Fall 2002. 10.34. Numerical Methods Applied to Chemical Engineering

Homework # 5. Boundary Value Problems

Assigned Friday 10/18/02. Due Friday 10/25/02

Problem 1. Green's function calculation of a 1-D temperature profile

Consider the heat transfer problem outlined in the figure below. We have a slab of material of thickness L. On one side of the slab is a fluid at a temperature $T_{f,1}$. On the other is a fluid at a temperature $T_{f,2}$. These fixed temperatures set the boundary conditions on the temperature field within the catalyst at $x = 0$ and $x = L$ respectively. The slab may be considered to be infinitely long and tall, so that the only variation of temperature that we wish to consider occurs in the x direction. Within the slab are located several regions in which electrical resistance is used to dissipate energy as heat. Within these heat generating regions, the rate of heat produced per unit volume is equal to a uniform specified value S in SI units of *J/(s-m^3)*.

We wish to calculate the temperature profile within the slab and the rate of heat transfer per unit area to the fluids on either side. To do so, we will apply Green's function analysis. The derivation is outlined below. You are to perform the calculation and plot the resulting temperature field. Then, compute the heat flux per unit area to the fluids on each side of the slab.

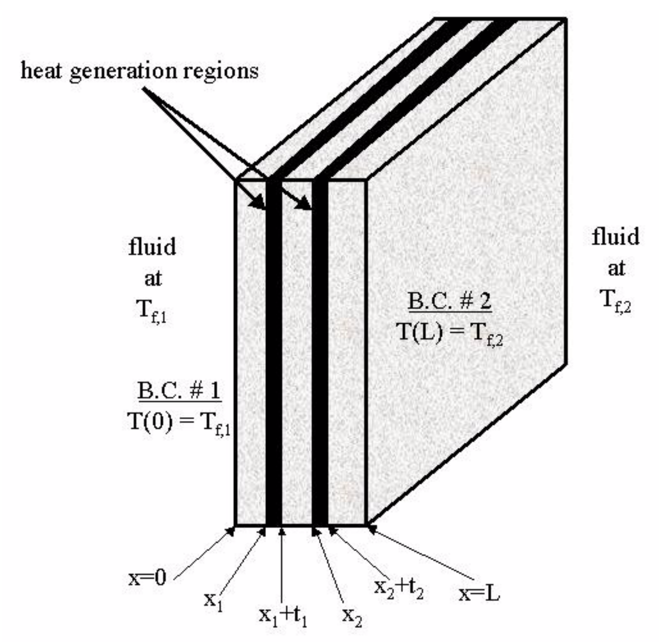

FIGURE 1. Geometry of 1-D heat transfer problem

First, we derive the governing differential equation for the temperature field. Let the rate of local heat generation per unit volume be a specified function $s(x)$ that we write as

$$s(x) = S \times H(x) \quad \text{(EQ 1)}$$

where $H(x)$ is equal to 1 if the point x is within a heat generating region and is 0 everywhere else. The boundary value problem for the steady state temperature field is then

$$-\lambda \frac{d^2 T}{dx^2} = s(x)$$
$$T(0) = T_{f,1} \qquad T(L) = T_{f,2} \quad \text{(EQ 2)}$$

λ is the thermal conductivity. To solve this boundary value problem, we will use the technique of Green's functions outlined below. To do so, we first must convert the boundary conditions by defining the "excess" temperature θ from the expression

$$T(x) = T_{f,1} + (T_{f,2} - T_{f,1})\left(\frac{x}{L}\right) + \theta(x) \quad \text{(EQ 3)}$$

In the absence of heat generation, this "excess" temperature will be uniformly equal to zero. We substitute this form of the temperature field into the heat equation to obtain the following boundary value problem for the excess temperature,

$$\frac{d^2\theta}{dx^2} = f(x) = -\frac{s(x)}{\lambda}$$
$$\theta(0) = 0 \qquad \theta(L) = 0 \quad \text{(EQ 4)}$$

This modified boundary value problem is of a form that we can solve using the Green's function approach outlined below.

<u>Your assignment is the following</u>

1.A. Using the Green's function method outlined above, compute the temperature profile for the following set of parameter values.

$$L = 1$$
$$T_{f,1} = 1 \qquad T_{f,2} = 2$$
$$x_1 = 0.2 \qquad t_1 = 0.1 \quad \text{(EQ 5)}$$
$$x_2 = 0.7 \qquad t_2 = 0.1$$
$$S = 10 \qquad \lambda = 1$$

1.B. From this solution, compute the heat flux across each side of the slab into the surrounding fluids.

A Primer on the use of Green's functions

We wish to solve a boundary value problem of the following form, where $f(x)$ is some known "data" function.

$$\frac{d^2u}{dx^2} = f(x) \qquad \text{(EQ 6)}$$
$$u(0) = 0 \qquad u(L) = 0$$

For this boundary value problem, we define the Green's function $g(x, \xi)$ as that satisfying the related boundary value problem,

$$\frac{d^2g}{dx^2} = \delta(x-\xi) \qquad \text{(EQ 7)}$$
$$g(0, \xi) = 0 \qquad g(L, \xi) = 0$$

The Dirac delta function $\delta(x-\xi)$ is a "function" that is zero everywhere but at $x = \xi$, and that at that point blows up to infinity such that

$$\int_{-\infty}^{\infty} \delta(x-\xi)d\xi = 1 \qquad \text{(EQ 8)}$$

We can represent the Dirac delta function by taking the following limit,

$$\delta(x-\xi) = \lim_{\sigma \to 0} \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(x-\xi)^2}{2\sigma^2}\right] \qquad \text{(EQ 9)}$$

The figure below shows how the Dirac delta function is approached as we shrink the standard deviation of the normal distribution to zero. As we reduce σ, the distribution becomes more sharply peaked, but the area under the integral remains equal to one.

