More Diffusion Equation Solutions

Larry Caretto
Mechanical Engineering 501B

Seminar in Engineering Analysis

February 2, 2009

California State University Northridge

Overview

- Review last class
  - Separation of variables and eigenfunction expansions for initial condition
- Gradient boundary condition
  - In-class exercise for one of the homework problems
- Convection boundary condition
  - Use variable transforms to get homogenous boundary conditions required for a Sturm-Liouville problem

California State University Northridge

Review Diffusion and Laplace

- Partial differential equations related to conservation principles of fluxes governed by potentials
  - Heat transfer from temperature gradient
  - Mass diffusion from concentration gradient
  - Current from electrostatic potential
  - Magnetic fluxes
  - Ideal fluid flow from velocity potential

California State University Northridge 3

Review Multidimensional PDEs

- General diffusion equation for three dimensions $\frac{\partial u}{\partial t} = \alpha \nabla^2 u$

- Laplace (steady) $\nabla^2 u = 0$

$$\text{Cartesian} \quad \nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}$$

$$\text{Cylindrical} \quad \nabla^2 u = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2} + \frac{\partial^2 u}{\partial z^2}$$

$$\text{Sphere} \quad \nabla^2 u = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial u}{\partial r}\right) + \frac{1}{r^2 \sin^2\phi}\frac{\partial^2 u}{\partial \theta^2} + \frac{1}{r^2}\frac{\partial^2 u}{\partial \phi^2} + \frac{\cot\phi}{r^2}\frac{\partial u}{\partial \phi}$$

California State University Northridge 4

Review Diffusion Solutions

- Governs heat conduction and species diffusion for $t \geq 0$ and $0 \leq x \leq x_{max}$
  - $u(x,t)$ is temperature, species concentration
  - Initial condition $u(x,0) = u_0(x)$
  - Boundaries $u(0,t) = u_L(t)$; $u(x_{max},t) = u_R(t)$
  - Started with $u(0,t) = u(x_{max},t) = 0$
- Diffusivity, α, is material property $(\text{length})^2/(\text{time})$

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$$

California State University Northridge 5

Review Separation of Variables

- Assume $u(x,t) = X(x)T(t)$

$$\frac{\partial u}{\partial t} = \frac{\partial[X(x)T(t)]}{\partial t} = X(x)\frac{\partial T(t)}{\partial t} =$$

$$\alpha\frac{\partial^2 u}{\partial x^2} = \alpha\frac{\partial^2[X(x)T(t)]}{\partial x^2} = \alpha T(t)\frac{\partial^2 X(x)}{\partial x^2}$$

- Dividing by $\alpha X(x)T(t)$ gives $f(t) = g(x)$ which must equal a constant

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

California State University Northridge 6

Review General Solution

- Solve two ODEs

$$\frac{dT(t)}{dt} + \lambda^2 \alpha T(t) = 0 \qquad T(t) = Ae^{-\lambda^2 \alpha t}$$

$$\frac{d^2 X(x)}{dx^2} + \lambda^2 X(x) = 0 \quad X(x) = B\sin(\lambda x) + C\cos(\lambda x)$$

$$u(x,t) = T(t)X(x) = Ae^{-\lambda^2 \alpha t}\left[B\sin(\lambda x) + C\cos(\lambda x)\right]$$

$$= e^{-\lambda^2 \alpha t}\left[C_1 \sin(\lambda x) + C_2 \cos(\lambda x)\right]$$

- Can use this as starting point for any boundary or initial conditions

California State University Northridge 7

Review Homogenous BCs

- Look at case where $u(0,t) = u(x_{max},t) = 0$
- In this case, X(x) is the solution to a Sturm-Liouville problem
- $X(x) = B\sin(\lambda x) + C\cos(\lambda x)$
- $X(0) = 0 = B\sin(0) + C\cos(0) =$ $C = 0$
- $X(x_{max}) = 0 = B\sin(\lambda x_{max})$
- Must have $\lambda x_{max} = n\pi$ (n an integer)
- Complete set of orthogonal eigenfunctions: $\sin(n\pi x/x_{max})$

