the general solution above to give

\[
T(x, t) = \sum_{n=1}^{\infty} T_n(x, t) = \sum_{n=1}^{\infty} \left[ \frac{2}{L} \int_0^L f(x') \sin(\frac{n\pi x'}{L}) dx' \right] \sin(\frac{n\pi x}{L}) \exp\left(-\frac{n^2\pi^2\alpha t}{L^2}\right)
\]

and for the specific \( f(x) \) given above

\[
T(x, t) = \frac{4L}{\pi^2} \left[ \exp\left(-\frac{\pi^2\alpha t}{L^2}\right) \sin(\frac{\pi x}{L}) - \frac{1}{9} \exp\left(-\frac{9\pi^2\alpha t}{L^2}\right) \sin(\frac{3\pi x}{L}) + \ldots \right]
\]

Another important special case is when the initial temperature \( f(x) = T_i = \text{constant} \). The result in this case is

\[
T(x, t) = \frac{4T_i}{\pi} \sum_{n=0}^{\infty} \frac{1}{(2n+1)} \sin(\frac{(2n+1)\pi x}{L}) \exp\left(-\frac{n^2\pi^2\alpha t}{L^2}\right)
\]

A similar approach can be used to obtain the solution to the analogous problem for the solid cylinder of radius \( a \) described by

\[
\frac{\partial T}{\partial t} = \alpha \left( \frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} \right)
\]

subject to

\[
T(r, 0) = T_i
\]
and

\[ k \frac{\partial T}{\partial r} + hT = 0 \]

at \( r = a \). The corresponding solution is

\[
T(r, t) = 2 \frac{T_i}{a \lambda_n} \sum_{n=1}^{\infty} e^{-a \lambda_n^2 t} \frac{J_1(\lambda_n a) J_0(\lambda_n r)}{J_0(\lambda_n a)^2 + J_1(\lambda_n a)^2} = 2 \left( \frac{h}{k} \right) \frac{T_i}{a} \sum_{n=1}^{\infty} e^{-a \lambda_n^2 t} \frac{J_0(r \lambda_n)}{[\left(\frac{h}{k}\right)^2 + \lambda^2] J_0(a \lambda_n)}
\]

where \( J_0 \) is the Bessel function of first kind, order zero. The eigenvalues \( \lambda_1, \lambda_2, \ldots \) are the roots of

\[
\lambda J_0'(\lambda a) + \left( \frac{h}{k} \right) J_0(\lambda a) = 0
\]

where \( J_0'(z) = -J_1(z) \), with \( J_1(z) \) being the Bessel function of first kind, order one. The above solution could represent the process of cooling a cylindrical shaft by exposure to a convective environment.

If the initial temperature is \( T_i = 0 \) and boundary condition is instead one of constant temperature, i.e. \( T(a, t) = T_S \) the solution becomes

\[
T(r, t) = T_S - 2 \frac{T_S}{a} \sum_{n=1}^{\infty} e^{-a \lambda_n^2 t} \frac{J_0(r \lambda_n)}{\lambda_n J_1(a \lambda_n)}
\]

where the eigenvalues are now the roots of

\[
J_0(\lambda a) = 0
\]

This solution could represent the sudden heating of a cylindrical shaft.

### 3 Mass Diffusion

As with the heat equation, fundamental solutions to the diffusion equation are solutions to selected fundamental problems in solid state diffusion. They include steady as well as transient situations in the three most commonly used coordinate systems. Solutions to selected multidimensional problems (steady and transient) in various coordinate systems are obtained using the separation of variables method.

Here we investigate solutions to special cases of the following form of the diffusion equation

\[
\frac{\partial c}{\partial t} = D \nabla^2 c
\]
subject to properly stated initial and boundary conditions.

Selected steady state problems will also be discussed. Recall that under steady state conditions with constant diffusivity the mass balance equation is

$$\nabla^2 c = 0$$

Finally, at steady state but in the presence of distributed internal substance generation processes the mass equation is

$$\nabla \cdot (D \nabla c) = -g(r)$$

proper formulation requires the statement of boundary conditions.