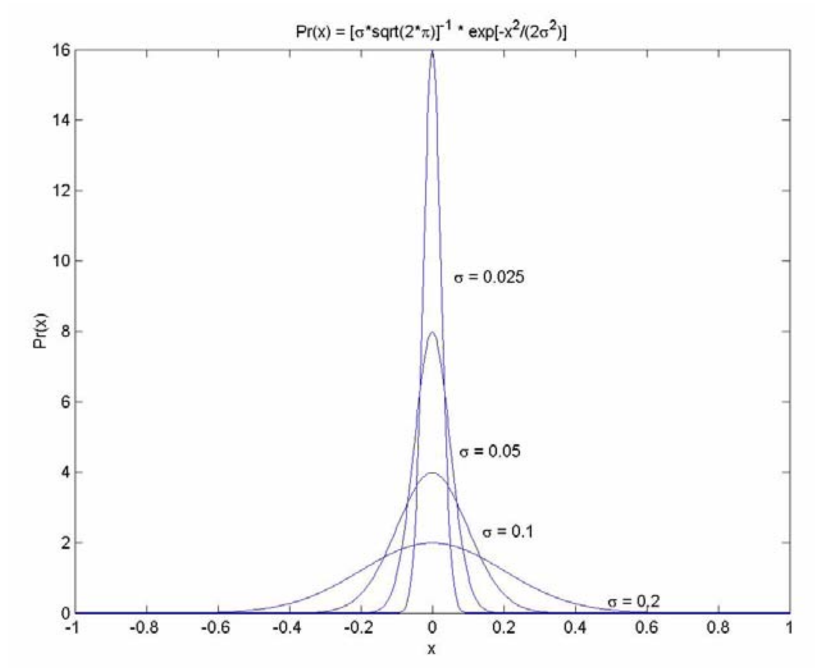

FIGURE 2. Dirac delta function as limit of Gaussian normal distribution as standard deviation approaches zero

We will never have to evaluate the Dirac delta function, but will only use the property that a function $f(x)$ defined on the domain $0 \le x \le L$ may be written as

$$f(x) = \int_0^L f(\xi)\delta(x-\xi)d\xi \qquad \text{(EQ 10)}$$

To see that this equation is valid, we note the Dirac delta function is zero except at $x = \xi$. We therefore can choose a very small, but non-zero, number ε and write this integral as

$$f(x) = \int_0^{(x-\varepsilon)} f(\xi)\delta(x-\xi)d\xi + \int_{(x-\varepsilon)}^{(x+\varepsilon)} f(\xi)\delta(x-\xi)d\xi + \int_{(x+\varepsilon)}^{L} f(\xi)\delta(x-\xi)d\xi$$

$$f(x) = \int_0^{(x-\varepsilon)} f(\xi)[0]d\xi + \int_{(x-\varepsilon)}^{(x+\varepsilon)} f(\xi)\delta(x-\xi)d\xi + \int_{(x+\varepsilon)}^{L} f(\xi)[0]d\xi \qquad \text{(EQ 11)}$$

$$f(x) = \int_{(x-\varepsilon)}^{(x+\varepsilon)} f(\xi)\delta(x-\xi)d\xi \approx f(x)\int_{(x-\varepsilon)}^{(x+\varepsilon)} \delta(x-\xi)d\xi$$

$$f(x) = f(x)$$

It is this property of the Dirac delta function, that upon integration it “extracts” the value of a function at a specific point, that makes it useful in the solution of boundary value problems involving linear differential equations.

We propose that the Green’s function $g(x, \xi)$ defined above can be used to express the solution to the boundary value problem as

$$u(x) = \int_0^L f(\xi) g(x, \xi) d\xi \qquad \text{(EQ 12)}$$

To see that this is true, we substitute this trial form of the solution into the differential equation,

$$\begin{aligned}
\frac{d^2 u}{dx^2} &= f(x) \\
\frac{d^2}{dx^2}\int_0^L f(\xi) g(x, \xi) d\xi &= \int_0^L f(\xi) \delta(x-\xi) d\xi \\
\int_0^L f(\xi)\left[\frac{d^2}{dx^2} g(x, \xi)\right] d\xi &= \int_0^L f(\xi) \delta(x-\xi) d\xi \\
\int_0^L f(\xi)\left[\frac{d^2}{dx^2} g(x, \xi) - \delta(x-\xi)\right] d\xi &= 0
\end{aligned} \qquad \text{(EQ 13)}$$

We therefore find that we can satisfy the differential equation for all possible functions $f(x)$ as long as the Green’s function satisfies the differential equation

$$\frac{d^2 g}{dx^2} = \delta(x-\xi) \qquad \text{(EQ 14)}$$

In particular, we want to find solutions to the differential equation that satisfy the boundary conditions,

$$u(0) = 0 = \int_0^L f(\xi) g(0, \xi) d\xi \qquad u(L) = 0 = \int_0^L f(\xi) g(L, \xi) d\xi \qquad \text{(EQ 15)}$$

This implies that the Green’s function must satisfy the boundary conditions,

$$g(0, \xi) = 0 \qquad g(L, \xi) = 0 \qquad \text{(EQ 16)}$$

as specified in the original definition of $g(x, \xi)$.