California State University Northridge 8

Review Initial Condition

- General solution: sum of all eigenfunctions

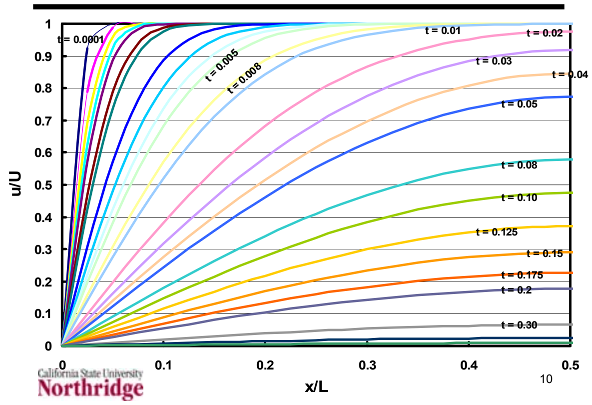
$$u(x,t) = \sum_{n=1}^{\infty} C_n e^{-\lambda_n^2 \alpha t} \sin(\lambda_n x) \qquad \lambda_n = \frac{n\pi}{x_{max}}$$

- Eigenfunction expansion gives any initial condition $u_0(x) = u(x,0) = \sum_{n=1}^{\infty} C_n \sin\left(\frac{n\pi x}{x_{max}}\right)$

$$C_m = \frac{\int_0^{x_{max}} u_0(x)\sin\left(\frac{m\pi x}{x_{max}}\right)dx}{\int_0^{x_{max}} \sin^2\left(\frac{m\pi x}{x_{max}}\right)dx} = \frac{2}{x_{max}}\int_0^{x_{max}} u_0(x)\sin\left(\frac{m\pi x}{x_{max}}\right)dx$$

California State University Northridge 9

Review Solution for $u_0(x) = U$



California State University Northridge 10

Review Nonzero Boundaries

- Sturm-Liouville eigenfunction expansion requires zero boundary conditions
- For nonzero boundaries, $u(0,t) = u_L$ and $u(x_{max},t) = u_R$ split solution into two functions $u(x,t) = v(x,t) + w(x)$
  - v satisfies diffusion equation with zero boundary conditions: $\partial v/\partial t = \alpha\partial^2 v/\partial x^2$ with $v(0,t) = v(x_{max},t) = 0$; $v(x,0) = u(x,0) - w(x)$
  - w satisfies ODE $d^2w/dx^2 = 0$ with boundary conditions $w(0) = u_L$ and $w(x_{max}) = u_R$
  - u = v + w satisfies PDEs, BC and ICs

California State University Northridge 11

Review Nonzero Boundaries II

- Eigenfunction expansion used for zero boundary solution v(x,0) gives

$$C_m = \frac{2}{x_{max}}\int_0^{x_{max}} \left[u_0(x) - u_L - \frac{u_R - u_L}{x_{max}}x\right]\sin\left(\frac{m\pi x}{x_{max}}\right)dx$$

$v(x,0) = u_0(x) - w(x)$

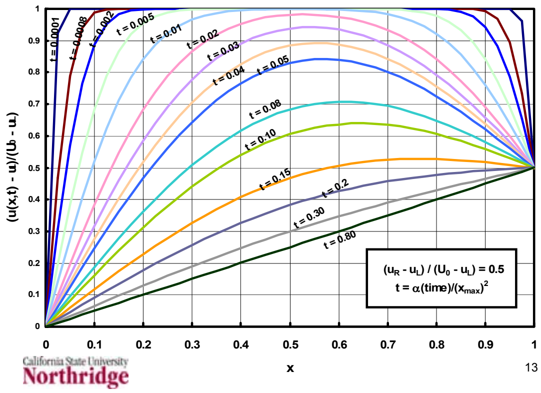
- After C_n is found, solution is

$$u(x,t) = \sum_{n=1}^{\infty} C_n e^{-\left(\frac{n\pi}{x_{max}}\right)^2 \alpha t} \sin\left(\frac{n\pi x}{x_{max}}\right) + u_L + \frac{u_r - u_L}{x_{max}}x$$

v(x,t) **w(x)**

California State University Northridge 12

Review $u_0(x) = U_0$ Example



California State University Northridge 13

Other Boundary Conditions

- Can have boundary conditions on gradients
  - Physical meaning is flux
    - Zero gradient of temperature, mass fraction, etc. means is zero flux of heat, diffusion, etc.
  - Sturm-Liouville problem requires zero gradient boundary condition
  - Start with separation of variables solution

$$u(x,t) = T(t)X(x) = Ae^{-\lambda^2 \alpha t}\left[B\sin(\lambda x) + C\cos(\lambda x)\right]$$
$$= e^{-\lambda^2 \alpha t}\left[C_1\sin(\lambda x) + C_2\cos(\lambda x)\right]$$

California State University Northridge 14

Homework Problem for 2/9

- Text, p 561, prob 13: find u(x,t) for 0 ≤ x ≤ L

$$\frac{\partial u}{\partial t} = \alpha\frac{\partial^2 u}{\partial x^2} \qquad \left.\frac{\partial u}{\partial x}\right|_{x=0} = \left.\frac{\partial u}{\partial x}\right|_{x=L} = 0 \qquad u(x,0) = f(x)$$