Exact solutions to selected special cases of the above equations are presented below.

3.1 Fundamental Solutions to Steady State Problems

Solutions to steady state problems in one dimensional systems exhibiting symmetry are easily obtained as solutions of ordinary differential equations by direct integration.

Consider a solid slab whose thickness $L$ is much smaller than its width and its height. In cartesian coordinates the steady state mass balance equation becomes

$$\frac{d^2 c}{dx^2} = 0$$

the general solution of which is

$$c(x) = Ax + B$$

where the constants $A$ and $B$ must be determined from the specific boundary conditions involved. This represents the steady state diffusional leakage of substance through a flat wall.

Similarly, consider the infinite hollow cylinder with inner and outer radii $a$ and $b$, respectively. At steady state the diffusion equation in cylindrical coordinates with azimuthal symmetry becomes

$$\frac{d}{dr}(r \frac{dc}{dr}) = 0$$

the general solution of which is

$$c(r) = A \ln r + B$$

where the constants $A$ and $B$ must be determined from the specific boundary conditions involved. This represents the steady state diffusional leakage of substance through a cylindrical wall.
Finally, consider the hollow sphere with inner and outer radii $a$ and $b$, respectively. At steady state the diffusion equation in spherical coordinates with azimuthal and poloidal symmetry becomes

$$\frac{d}{dr} \left( r^2 \frac{dc}{dr} \right) = 0$$

the general solution of which is

$$c(r) = \frac{A}{r} + B$$

where the constants $A$ and $B$ must be determined from the specific boundary conditions involved. This represents the steady state diffusional leakage of substance through a spherical shell.

### 3.2 Fundamental Solutions to Transient Problems

As in the case of the heat equation, transient problems resulting from the effect of instantaneous point, line and planar sources of substance lead to useful fundamental solutions of the diffusion equation. By considering media of infinite or semi-infinite extent one can conveniently ignore the effect of boundary conditions on the resulting solutions.

Let a fixed amount of substance $M$ be released at time $t = 0$ at the origin of the three dimensional solid of infinite extent, initially at $c = 0$ everywhere. The diffusion equation is

$$\frac{1}{D} \frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2}$$

and this must be solved subject to

$$c(x, y, z, 0) = 0$$

for all $x, y, z$ and with the amount of substance $M$ released instantaneously at $t = 0$ at the origin.

The fundamental solution of this problem is

$$c(x, y, z, t) = \frac{M}{(4\pi Dt)^{3/2}} e^{-\frac{x^2+y^2+z^2}{4Dt}}$$

Similarly, if the substance is released instantaneously at $t = 0$ but along the $z-$axis, the corresponding fundamental solution is

$$c(x, y, z, t) = \frac{M}{4\pi Dt} e^{-\frac{x^2+y^2}{4Dt}}$$

where $M$ is now the amount of substance released per unit length.
Finally, if the substance is released instantaneously at \( t = 0 \) but on the entire the \( y - z \) plane at \( x = 0 \) the corresponding fundamental solution is

\[
c(x, y, z, t) = \frac{M}{(4\pi Dt)^{1/2}} e^{-\frac{x^2}{4Dt}}
\]

where \( M \) is now the amount of substance released per unit area. This solution is useful in solid state diffusion studies of sandwich-type specimens produced by depositing a thin film of diffusant on the clean surface of a cut sample which is then sandwiched by rejoining the sample. The specimen is subsequently exposed for selected periods of time at temperature, quenched and resulting distribution of diffusant measured by analytical means.