The whole idea behind the use of Green's functions is that once we find the functional form of $g(x, \xi)$, we can solve the problem for any given function $f(x)$ merely by evaluating a single definite integral,

$$u(x) = \int_0^L f(\xi) g(x, \xi) d\xi \quad \text{(EQ 17)}$$

There are two approaches that we may use to compute the Green's function for this problem. The first is a rather straight-forward method of writing the Green's function as a linear combination of the eigenfunctions of the second derivative.

$$g(x, \xi) = \sum_{m=1}^{\infty} c_m(\xi) \chi_m(x) \qquad \chi_m(x) = \left(\frac{2}{L}\right)^{\frac{1}{2}} \sin(m\pi x/L) \quad \text{(EQ 18)}$$

We substitute this expression into the differential equation and use the fact that $\chi_m(x)$ is an eigenfunction of the second derivative to obtain

$$\frac{d^2 g}{dx^2} = \sum_{m=1}^{\infty} c_m(\xi) \frac{d^2 \chi_m}{dx^2} = \delta(x - \xi)$$

$$\sum_{m=1}^{\infty} c_m(\xi) [-(m\pi/L)^2] \chi_m(x) = \delta(x - \xi) \quad \text{(EQ 19)}$$

We next use the fact that sine functions are orthogonal,

$$\langle \chi_m | \chi_n \rangle = \left(\frac{2}{L}\right) \int_0^L \sin(m\pi x/L) \sin(n\pi x/L) dx = \delta_{mn} = \begin{cases} 1, m = n \\ 0, m \neq n \end{cases} \quad \text{(EQ 20)}$$

to compute the coefficient functions $c_m(\xi)$. To do so, we multiply the differential equation by $\chi_n(x)$ and integrate over the domain $[0,L]$. All terms in the summation are zero except for that with $m = n$, yielding the coefficient function $c_n(\xi)$.

$$\sum_{m=1}^{\infty} c_m(\xi)[-(m\pi/L)^2]\left[\int_0^L \chi_m(x)\chi_n(x)dx\right] = \int_0^L \delta(x-\xi)\chi_n(x)dx$$

$$\sum_{m=1}^{\infty} c_m(\xi)[-(m\pi/L)^2]\langle\chi_m|\chi_n\rangle = \int_0^L \delta(x-\xi)\chi_n(x)dx$$

$$\sum_{m=1}^{\infty} c_m(\xi)[-(m\pi/L)^2]\delta_{mn} = \chi_n(\xi) \tag{EQ 21}$$

$$c_n(\xi)[-(n\pi/L)^2] = \chi_n(\xi)$$

$$c_n(\xi) = -\frac{\chi_n(\xi)L^2}{n^2\pi^2}$$

In terms of this eigenfunction expansion, the Green’s function takes the form

$$g(x,\xi) = -\sum_{m=1}^{\infty}\frac{\chi_m(\xi)\chi_m(x)L^2}{m^2\pi^2} = -\sum_{m=1}^{\infty}\frac{2L\sin(m\pi\xi/L)\sin(m\pi x/L)}{m^2\pi^2} \tag{EQ 22}$$

While this form of the Green’s function can be used to perform calculations, with a bit of physical insight, we can obtain an equivalent functional form of $g(x,\xi)$ that is much easier to use. To do so, we note that since the Dirac delta function $\delta(x-\xi)$ is non-zero only at $x = \xi$, we can write for $x < \xi$,

$$\left.\frac{d^2}{dx^2}g(x,\xi)\right|_{x<\xi} = 0 \tag{EQ 23}$$

Therefore, in this region, the form of the Green’s function must be

$$g(x<\xi,\xi) = A_0(\xi) + A_1(\xi)x \tag{EQ 24}$$

But, we know that at $x = 0$, we have the boundary condition $g(0,\xi) = 0$, requiring that

$$g(0,\xi) = A_0(\xi) + A_1(\xi)(0) = A_0(\xi) = 0 \tag{EQ 25}$$

Therefore, we have determined that for $x < \xi$, the Green’s function must be of the form

$$g(x<\xi,\xi) = A_1(\xi)x \tag{EQ 26}$$

Next, we look at the region $x > \xi$, where

$$\left.\frac{d^2}{dx^2}g(x, \xi)\right|_{x > \xi} = 0 \qquad \text{(EQ 27)}$$

that implies that for this region, the Green's function is of the form

$$g(x > \xi, \xi) = B_0(\xi) - B_1(\xi)x \qquad \text{(EQ 28)}$$

The boundary condition that $g(L, \xi) = 0$ requires that

$$\begin{aligned} g(L, \xi) &= B_0(\xi) - B_1(\xi)L = 0 \\ B_0(\xi) &= B_1(\xi)L \end{aligned} \qquad \text{(EQ 29)}$$

so that for $x > \xi$, the Green's function is

$$g(x > \xi, \xi) = B_1(\xi)L - B_1(\xi)x = B_1(\xi)(L - x) \qquad \text{(EQ 30)}$$

We have reasoned that the Green's function must be of the functional form,

$$g(x, \xi) = \begin{cases} A_1(\xi)x, 0 \le x < \xi \\ B_1(\xi)(L - x), \xi < x \le L \end{cases} \qquad \text{(EQ 31)}$$

