Derivation of Diffusion Equation

The diffusion equation (5.30) is one of the most important PDE applications, so let's see how it is derived. We let $C(x, y, z, t)$ be the density (mass per unit volume) of a diffusing substance X, and let E be any small subregion of the region where diffusion is occurring. Then the total mass of X within the subregion is $\int \int \int_E C \, dV$, and

$$\frac{d}{dt} \int \int \int_E C \, dV = \int \int_{\partial E} \mathbf{J} \bullet (-\mathbf{n}) \; dA + \int \int \int_E q \, dV$$

This equation says that the rate of change of the total mass of X in E is equal to the net rate at which X is entering from outside plus the net rate at which X is being created internally due to sources and sinks. The flux vector $\mathbf{J}$ represents the net flow of X, in mass per unit area per unit time, due to diffusion or convection, and can be thought of as the density C times the average velocity of the particles. Thus the dot product of the flux vector with the unit inward normal vector $(-\mathbf{n})$ is the density times the component of the average velocity inward through the boundary, so the above boundary integral gives the total mass per unit time entering the subregion E. $q(x, y, z, t)$ is the net rate, in mass per unit volume per unit time, that X is being created within E, so the second integral on the right gives the total mass per unit time created (or destroyed) inside E.

Now if we use the divergence theorem (see the "Review of Multivariate Calculus" link near the bottom of the class web page) we see that

$$\int \int \int_E [C_t + \nabla \bullet \mathbf{J} - q] \; dV = 0$$

Since E is an arbitrary, small, subregion, this means that the integrand must be zero everywhere.

Now Fick's Law (9.8 is the 1D version) says that the flux due to (isotropic) diffusion is in the direction of most rapid decrease in concentration $(-\nabla C)$, and its magnitude is proportional to the rate of decrease in that direction, $\mathbf{J} = -D\nabla \mathbf{C}$, where the proportionality constant $D(x, y, z)$ is the diffusion coefficient. Using Fick's Law, then, our partial differential equation becomes:

$$C_t = \nabla \bullet [D\nabla \mathbf{C}] + q$$

which is (5.30). However, if there also convection, there is an additional flux of X which is equal to the density times the wind or current velocity vector $\mathbf{v}$, and then

the total flux, due to both diffusion and convection, is $\mathbf{J} = -D\nabla C + C\mathbf{v}$, and the equation becomes

$$C_t = \nabla \bullet [D\nabla \mathbf{C} - C\mathbf{v}] + q$$

Equation (9.30) is a 1D version of this diffusion/convection/reaction equation. In problem 2, you solved the 1D problem (6.4), which is essentially this same equation, where heat is what is diffusing and convecting and being generated.
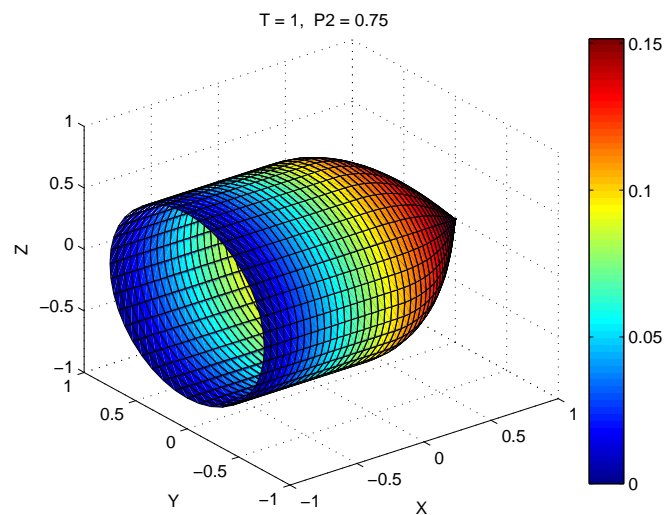
Problems

8.   a. Now we will solve the steady-state diffusion problem 5.30 (p102), where the time derivative term is set to zero, in a 3D bullet-shaped region. The region is a cylinder whose axis is the x-axis, and whose radius varies with x: $r(x) = 1$ for $-1 \le x \le 0$ and $r(x) = cos(\pi x/2)$ for $0 < x \le 1$.