Another important solution is obtained for the case of a semi-infinite solid \( (x \geq 0) \) initially at \( c = 0 \) everywhere and whose surface at \( x = 0 \) is maintained at \( c = c_S \) for \( t > 0 \). The statement of the problem is

\[
\frac{1}{D} \frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial x^2}
\]

subject to

\[
c(x, 0) = 0
\]

and

\[
c(0, t) = c_S
\]

The solution is easily obtained using again the Laplace transform. Multiply the diffusion equation by \( \exp(-st) \), where \( s \) is the parameter of the transform, and integrate with respect to \( t \) from 0 to \( \infty \), i.e.

\[
\frac{1}{D} \int_0^\infty \exp(-st) \frac{\partial c}{\partial t} dt = \int_0^\infty \exp(-st) \frac{\partial^2 c}{\partial x^2} dt
\]

introducing the notation \( L[c] = c^* = \int_0^\infty \exp(-st)c dt \) the transformed heat equation becomes

\[
\frac{d^2 c^*}{dx^2} = \frac{s}{D} c^*
\]

an ordinary differential equation which is readily solved for \( c^* \). The desired result \( c(x, t) \) is finally obtained from \( c \) by inverting the transform and is

\[
c(x, t) = c_S erf c\left(\frac{x}{2\sqrt{Dt}}\right)
\]

where the complementary error function, \( erf c \) is defined as

\[
erf c(z) = 1 - erf(z) = \frac{2}{\sqrt{\pi}} \int_z^\infty \exp(-\xi^2) d\xi
\]

The above solution is an approximate mathematical representation of the process of gas carburization of bulk iron samples.
3.3 Solution to Steady State Problems in Finite Media by Separation of Variables

Consider the problem of determining the steady state distribution of diffusing substance in a thin annular plate where the concentrations are specified at the inner and outer radii \( r_1 \) and \( r_2 \) as

\[
c(r_1, \theta) = f_1(\theta)
\]

\[
c(r_2, \theta) = f_2(\theta)
\]

Laplace’s equation in this case is

\[
\nabla^2 c = \frac{\partial^2 c}{\partial r^2} + \frac{1}{r} \frac{\partial c}{\partial r} + \frac{1}{r^2} \frac{\partial^2 c}{\partial \theta^2} = 0
\]

Assume now a particular solution is of the form

\[
c_p(r, \theta) = R(r) \Phi(\theta)
\]

Substituting leads to the following two ODEs

\[
r^2 R'' + r R' - k^2 R = 0
\]

\[
\Phi'' + k^2 \Phi = 0
\]

where the separation constant as been chosen as \( k^2 \) in order to obtain periodic trigonometric functions as the solutions for \( \Phi \).

The general solution for \( R \) is

\[
R = \begin{cases} 
A_k r^k + B_k r^{-k}; & k \neq 0 \\
A_0 + B_0 \ln r; & k = 0 
\end{cases}
\]

whereas that for \( \Phi \) is

\[
\Phi = \begin{cases} 
C_k \cos(k\theta) + D_k \sin(k\theta); & k \neq 0 \\
C_0 + D_0 \theta; & k = 0 
\end{cases}
\]

The periodicity requirement is satisfied by taking \( k = n \), with \( n = 1, 2, 3, \ldots \).

The particular single valued solution \( c \) is then

\[
c = (a_0 + b_0 \ln r) + \sum_{n=1}^{\infty} [(a_n r^n + b_n r^{-n}) \cos(n\theta) + (c_n r^n + d_n r^{-n}) \sin(n\theta)]
\]
Finally, the desired solution must satisfy the stated boundary conditions. Substituting \( f_1 \) and \( f_2 \) leads to Fourier series representations and the relationships

\[
a_0 + b_0 \ln r_1 = \frac{1}{2\pi} \int_0^{2\pi} f_1(\theta)d\theta
\]

\[
a_0 + b_0 \ln r_2 = \frac{1}{2\pi} \int_0^{2\pi} f_2(\theta)d\theta
\]

\[
a_n r_1^n + b_n r_1^{-n} = \frac{1}{\pi} \int_0^{2\pi} f_1(\theta) \cos(n\theta)d\theta
\]

\[
a_n r_2^n + b_n r_2^{-n} = \frac{1}{\pi} \int_0^{2\pi} f_2(\theta) \cos(n\theta)d\theta
\]

\[
c_n r_1^n + d_n r_1^{-n} = \frac{1}{\pi} \int_0^{2\pi} f_1(\theta) \sin(n\theta)d\theta
\]

\[
c_n r_2^n + d_n r_2^{-n} = \frac{1}{\pi} \int_0^{2\pi} f_2(\theta) \sin(n\theta)d\theta
\]