We now need to establish two independent relations between $A_1(\xi)$ and $B_1(\xi)$ to specify exactly the Green's function. The first is rather straightforward; we require that the Green's function be continuous at $x = \xi$. This yields

$$A_1\xi = B_1(L - \xi) \qquad \text{(EQ 32)}$$

The second relation between $A_1(\xi)$ and $B_1(\xi)$ comes from a bit of physical insight into how the differential equation for the Green's function arises. Let us say that we have an equation of the form,

$$\frac{d^2u}{dx^2} = f(x) \qquad \text{(EQ 33)}$$

This equation is obtained from a conservation equation on the quantity of $u(x)$ where $-f(x)$ is a source term. To see that this is so, we write a balance on u in a differential control volume between $x - \Delta x$ and $x + \Delta x$,

$$\left.\frac{du}{dx}\right|_{x - \Delta x} - \left.\frac{du}{dx}\right|_{x + \Delta x} = \int_{(x - \Delta x)}^{(x + \Delta x)} (-f(x'))dx' \approx -f(x)2\Delta x \qquad \text{(EQ 34)}$$

The first term on the left is the "diffusive" flux into the control volume at $x - \Delta x$ and the second term is the "diffusive" flux out the other side. The term on the right is the "source" term and is the rate of generation of u within the control volume. Dividing this balance by $2\Delta x$ yields the equation

$$\frac{\left.\frac{du}{dx}\right|_{x-\Delta x} - \left.\frac{du}{dx}\right|_{x+\Delta x}}{2\Delta x} = -f(x) \tag{EQ 35}$$

At $\Delta x \to 0$,

$$\frac{\left.\frac{du}{dx}\right|_{x-\Delta x} - \left.\frac{du}{dx}\right|_{x+\Delta x}}{2\Delta x} \to -\frac{d^2 f}{dx^2} \tag{EQ 36}$$

and we obtain the differential equation

$$\frac{d^2 u}{dx^2} = f(x) \tag{EQ 37}$$

We now apply this same concept to the Green's function equation,

$$\frac{d^2 g}{dx^2} = \delta(x-\xi) \tag{EQ 38}$$

We form a balance for $g(x, \xi)$ on a small region surrounding the point $x = \xi$,

$$\left.\frac{dg}{dx}\right|_{\xi-\Delta x} - \left.\frac{dg}{dx}\right|_{\xi+\Delta x} = \int_{(\xi-\Delta x)}^{(\xi+\Delta x)} (-\delta(x-\xi))dx = -1 \tag{EQ 39}$$

This suggests that the first derivative of the Green's function is discontinuous at $x = \xi$ and experiences a "jump". On either side of $x = \xi$ we can compute the first derivative with respect to x,

$$\left.\frac{dg}{dx}\right|_{\xi-\Delta x} = A_1(\xi) \qquad \left.\frac{dg}{dx}\right|_{\xi+\Delta x} = -B_1(\xi) \tag{EQ 40}$$

We then use these results in the shell balance around $x = \xi$ to obtain the "jump" condition,

$$A_1(\xi) + B_1(\xi) = -1 \tag{EQ 41}$$

The two conditions for $A_1(\xi)$ and $B_1(\xi)$ generated by the condition that the Green's function be continuous at $x = \xi$ and the "jump" condition are

$$A_1\xi = B_1(L-\xi)$$
$$A_1 + B_1 = -1 \tag{EQ 42}$$

These two equations are readily solved to yield

$$A_1(\xi) = -\frac{(L-\xi)}{L} \qquad B_1(\xi) = -\frac{\xi}{L} \tag{EQ 43}$$

The Green’s function for this problem therefore takes the simple form,

$$g(x,\xi) = \begin{cases} -\frac{(L-\xi)x}{L}, \; 0 \le x < \xi \\ -\frac{\xi(L-x)}{L}, \; \xi < x \le L \end{cases} \tag{EQ 44}$$

This means that the solution to the boundary value problem,

$$\frac{d^2u}{dx^2} = f(x)$$
$$u(0) = 0 \qquad u(L) = 0 \tag{EQ 45}$$

is computed very simply by taking the integral

$$u(x) = \int_0^L f(\xi)g(x,\xi)d\xi$$
$$u(x) = \int_0^x f(\xi)g(x>\xi,\xi)d\xi + \int_x^L f(\xi)g(x<\xi,\xi)d\xi \tag{EQ 46}$$
$$u(x) = \int_0^x f(\xi)\left[-\frac{\xi(L-x)}{L}\right]d\xi + \int_x^L f(\xi)\left[-\frac{(L-\xi)x}{L}\right]d\xi$$

It is hard to find a simpler approach to solving a boundary value problem than by performing an integration with a known Green’s function. Unfortunately, not all boundary value problems can be solved using a Green’s function approach. Therefore, it is worthwhile to see what it is about this particular problem that allows the Green’s function technique to succeed.