- Show that the solution is

Note: Kreyszig uses $c^2 = \alpha$

$$u(x,t) = A_0 + \sum_{n=1}^{\infty} A_n e^{-\lambda_n^2 \alpha t}\cos(\lambda_n x) \qquad \lambda_n = \frac{n\pi}{L}$$
$$A_0 = \frac{1}{L}\int_0^L f(x)dx \qquad A_n = \frac{2}{L}\int_0^L f(x)\cos\left(\frac{n\pi x}{L}\right)dx$$

California State University Northridge 15

Class Exercise

- Work problem on previous chart
- Start with separation of variables result

$$u(x,t) = T(t)X(x) = Ae^{-\lambda^2 \alpha t}\left[B\sin(\lambda x) + C\cos(\lambda x)\right]$$
$$= e^{-\lambda^2 \alpha t}\left[C_1\sin(\lambda x) + C_2\cos(\lambda x)\right]$$

- Apply zero gradient boundary conditions to get eigenfunction solution
- Use eigenfunction expansion for initial conditions

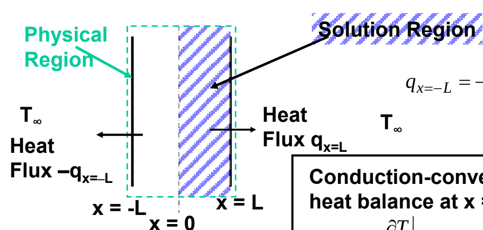
California State University Northridge 16

Convection Boundary Condition

- Look at gradient and mixed boundary conditions
- Show how making differential equation dimensionless can lead to Sturm-Liouville problem in initial formulation
- Consider convective heat transfer to sides of slab in region –L ≤ x ≤ L
  - Because of symmetry solve 0 ≤ x ≤ L with zero gradient (symmetry) condition at x = 0

California State University Northridge 17

Problem Diagram



$$q_{x=-L} = -q_{x=L}$$

Conduction-convection heat balance at x = L

$$q_{x=L} = -k\left.\frac{\partial T}{\partial x}\right|_{x=L} = h(T_{x=L} - T_\infty)$$

Symmetry Condition at x = 0 $\left.\frac{\partial T}{\partial x}\right|_{x=0} = 0$

$$q_{x=-L} = -k\left.\frac{\partial T}{\partial x}\right|_{x=-L} = h(T_\infty - T_{x=-L})$$

California State University Northridge 18

Problem Definition

- Diffusion equation $\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$
- Initial condition $T(x,0) = f_0(x)$
- Symmetry boundary condition $\left.\frac{\partial T}{\partial x}\right|_{x=0} = 0$
- Convection boundary condition

$$k\left.\frac{\partial T}{\partial x}\right|_{x=L} + h(T_{x=L} - T_\infty) = 0 \quad \Rightarrow \quad k\left.\frac{\partial T}{\partial x}\right|_{x=L} + hT_{x=L} = hT_\infty$$

Nonhomogenous boundary condition

California State University Northridge 19

Dimensionless Variables

- We can convert the boundary condition at x = L to a Sturm-Liouville problem by defining a new variable like $\theta = T - T_\infty$
- All other occurrences of T, which are in derivatives, will not change
- For convenience we typically define the following dimensionless variables (based on previous results)

$$\Theta = \frac{T - T_\infty}{T_0 - T_\infty} \qquad \xi = \frac{x}{L} \qquad \tau = \frac{\alpha t}{L^2}$$

Reference value (constant initial value)

California State University Northridge 20

Substitute Dimensionless

$$\frac{\partial T}{\partial t} = \frac{\partial[(T_0 - T_\infty)\Theta + T_\infty]}{\partial\left(\frac{L^2\tau}{\alpha}\right)} = \frac{\alpha(T_0 - T_\infty)}{L^2}\frac{\partial\Theta}{\partial\tau}$$

=

$$= \alpha\frac{\partial^2 T}{\partial x^2} = \alpha\frac{\partial^2[(T_0 - T_\infty)\Theta + T_\infty]}{\partial(L\xi)^2} = \frac{\alpha(T_0 - T_\infty)}{L^2}\frac{\partial^2\Theta}{\partial\xi^2}$$

$$0 = \frac{\partial T}{\partial x} = \frac{\partial[(T_0 - T_\infty)\Theta + T_\infty]}{\partial(L\xi)} = \frac{(T_0 - T_\infty)}{L}\frac{\partial\Theta}{\partial\xi} = 0$$

$$k\frac{\partial T}{\partial x} + h(T - T_\infty) = \frac{k(T_0 - T_\infty)}{L}\frac{\partial\Theta}{\partial\xi} + h(T_0 - T_\infty)\Theta = 0$$