A special case of interest is steady state diffusion in a disk \((r_1 = 0)\) of radius \(r_2 = a\) subject to a concentration of diffusant \(f(\theta)\) at its boundary. In this case, the solution is

\[
c(r, \theta) = A_0 + \sum_{n=1}^{\infty} \left(\frac{r}{a}\right)^n [A_n \cos(n\theta) + C_n \sin(n\theta)]
\]

with

\[
A_0 = \frac{1}{2\pi} \int_0^{2\pi} f(\theta)d\theta
\]

\[
A_n = \frac{1}{\pi} \int_0^{2\pi} f(\theta) \cos(n\theta)d\theta
\]

\[
C_n = \frac{1}{\pi} \int_0^{2\pi} f(\theta) \sin(n\theta)d\theta
\]

for \(n = 1, 2, \ldots\). Note that the concentration at the center of the disk is simply the average value of the boundary concentration.
Poisson’s integral formula allows direct determination of the concentration \( c(r, \theta) \) from the values of it at its boundary as follows

\[
c(r, \theta) = \frac{1}{2\pi} \int_0^{2\pi} \frac{a^2 - r^r}{a^2 - 2ar \cos(\theta - \psi) + r^2} c(a, \psi) d\psi
\]

Another important special case is that of computing the concentration field around a circular hole \((r_2 \rightarrow \infty)\) of radius \( r_1 = a \) subject to a concentration distribution \( c(a, \theta) = f(\theta) \) at the hole boundary. In this case

\[
c(r, \theta) = A_0 + \sum_{n=1}^{\infty} \left( \frac{a}{r} \right)^n [B_n \cos(n\theta) + D_n \sin(n\theta)]
\]

with

\[
A_0 = \frac{1}{2\pi} \int_0^{2\pi} f(\theta) d\theta
\]

\[
B_n = \frac{1}{\pi} \int_0^{2\pi} f(\theta) \cos(n\theta) d\theta
\]

\[
D_n = \frac{1}{\pi} \int_0^{2\pi} f(\theta) \sin(n\theta) d\theta
\]

for \( n = 1, 2, ..., \). Note that the concentration at infinity is simply the average value of the boundary concentration.

### 3.4 Solution to Transient Problems in Finite Media by Separation of Variables

The separation of variables method can also be used when the boundary conditions specify values of the normal derivative of the concentration (Newmann conditions) or when linear combinations of the normal derivative and the concentration itself are used (Convective conditions; Mixed conditions; Robin conditions). Consider the homogeneous problem of transient diffusion in a slab initially containing a concentration \( c = f(x) \) of diffusant and subject to convective losses into a medium with \( c = 0 \) at \( x = 0 \) and \( x = L \). Convection mass transfer coefficients at \( x = 0 \) and \( x = L \) are, respectively \( h_1 \) and \( h_2 \). Assume the diffusivity \( D \) is constant.

The mathematical formulation of the problem is to find \( c(x, t) \) such that

\[
\frac{\partial^2 c(x, t)}{\partial x^2} = \frac{1}{D} \frac{\partial c(x, t)}{\partial t}
\]
\[-D \frac{\partial c}{\partial x} + h_1 c = 0\]

at \(x = 0\) and

\[D \frac{\partial c}{\partial x} + h_2 c = 0\]

at \(x = L\), with

\[c(x, 0) = f(x)\]

for all \(x\) when \(t = 0\).