The existence of a Green’s function for this problem is a consequence of the fact that the differential operator, in this case the second derivative, is linear. That is,

$$\hat{L}u \equiv \frac{d^2u}{dx^2}$$
$$\hat{L}(u_1 + u_2) = \hat{L}u_1 + \hat{L}u_2 \quad \text{(EQ 47)}$$

Therefore, if we have a "data" function that is the sum of two terms,

$$f(x) = f_1(x) + f_2(x) \quad \text{(EQ 48)}$$

we can write the differential equation as

$$\hat{L}u = \hat{L}u_1 + \hat{L}u_2 = f_1(x) + f_2(x) \quad \text{(EQ 49)}$$

so that we write the solution as

$$u(x) = u_1(x) + u_2(x) \quad \text{(EQ 50)}$$

where the two "contributions" to the solutions from each data function are computed individually.

$$\begin{array}{ll} \hat{L}u_1 = f_1(x) & \hat{L}u_2 = f_2(x) \\ u_1(0) = 0 & u_2(0) = 0 \\ u_1(L) = 0 & u_2(L) = 0 \end{array} \quad \text{(EQ 51)}$$

The Green's function formalism is an extension of this idea to the limit where we express the data function not as summation of a finite number of contributions, but rather as an integral (a continuos form of summation). To see how the Green's function is reached in this limit, let us approximate the solution to the problem by placing a grid of points separated by a uniform distance Δx. We then approximate the function $f(x)$ by interpolating between the function values at each point using "hat" functions (see figure below).

$$f(x) \approx \sum_{m=1}^{N} f(x_m)\Delta_m(x)(\Delta x) \quad \text{(EQ 52)}$$

The hat function for grid point x_m is defined as

$$\Delta_m(x) \equiv \begin{cases} \left(\frac{1}{\Delta x}\right)\frac{x - x_{m-1}}{x_m - x_{m-1}}, \ x_{m-1} \le x \le x_m \\ \left(\frac{1}{\Delta x}\right)\frac{x_{m+1} - x}{x_{m+1} - x_m}, \ x_m \le x \le x_{m+1} \\ 0, \ \text{otherwise} \end{cases} \quad \text{(EQ 53)}$$

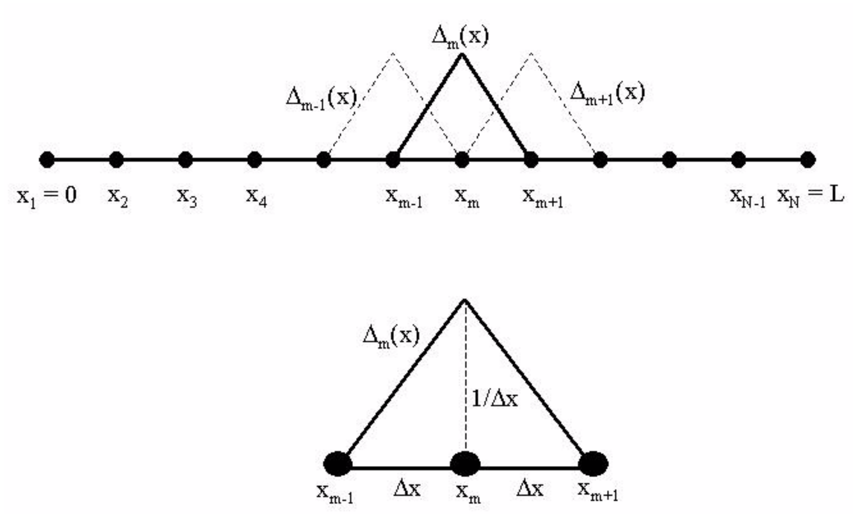

FIGURE 3. "Hat" functions used to approximate $f(x)$ from its values at distinct grid points

We see that this hat function has the following properties:

1. It is zero outside of a small interval $x_m - \Delta x \le x \le x_m + \Delta x$

2. For any grid point x_n, $\Delta_m(x_n) = \left(\frac{1}{\Delta x}\right)\delta_{mn}$

3. The area under each hat function is always equal to one, but as $\Delta x \to 0$, the hat function becomes more sharply peaked around x_m

4. For any value of x that is not a grid point, the approximation for $f(x)$ presented above interpolates linearly between the two nearest grid points to estimate the local value of $f(x)$

Using the property of linearity, we write the solution as

$$u(x) = \sum_{m=1}^{N} u_m(x) \quad \text{(EQ 54)}$$

where $u_m(x)$ is the solution to the boundary value problem

$$\begin{gathered} \hat{L}u_m = f(x_m)\Delta_m(x)(\Delta x) \\ u_m(0) = 0 \qquad u_m(L) = 0 \end{gathered} \quad \text{(EQ 55)}$$

We note that the product $f(x_m)(\Delta x)$ is merely some number, so we define the function $g_m(x)$ such that

$$u_m(x) = [f(x_m)(\Delta x)]g_m(x) \quad \text{(EQ 56)}$$

The boundary value problem for $g_m(x)$ is

$$\hat{L}g_m = \Delta_m(x)$$
$$g_m(0) = 0 \qquad g_m(L) = 0 \tag{EQ 57}$$

From the functions $g_m(x)$, we can compute the solution for any $f(x)$ from the summation,

$$u(x) = \sum_{m=1}^{N} f(x_m)g_m(x)(\Delta x) \tag{EQ 58}$$

We see that as $\Delta x \to 0$, the discrete grid point values x_m become the continuous variable ξ, $\Delta x \to d\xi$, and the hat functions become Dirac delta functions, $\Delta_m(x) \to \delta(x-\xi)$. In this limit, the approximation for $f(x)$ becomes

$$\sum_{m=1}^{N} f(x_m)\Delta_m(x)(\Delta x) \to \int_0^L f(\xi)\delta(x-\xi)d\xi = f(x) \tag{EQ 59}$$

The expression for the solution, obtained through the linearity property, becomes

$$\sum_{m=1}^{N} f(x_m)g_m(x)(\Delta x) \to \int_0^L f(\xi)g(x,\xi)d\xi = u(x) \tag{EQ 60}$$

There are many important boundary value problems that do possess this linearity property, and are defined on a simple enough geometry that the Green's function can be derived analytically. In such a case, solving the boundary value problem is very simple.