California State University Northridge 21

Dimensionless Problem

- Diffusion equation $\frac{\partial T}{\partial t} = \alpha\frac{\partial^2 T}{\partial x^2}$ | $\frac{\partial\Theta}{\partial\tau} = \frac{\partial^2\Theta}{\partial\xi^2}$
- Initial condition $T(x,0) = f_0(x)$ | $\Theta(\xi,0) = \frac{f_0(\xi L) - T_\infty}{T_0 - T_\infty}$
- Symmetry boundary condition $\left.\frac{\partial T}{\partial x}\right|_{x=0} = 0$ | $\left.\frac{\partial\Theta}{\partial\xi}\right|_{\xi=0} = 0$
- Convection boundary condition

$$k\left.\frac{\partial T}{\partial x}\right|_{x=L} + h(T_{x=L} - T_\infty) = 0 \quad \Big| \quad \left.\frac{\partial\Theta}{\partial\xi}\right|_{\xi=1} + \frac{hL}{k}\Theta_{\xi=1} = 0$$

Homogenous boundary condition

California State University Northridge 22

General Solution

- Start with separation of variables solution in dimensionless coordinates

$$\Theta(\xi,\tau) = e^{-\lambda^2\tau}[C_1\sin(\lambda\xi) + C_2\cos(\lambda\xi)]$$

$$\frac{\partial\Theta}{\partial\xi} = \lambda e^{-\lambda^2\tau}[C_1\cos(\lambda\xi) - C_2\sin(\lambda\xi)]$$

- Boundary condition of zero gradient at ξ = 0 requires $C_1 = 0$

$$\left.\frac{\partial\Theta}{\partial\xi}\right|_{\xi=0} = 0 = \lambda e^{-\lambda^2\tau}[C_1\cos(0) - C_2\sin(0)] = C_1\lambda e^{-\lambda^2\tau}$$

California State University Northridge 23

Boundary at ξ = 1

- Substitute solution into dimensionless convection boundary condition at ξ = 1

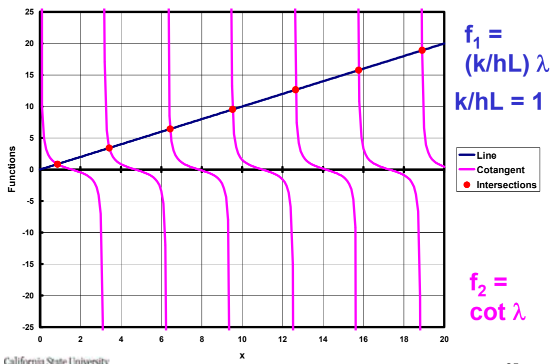
$$\left.\frac{\partial\Theta}{\partial\xi}\right|_{\xi=1} + \frac{hL}{k}\Theta_{\xi=1} = -\lambda e^{-\lambda^2\tau}C_2\sin(\lambda) + \frac{hL}{k}e^{-\lambda^2\tau}C_2\cos(\lambda) = 0$$

- Get equation to be solved for λ

$$\frac{k}{hL}\lambda = \frac{\cos(\lambda)}{\sin(\lambda)} = \cot(\lambda)$$

California State University Northridge 24

Finding λ_n



Getting Initial Conditions

- Solution as sum of all eigenfunctions

$$\Theta(\xi,\tau) = \sum_{m=1}^{\infty} C_m e^{-\lambda_m^2 \tau} \cos(\lambda_m \xi) \qquad \lambda_m = \frac{hL}{k}\cot(\lambda_m)$$

- Eigenfunction expansion for initial condition
  - Valid because Θ are eigenfunctions for a Sturm-Liouville problem even though eigenvalues are not evenly spaced

$$\Theta(\xi,0) = \Theta_0(\xi) = \sum_{m=1}^{\infty} C_m \cos(\lambda_m \xi) \qquad \lambda_m = \frac{hL}{k}\cot(\lambda_m)$$

Getting Initial Conditions II

- Usual formula for C_m but $\lambda_m \neq m\pi$ $\qquad \Theta = \frac{T - T_\infty}{T_0 - T_\infty}$

$$C_m = \frac{\int_0^1 \Theta_0(\xi)\cos(\lambda_m \xi)d\xi}{\int_0^1 \cos^2(\lambda_m \xi)d\xi} = \frac{2\lambda_m \int_0^1 \Theta_0(\xi)\cos(\lambda_m \xi)d\xi}{\cos(\lambda_m)\sin(\lambda_m) + \lambda_m}$$