Assume the solution is of the form \(c(x, t) = X(x)\Theta(t)\) and substitute to obtain

\[
\frac{1}{X} \frac{d^2 X}{dx^2} = \frac{1}{\alpha \Theta} \frac{d\Theta}{dt} = -\beta^2
\]

The solution for \(\Theta(t)\) is

\[\Theta(t) = \exp(-D \beta^2 t)\]

while \(X(x)\) is the solution of the following eigenvalue (Sturm-Liouville) problem

\[
\frac{d^2 X}{dx^2} + \beta^2 X = 0
\]

with

\[-D \frac{dX}{dx} + h_1 X = 0\]

at \(x = 0\) and

\[D \frac{dX}{dx} + h_2 X = 0\]

at \(x = L\).

Let the eigenvalues of this problem be \(\beta_m\) and the eigenfunctions \(X(\beta_m, x)\). Since the eigenfunctions are orthogonal

\[
\int_0^L X(\beta_m, x)X(\beta_n, x)dx = \begin{cases} 
0, & n \neq m \\
N(\beta_m), & n = m
\end{cases}
\]

where

\[N(\beta_m) = \int_0^L X(\beta_m, x)^2dx\]
is the norm of the problem.

It can be shown that for the above problem the eigenfunctions are

\[ X(\beta_m, x) = \beta_m \cos \beta_m x + \frac{h_1}{k_1} \sin \beta_m x \]

while the eigenvalues are the roots of the transcendental equation

\[ \tan \beta_m L = \frac{\beta_m \left( \frac{h_1}{k_1} + \frac{h_2}{k_2} \right)}{\beta_m^2 - \frac{h_1}{k_1} \frac{h_2}{k_2}} \]

Therefore, the complete solution is of the form

\[ c(x, t) = \sum_{m=1}^{\infty} A_m X(\beta_m, x) \exp(-D\beta_m^2 t) \]

The specific eigenfunctions are obtained by incorporating the initial condition

\[ f(x) = \sum_{m=1}^{\infty} A_m X(\beta_m, x) \]

which expresses the representation of \( f(x) \) in terms of eigenfunctions and requires that

\[ A_m = \frac{1}{N(\beta_m)} \int_0^L X(\beta_m, x) f(x) dx \]

Many problems are special cases of the above generalization. For example, the problem of diffusion out of the slab when its boundaries are maintained at constant concentration (homogeneous Dirichlet conditions) is a special case of the above in which the eigenfunctions are

\[ X(\beta_m, x) = \sin(\beta_m x) \]

the eigenvalues are the roots of \( \sin(\beta_m L) \), i.e.

\[ \beta_m = \frac{m\pi}{L} \]

and the norm is simply

\[ N(\beta_m) = \int_0^L X(\beta_m, x)^2 dx = \int_0^L \sin(\beta_m x)^2 = \frac{L}{2} \]

As another example, the case when \( h_1 = 0 \) and \( h_2 = h \) yields the eigenfunctions

\[ X(\beta_m, x) = \cos(\beta_m x) \]
and the eigenvalues are the roots of \( \beta_m \tan(\beta_m L) = h/D \). Note that the eigenvalues in this case cannot be given explicitly but must be determined by numerical solution of the given transcendental equation. For this purpose, it is common to rewrite the transcendental equation as

\[
cot(\beta_m L) = \frac{\beta_m L}{Bi}
\]

where \( Bi = hL/D \) is the Biot number for mass transfer. This can be easily solved either graphically or numerically by bisection, Newton’s or secant methods. Finally, the norm in this case is

\[
N(\beta_m) = \int_0^L X(\beta_m, x)^2 \, dx = \int_0^L \cos(\beta_m x)^2 \, dx = \frac{1}{2} \frac{\cos(\beta_m L) \sin(\beta_m L) + \beta_m L}{\beta_m} = \frac{L(\beta_m^2 + (h/D)^2) + (h/D)}{2(\beta_m^2 + (h/D)^2)}
\]