Unfortunately many important problems involve either complex geometries for which the Green's function itself must be computed numerically, or the differential equation is not linear. The latter is the typical case for problems involving both nonlinear reaction terms. For these problems, we will use the real-space methods - such as finite differences - to be developed in chapter 5.

Problem 2. Temperature distribution on a stove top

Consider the following “kitchen” transport problem. We have an electric stove top comprised of several heating elements. Each element contains within a ceramic matrix two annular regions in which heat is generated by electrical resistance (see figure below).

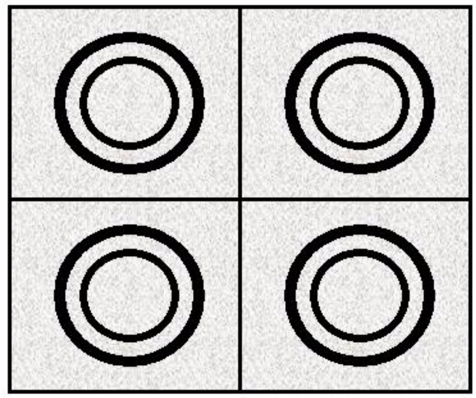

FIGURE 4. Stove top geometry showing 2x2 grid of heating elements

The geometry of an individual heating element in shown in the figures below. The first figure shows a top view of the geometry in the (x, y) plane. Each of the two heat generation regions is described by an annular region of specified inner radius and thickness. A side view in the second figure shows that these heat generation regions penetrate to a specified depth d_1. The thermal conductivities of the ceramic matrix and the heat generation material are assumed to equal a common value λ. Within the heat generation regions, the specified volumetric rate of heat generation is S.

We wish to calculate the temperature profile within the heat element. Since we are considering but a single element within a periodic array of identical copies, we employ periodic boundary conditions in the (x, y) plane. In the z direction, we assume that on top of the heating element ($z = 0$) a metal pot has been placed containing boiling water. If the thermal conductivity of the metal pot is much higher than the thermal conductivity of the ceramic matrix, we expect that at steady state, the temperature of the upper surface will be equal uniformly to that of boiling water, T_b (100 C under standard conditions). On the bottom surface, we assume that there is an underlying insulator layer, so that the heat flux out the bottom is zero. This implies a zero normal gradient at the bottom surface, $z = -D$.

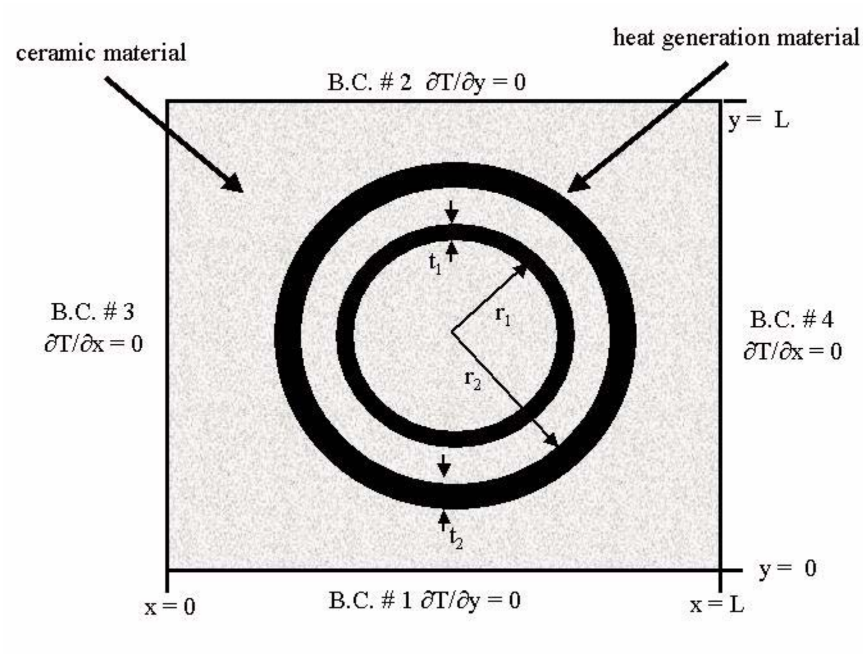

FIGURE 5. Top view of heating element geometry in (*x*,*y*) plane

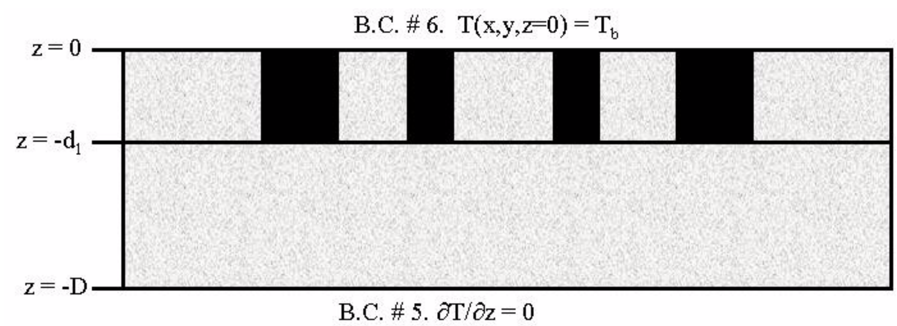

FIGURE 6. Side view of heating element showing depth profile

We can simplify the boundary conditions for this system by defining a dimensionless temperature field,

$$\theta = \frac{T - T_b}{T_b} \qquad T = T_b(1 + \theta) \tag{EQ 61}$$

and dimensionless coordinates

$$\chi = \frac{x}{L} - \frac{1}{2} \qquad \eta = \frac{y}{L} - \frac{1}{2} \qquad \zeta = \frac{z}{L} \tag{EQ 62}$$