Output grid
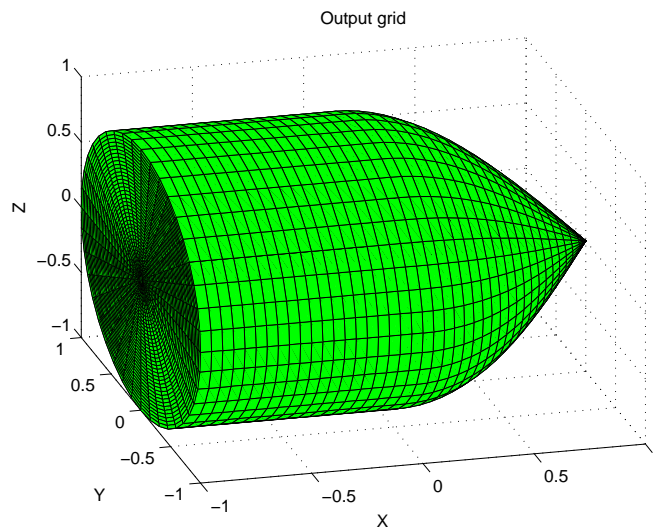
We will take the diffusion coefficient $D = 5$, and the source term q will be 1 for $x > 0$ and zero otherwise. Thus, the diffusing element C is being created by a chemical reaction in the forward (nose cone) half of the bullet, but not in the back half. The rear surface is in contact with another material which has no C, so the boundary condition at $x = -1$ will be $C = 0$. The rest of the boundary is insulated, so the normal derivative (see 5.25, p97) is zero, $\frac{\partial C}{\partial n} = 0$, that is, there is no flux across the sides of the bullet. Solve for the concentration C

and calculate the integral of C over the entire bullet, and make some MATLAB cross-sectional plots of C. It is important for good accuracy to make sure there is a gridline at $x = 0$, where the source term q is discontinuous.

If you need to define any coefficients, such as q, using an IF statement, remember that you can simply reference a Fortran function and supply the function at the end (see function TRUE(X,Y) in interactive driver example 2). Alternatively, you can add the IF statements when prompted right before the coefficient is used (see D(Z) in interactive driver example 12).

T = 1, P2 = 0.75

b. If this 3D problem is solved in cylindrical coordinates, that is, if y, z are replaced by polar coordinates r, ϕ, the solution will obviously not depend on the polar angle ϕ, so then 5.30 can be written in the "axi-symmetric" form (cf. formula 5.24b):

$\frac{\partial C}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(rD\frac{\partial C}{\partial r}\right) + \frac{\partial}{\partial x}\left(D\frac{\partial C}{\partial x}\right) + q$

Re-solve the problem of part "a" as a 2D steady-state axi-symmetric problem, using the Galerkin method, and again compute the integral of C over the entire bullet (hint: this means you must integrate $2\pi\, r\, C$ over the 2D axi-symmetric cross-section). You will of course have to use "y" for "r", and again it is important that there be no triangles in the initial triangulation (and thus none in the final triangulation) which straddle the interface $x = 0$. On the bottom of the region ($r = 0$) you can use either the boundary condition $\frac{\partial C}{\partial r} = 0$ or "no" boundary

condition. Create a MATLAB surface plot of $C(x, y)$.

c. Finally, re-solve the axi-symmetric problem "b" but now with D decreased to 1 in the "nose cone" half of the bullet ($x > 0$) only. Thus the nose cone and the back half of the bullet are made out of different materials, diffusion is slower in the nose cone. Recall that the chemical reaction which is creating C only occurs in the nose cone. It is very easy to treat composite materials such as this using the Galerkin method, one simply defines D to be a discontinuous function of position. Note that $D(x)$ is not constant (even though it is piecewise constant) so you cannot take it out of the brackets in $\frac{\partial}{\partial x}\left[D\frac{\partial C}{\partial x}\right]$. However, $D\frac{\partial C}{\partial x}$ must be continuous, otherwise its derivative would not exist, so $\frac{\partial C}{\partial x}$ must be discontinuous also, see plot of C below. The collocation method cannot handle such problems as easily, because to put this term in the form required by the collocation method, we would have to write as $D\frac{\partial^2 C}{\partial x^2} + \frac{\partial D}{\partial x}\frac{\partial C}{\partial x}$ and $\frac{\partial D}{\partial x}$ would be infinite at $x = 0$.