Using the above for the case when \( f(x) = c_i \) and simplifying yields the solution

\[
c(x, t) = 2c_i \sum_{m=1}^{\infty} \frac{\sin(\beta_m L) \cos(\beta_m x)}{\beta_m L + \sin(\beta_m L \cos(\beta_m L))} e^{-D\beta_m^2 t}
\]

A similar approach can be used to obtain the solution of the analogous problem for a sphere of radius \( a \) described by

\[
\frac{\partial c}{\partial t} = D\left(\frac{\partial^2 c}{\partial r^2} + \frac{2}{r} \frac{\partial c}{\partial r}\right)
\]

subject to

\[
c(r, 0) = c_i
\]

and

\[
D \frac{\partial c}{\partial r} + hc = 0
\]

at \( r = a \). The solution is

\[
c(r, t) = 2\left(\frac{h}{D}\right)\left(\frac{c_i}{a}\right) \sum_{n=1}^{\infty} e^{-D\lambda_n^2 t}\frac{a^2 \lambda_n^2 + (a(h/D) - 1)^2}{\lambda_n^2(a^2 \lambda_n^2 + a(h/D)(a(h/D) - 1))} \sin(a\lambda_n) \sin(r\lambda_n)
\]

where \( \lambda_1, \lambda_2, \ldots \) are the roots of

\[
a\lambda \cot(a\lambda) + a \frac{h}{D} - 1 = 0
\]

Finally, for the sphere containing initially no diffusant and whose surface in suddenly exposed to a constant concentration of diffusant \( c_S \), the solution is

\[
c(r, t) = c_S + \frac{2ac_S}{\pi r} \sum_{n=1}^{\infty} \frac{(-1)^n}{n} e^{-an^2\pi^2 t/a^2} \sin\left(\frac{n\pi r}{a}\right)
\]
4 Exercises

**Exercise 1.** Obtain the solutions to 1D steady state problems with constant internal heat generation for rectangular, cylindrical and spherical coordinates.

**Exercise 2.** A large Titanium component at uniform initial temperature $T_i = 25$ degrees Celsius is exposed to an extreme environment which fixes the temperature of its surface to $T_0 = 525$ degrees Celsius. Use the appropriate fundamental solution to investigate the heat conduction rate into the component. Assume $k = 22W/mK$, $\rho = 4540kg/m^3$ and $C_p = 522J/kgK$.

**Exercise 3.** Derive the expression given for $B_n$ obtained in the solution to the transient 1D heat conduction problem obtained by separation of variables. Then derive the infinite series solution for the special case of uniform initial temperature $T_i$.

**Exercise 4.** A diffusion specimen is prepared by depositing diffusant atoms on the surface of the sample ($10^{24}$ atoms per square meter. The surface is then sealed and the specimen placed in a high temperature environment where the diffusivity is $D = 10^{-18}m^2/s$ for 4800 seconds. Use the appropriate fundamental solution to estimate the diffusion rate of diffusant into the sample.

**Exercise 5.** Derive the expression for $N(\beta_m)$ obtained for to the transient 1D diffusion problem obtained by separation of variables.

**Exercise 6.** A solid aluminum cylinder of radius $a = 0.1$ m initially at a uniform temperature of 500 degrees Celsius is cooled by convection into an environment at zero temperature. The heat transfer coefficient is $100 \ W/m^2K$ and the thermal diffusivity is $\alpha = 10^{-4}m^2/s$. Use the series solution to map out the cooling process of the cylinder.

**Exercise 7.** A solid iron sphere is suddenly exposed to an environment which fixes the carbon concentration at its surface to 1 percent (i.e. $c_S = 0.01$). Use the series solution to map out the carburization process in the sphere.

**Exercise 8.** Pure titanium samples are extracted from a furnace at a uniform temperature of 525 degrees Celsius and exposed to an environment at zero degrees. Samples are a slab 0.1 m in thickness, a cylinder 0.1 m in diameter and a sphere 0.1 m in diameter. Use the given series solutions to determine the time required for the center of each sample to reach 100 degrees. Assume $h = 1000W/m^2K$. 
5 References