- Constant initial temperature, T_0, gives $\Theta_0 = 1$

$$C_m = \frac{2\lambda_m \int_0^1 (1)\cos(\lambda_m \xi)d\xi}{\cos(\lambda_m)\sin(\lambda_m) + \lambda_m} = \frac{2\sin(\lambda_m)}{\cos(\lambda_m)\sin(\lambda_m) + \lambda_m}$$

Solution

- Substitute formula for C_m into previous solution

$$\Theta(\xi,\tau) = \sum_{m=1}^{\infty} C_m e^{-\lambda_m^2 \tau} \cos(\lambda_m \xi) \qquad \lambda_m = \frac{hL}{k}\cot(\lambda_m)$$

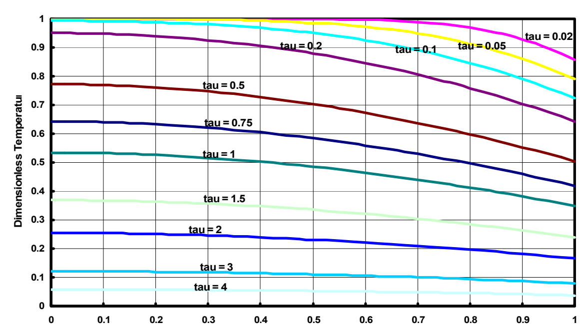
$$\Theta(\xi,\tau) = \sum_{m=1}^{\infty} \frac{2\sin(\lambda_m) e^{-\lambda_m^2 \tau} \cos(\lambda_m \xi)}{\cos(\lambda_m)\sin(\lambda_m) + \lambda_m} \qquad \lambda_m = \frac{hL}{k}\cot(\lambda_m)$$

- Need root-finding method to obtain eigenvalues, λ_m
  - For typical accuracy, can use only first term in sum if $\tau = \alpha t/L^2 > 0.2$

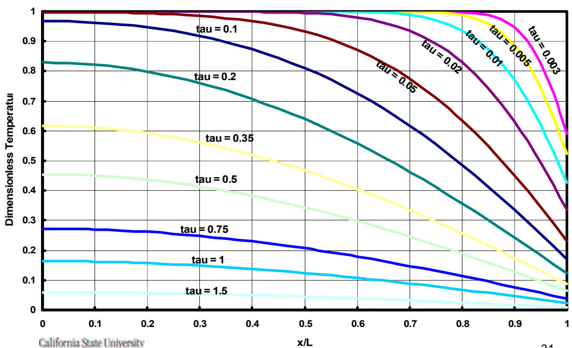
Values for λ_n

n	hL/k = .1	hL/k = 1	hL/k = 10
1	0.3111	0.8603	1.4289
2	3.1731	3.4256	4.3058
3	6.2991	6.4373	7.2281
4	9.4354	9.5293	10.2003
5	12.5743	12.6453	13.2142
6	15.7143	15.7713	16.2594
7	18.8549	18.9024	19.3270
8	21.9957	22.0365	22.4108
9	25.1367	25.1724	25.5064

Solution for hL/k = 1



Solution for hL/k = 10



California State University Northridge 31

Diffusion Equation Summary

- Create Sturm-Lioville problem for non-zero spatial boundary conditions
  - Define u(x,t) = v(x,t) + w(x)
  - Use u – u_{ref} in original equation
- Solve by separation of variables
  - Product solution X(x)T(t)
  - Time solution, T(t), will be exponential
  - X(x) is sine and cosine for Cartesian
- Apply boundary conditions to determine eigenvalues and eigenfunctions

California State University Northridge 32

Diffusion Equation Summary II

- Write solution as sum of all possible eigenfunctions with individual constants
- Use eigenfunction expansion to match initial conditions
  - If a solution for u(x,t) = v(x,t) + w(x) is used the eigenfunction expansion must be for $u_0(x)$ – w(x)
- Solution is sum of all eigenfunctions with constants determined from matching initial conditions.

California State University Northridge 33

Diffusion Equation Summary III

- Sine eigenfunctions start at n = 1
- Cosine eigenfunctions start at n = 0 and C_0 equation has factor of 1/L not 2/L
- Can convert diffusion equation with source term into homogenous equation
  - Homework problem 27 (K, p 561): Find w(x) such that u(x,t) = v(x,t) + w(x), where v(x) satisfies diffusion equation with v(0,t) = v(L,t) = 0 to solve $\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} + Ne^{-ax}$

California State University Northridge 34