If we convert the governing differential equation to dimensionless form, we reduce the set of independent system parameters to the following,

$$
\begin{array}{cc}
r_1/L & t_1/L \\
r_2/L & t_2/L \\
a \equiv L/D & b \equiv d_1/L
\end{array}
\qquad \text{(EQ 63)}
$$

$$
\sigma \equiv \frac{SL^2}{T_b\lambda}
$$

The boundary value problem, in these dimensionless variables, is

$$
-\frac{\partial^2\theta}{\partial\chi^2}-\frac{\partial^2\theta}{\partial\eta^2}-\frac{\partial^2\theta}{\partial\zeta^2} = \sigma H(\chi, \eta, \zeta)
$$

$$
\begin{array}{llllll}
\text{BC \# 1} & \eta = -\frac{1}{2} & -\frac{1}{2} \le \chi \le \frac{1}{2} & -\frac{1}{a} \le \zeta \le 0 & \frac{\partial\theta}{\partial\eta} = 0 \\
\text{BC \# 2} & \eta = \frac{1}{2} & -\frac{1}{2} \le \chi \le \frac{1}{2} & -\frac{1}{a} \le \zeta \le 0 & \frac{\partial\theta}{\partial\eta} = 0 \\
\text{BC \# 3} & \chi = -\frac{1}{2} & -\frac{1}{2} \le \eta \le \frac{1}{2} & -\frac{1}{a} \le \zeta \le 0 & \frac{\partial\theta}{\partial\chi} = 0 \\
\text{BC \# 4} & \chi = \frac{1}{2} & -\frac{1}{2} \le \eta \le \frac{1}{2} & -\frac{1}{a} \le \zeta \le 0 & \frac{\partial\theta}{\partial\chi} = 0 \\
\text{BC \# 5} & \zeta = -\frac{1}{a} & -\frac{1}{2} \le \chi \le \frac{1}{2} & -\frac{1}{2} \le \eta \le \frac{1}{2} & \frac{\partial\theta}{\partial\zeta} = 0 \\
\text{BC \# 6} & \zeta = 0 & -\frac{1}{2} \le \chi \le \frac{1}{2} & -\frac{1}{2} \le \eta \le \frac{1}{2} & \theta = 0
\end{array}
\qquad \text{(EQ 64)}
$$

The following function “switches on” the heat generation only within the specified annular regions,

$$
H(\chi, \eta, \zeta) = \begin{cases} 1, \text{ if } (\chi, \eta, \zeta) \text{ is within annular region} \\ 0, \text{ otherwise} \end{cases} \qquad \text{(EQ 65)}
$$

Note that the geometry of the problem is highly symmetric, so that we expect the solution to possess the symmetry,

$$
\theta(\chi, \eta, \zeta) = \theta(-\chi, \eta, \zeta) \qquad \theta(\chi, \eta, \zeta) = \theta(\chi, -\eta, \zeta) \qquad \text{(EQ 66)}
$$

Your assignment is the following

1.A. Propose a general form for $\theta(\chi, \eta, \zeta)$ as a linear combination

$$\theta(\chi, \eta, \zeta) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} c_{m,n,k} X_m(\chi) Y_n(\eta) Z_k(\zeta) \qquad \text{(EQ 67)}$$

where the functions $X_m(\chi)$, $Y_n(\eta)$, and $Z_k(\zeta)$ are either sine or cosine functions that satisfy the boundary conditions of the problem and possess the desired symmetry. Note that $\cos(x) = \cos(-x)$ and $\sin(x) = -\sin(-x)$. These sine and cosine functions are eigenfunctions of the second derivative,

$$-\frac{d^2}{dx^2}\cos(Ax) = A^2\cos(Ax) \qquad -\frac{d^2}{dx^2}\sin(Ax) = A^2\sin(Ax) \qquad \text{(EQ 68)}$$

1.B. Substitute the general form of the dimensionless temperature profile into the governing equation, and compute the temperature profile for the following parameter values.

$$\begin{aligned} a &= \frac{2}{3} & b &= 0.5 \\ r_1/L &= 0.1 & t_1/L &= 0.05 \\ r_2/L &= 0.25 & t_2/L &= 0.05 \end{aligned} \qquad \text{(EQ 69)}$$

Note that due to the linearity of the differential equation, we need solve the problem only once for a value of $\sigma = 1$. Let this solution be $\theta(\chi, \eta, \zeta; \sigma = 1)$. Then, if we require the solution for other values of the heat generation rate, we need merely multiply this solution by the desired value of σ to obtain the new solution,

$$\theta(\chi, \eta, \zeta; \sigma) = \sigma \times \theta(\chi, \eta, \zeta; \sigma = 1) \qquad \text{(EQ 70)}$$

From your results, plot the dimensionless temperature field in the mid-plane in (χ, ζ) defined by $\eta = 0$.

