<u>**Recitation Notes**</u>

September 18/19, 2003

Topics covered

- Fourier series solution
- Q&A: Steady state and Transient state diffusion

The story of the **Fourier series solution**…

The Fourier series solution of a diffusion equation is the result of a method called *Separation of Variables*. We assume that the solution for the diffusion equation can be written as a product of two functions, each depended on only one variable. In this case, the concentration profile is written as a product of a "x-only" function, X*(x)*, and a "t-only" function, T*(t)*.

$$c(x,t) = X(x)T(t)$$

When we substitute this trial solution into the diffusion equation, we get

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}$$

$$\frac{\partial (X(x)T(t))}{\partial t} = D\frac{\partial^2 (X(x)T(t))}{\partial x^2}$$

$$X(x)\frac{\partial T(t)}{\partial t} = DT(t)\frac{\partial^2 X(x)}{\partial x^2}$$

$$\frac{1}{DT(t)}\frac{\partial T(t)}{\partial t} = \frac{1}{X(x)}\frac{\partial^2 X(x)}{\partial x^2}$$

Note that the left hand side is in terms of t only, and similarly, the right hand side is in terms of x only. The only condition under which the equality between the LHS and the RHS is satisfied is if they both evaluate to a constant. Let's suppose that constant is $-\lambda$, and then write the LHS and the RHS into two separate equations.

$$\frac{\partial T(t)}{\partial t} = -\lambda DT(t)$$

$$\frac{\partial^2 X(x)}{\partial x^2} = -\lambda X(x)$$

By inspection, the T function is going to be an exponential function (not very interesting). On the other hand, the X function can either be an exponential function or a trigonometric function depending on λ (as you have seen in your first assignment).

$$X(x) = \begin{cases} A\sin\left(\sqrt{\lambda}x\right) + B\cos\left(\sqrt{\lambda}x\right) & (\lambda > 0) \\ A'e^{\sqrt{-\lambda}x} + B'e^{-\sqrt{-\lambda}x} & (\lambda < 0) \\ A''x + B'' & (\lambda = 0) \end{cases}$$

The specific boundary conditions and initial conditions of a given problem determine the form of the solution.

Let's focus on the $\lambda > 0$ case. This solution leads to a Fourier series due to the periodicity of sinusoidal functions. Hence, the *X* function can be expressed as a summation of the set of sine/cosine curves that satisfies the initial condition. However, each element in the series brings an "amplitude" term (called the Fourier coefficients) that need to be determined; e.g.

$$c_o = \sum_{n=1}^{\infty} A_n \sin\left(n\pi \frac{x}{L}\right)$$

The need to figure out each and every A_n makes the solution process a lot harder and much more tedious than it first appears to be. Refer to your calculus textbook on how to find the Fourier coefficients for general case.

Summary on Diffusion

Consider the following questions when approaching a diffusion problem:

1. Is the system in a (quasi) steady state or in a transient state?
2. Define the boundary of the system.
3. Which type of boundary conditions does the system have?
    a. Constant concentration
    b. Constant flux
    c. Surface flux depends on surface concentration
4. What is the initial condition? (esp. important in transient problems)
5. What is the most appropriate coordinate system (Cartesian, cylindrical or spherical) for representing the physical system?

If the system is in a (quasi) steady state…

6. Is there any reaction/production occurring within the boundary of the system?
7. Can you write the mass or mole balance equation for the system (i.e. Flux in – Flux out + Reaction/Production = 0)?
8. Can you express the mass/mole balance equation into a differential equation and then solve it?
9. Can you determine the integration constants with the boundary conditions identified earlier?

If the system in a transient state…

6. Can the system be approximated as having an infinite or semi-infinite domain? If yes, until when is the solution valid?
7. For systems with (semi-) infinite domain, does the initial concentration profile resemble that of a step function or a delta function?
8. If the initial concentration profile resembles a delta function, does the "point source" on the boundary changes with time or remains constant with time?
9. For systems with finite domain, can an infinite domain solution be applied for small time t?
10. If the Fourier series solution is needed, is it possible to modify the standard square wave solution given in class to correctly depict the actual system?
11. In all cases, when will steady state be achieved?