Hints:

1. Use the fact that cosine and sine functions have orthogonality conditions to calculate the coefficients in your expansion. For example, consider the integral

$$\int_{-1/2}^{1/2} \cos(2m\pi x)\cos(2n\pi x)dx = \frac{1}{2}\delta_{mn} \qquad \text{(EQ 71)}$$

We could establish this orthogonality condition analytically, probably by consulting a table of integrals. More easily, we could check that it is valid by using the MATLAB functions *trapz()* or *quad()* to compute the value of the integral numerically for different values of m and n. Using this latter approach, you should be able to quickly establish the orthogonality relations for the basis functions that you select in 2.A.

2. The values of your coefficients will be proportional to integrals of the form

$$\langle H|(m,n,k)\rangle = \int_{-\frac{1}{2}}^{\frac{1}{2}}\int_{-\frac{1}{2}}^{\frac{1}{2}}\int_{-\frac{1}{a}}^{0} H(\chi,\eta,\zeta)X_m(\chi)Y_n(\eta)Z_k(\zeta)d\zeta d\eta d\chi \qquad \text{(EQ 72)}$$

For the annular geometry of the system, you can evaluate these integrals with little effort. First, you may note that since there are no heat generation regions for $\zeta < -b$, you can rewrite the integral as

$$\langle H|(m,n,k)\rangle = \int_{-\frac{1}{2}}^{\frac{1}{2}}\int_{-\frac{1}{2}}^{\frac{1}{2}}\int_{-b}^{0} H(\chi,\eta,\zeta)X_m(\chi)Y_n(\eta)Z_k(\zeta)d\zeta d\eta d\chi \qquad \text{(EQ 73)}$$

Next, we use the annular nature of the heat generation regions to note that for $\zeta > -b$, the function $H(\chi, \eta, \zeta)$ is solely a function of $r = \sqrt{\chi^2 + \eta^2}$ to write

$$\langle H|(m,n,k)\rangle = \left[\int_{-\frac{1}{2}}^{\frac{1}{2}}\int_{-\frac{1}{2}}^{\frac{1}{2}} H(r)X_m(\chi)Y_n(\eta)d\eta d\chi\right]\left[\int_{-b}^{0} Z_k(\zeta)d\zeta\right] \qquad \text{(EQ 74)}$$

At this point it is best to convert the first integral to polar coordinates. Rather than evaluate this integral analytically, you may use the MATLAB function *dblquad()*. You can evaluate the second integral using the MATLAB function *quad()*. These routines work by evaluating the integrand function at a finite number of grid points that break up the integration domain into a number of non-overlapping subintervals. On each subinterval, a polynomial of low degree is constructed to interpolate between the grid point values. The integral of this local polynomial approximation over the subinterval is calculated analytically and the sum of these integrals on each subinterval are added together to yield the numerical value of the definite integral. The number of grid points is increased until the estimated error in the calculated integral value is smaller than some allowable tolerance. For more details, see section 4.2.4 of the notes. The availability of these robust, accurate methods to calculate definite integrals saves us much effort in the solution of this problem.

3. The plot that you obtain should look like the following,

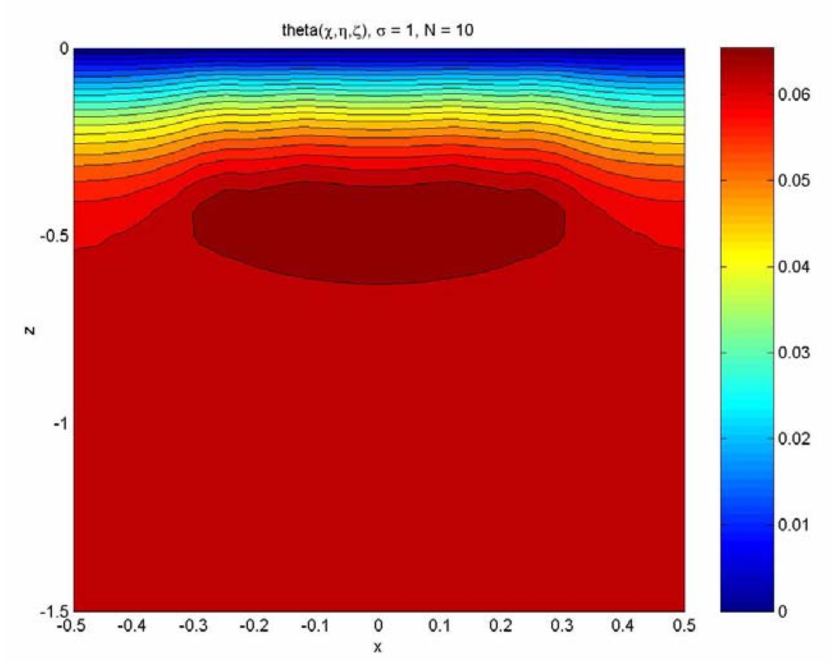

FIGURE 7. Dimensionless temperature field within heating element. Slice at $\eta = 0$

1.C. Compute the gradient of the temperature normal to the top surface as a function of χ and η. Make a color contour plot of this quantity, as it is proportional to the local heat flux into the metal pot. Where is the flux of heat out of the heating element into the pot the greatest?

Integrate the normal gradient over the top surface to get a measure of the total flux into the metal pot. How does this value relate to the total rate of heat generated by the annular regions in the element?