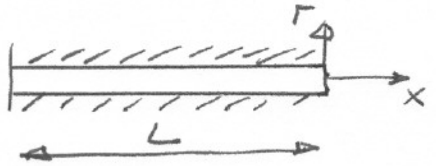
Non-Homogeneous Boundary Conditions

Motivation Example: Transient heat transfer along a thin-rod



IC $T(x,0) = f(x)$

BC's $\begin{cases} T(0,t) = 0 \\ T(L,t) = T_0 \end{cases}$

The equation is as before:

$$\frac{\partial T}{\partial t} = c^2 \frac{\partial^2 T}{\partial x^2} \qquad (1)$$

The solution to (1) is as before:

$$T(x,t) = De^{-p^2c^2t}(A\cos px + B\sin px) \qquad (2)$$

Substitute $x=0$ $T(0,t)=0$ $\Rightarrow A=0$

" $x=L$ $T(L,t) = \underbrace{B\sin(pL)De^{-p^2c^2t} = T_0}_{\text{impossible to satisfy!}}$

We have obtained a $f(t) \stackrel{?}{=} \text{const}$ impossible!

Look for a solution

$$T(x,t) = T'(x,t) + T_{ss}(x) \qquad (3)$$

T_{ss} - steady state solution.

The idea is to absorb the non homogeneous BC's into the T_{ss} problem as follows:

Solve 2 problems:

① $$\frac{\partial T'}{\partial t} = c^2 \frac{\partial^2 T'}{\partial x^2}$$

I.C. $T'(x,0) = f(x) - T_{ss}(x)$

$$\left.\begin{array}{l} T'(0,t) = 0 \\ T'(L,t) = 0 \end{array}\right\} BC$$

② $$\frac{\partial T_{ss}}{\partial t} = 0$$

$$\Rightarrow c^2 \frac{\partial^2 T_{ss}}{\partial x^2} = 0$$

$$BC \left\{\begin{array}{l} T_{ss}(0,t) = 0 \\ T_{ss}(L,t) = T_0 \end{array}\right.$$

Problem ① is exactly as before!! (except I.C.)

$$\Rightarrow T'(x,t) = \sum_{n=0}^{\infty} E_n e^{-p^2c^2t} \sin(px) \qquad p = n\frac{\pi}{L} \quad (4)$$

E_n is obtained from Fourier Series

$$E_n = \frac{2}{L}\int_0^L (f(x) - T_{ss}) \sin px \, dx \qquad (5)$$

In summary, the solution to problem (1), from (4),(5)

$$T'(x,t) = \sum_{n=0}^{\infty} \left\{ \frac{2}{L} \int_0^L [f(x) - T_{ss}] \sin px \, dx \right\} e^{-p^2c^2t} \sin(px) \quad (6)$$

The solution to Problem (2) is:

$$\frac{\partial^2 T_{SS}}{\partial x^2} = 0 \Rightarrow T_{SS} = \alpha x + \beta \qquad (7)$$

From boundary conditions of Problem (2)

$$T_{SS}(0) = 0 \Rightarrow \beta = 0$$

$$T_{SS}(L) = T_0 \Rightarrow \alpha = \frac{T_0}{L} \Rightarrow T_{SS} = \frac{T_0}{L} x \quad (8)$$

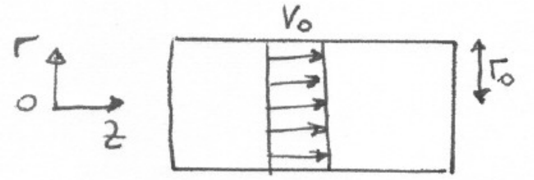
The general solution from (3), (6) and (8)

$$T(x,t) = \underbrace{\sum_{n=0}^{\infty} \left\{ \frac{2}{L} \int_0^L \left[f(x) - \frac{T_0}{L} x \right] \sin px \, dx \right\} e^{-p^2 c^2 t} \sin(px)}_{T'(x,t)} + \underbrace{\frac{T_0}{L} x}_{T_{SS}(x)}$$

$$p = \frac{n\pi}{L} \qquad n = 0, 1, 2 \ldots.$$

PDE's in cylindrical coordinates

Example: Coated Wall Reactor



1- Plug Flow , Inlet $C_A = C_{A0}$

2- Catalytic wall $\quad A \to$ product B

at the wall $-D_A \frac{\partial C_A}{\partial r}\Big|_{r_0} = K\, C_A(r_0, z)$

Neglecting axial diffusion and assuming steady state:

$$V_0 \frac{\partial C_A}{\partial z} = \frac{D_A}{r} \frac{\partial}{\partial r}\left(r \frac{\partial C_A}{\partial r}\right) \qquad (1)$$

Assume $\quad C_A(r, z) = Z(z)\, R(r) \qquad (2)$

(2) into (1) $\quad V_0 Z' R = \frac{D_A}{r}\left(Z R' + r Z R''\right)$

$$\Rightarrow \quad \frac{V_0}{D_A} \frac{Z'}{Z} = \frac{1}{r}\left(\frac{R'}{R} + \frac{r R''}{R}\right) = -\alpha^2 \qquad (3)$$

As before, it can be shown that $+\alpha^2$ will result in infinite C_A at $Z \to \infty$ $\quad (C_A \to \infty)$

Define $\frac{V_0}{D_A} = \beta$, from (3):

$$\beta Z' + \alpha^2 Z = 0 \Rightarrow Z' + \frac{\alpha^2}{\beta} Z = 0 \Rightarrow Z = A e^{-\frac{\alpha^2}{\beta} z} \qquad (4)$$

$$R'' + \frac{R'}{r} + \alpha^2 R = 0 \Rightarrow r^2 R'' + r R' + \alpha^2 r^2 R = 0$$

or defining $\xi = \alpha r$ $\quad \xi^2 \frac{d^2 R}{d\xi^2} + \xi \frac{dR}{d\xi} + \xi^2 R = 0 \qquad (5)$

Bessel Equation?!

Review : Bessel Functions

Bessel Equation $$x^2\frac{d^2y}{dx^2} + x\frac{dy}{dx} + (x^2-p^2)y = 0 \qquad (1)$$

Solution by series $$y = \sum_{n=0}^{\infty} a_n x^{n+c} \qquad (2)$$

Substituting (2) into (1), y can be obtained:

case i - $p \neq$ integer $$y(x) = A J_p(x) + B J_{-p}(x) \qquad (3)$$

case ii - $p =$ integer $$y(x) = A J_p(x) + B Y_p(x) \qquad (4)$$

For example: $$J_0(x) = \sum_{n=0}^{\infty} \frac{(-1)^n (\frac{1}{2}x)^{2n}}{n!\,n!} \qquad (5)$$

Modified Bessel Equation $$x^2\frac{d^2y}{dx^2} + x\frac{dy}{dx} - (x^2+p^2)y = 0 \qquad (6)$$

Notice that if $x' = ix \Rightarrow x'^2\frac{d^2y}{dx'^2} + x'\frac{dy}{dx'} + (x^2-p^2)y = 0$

$\Rightarrow$ the solution is $y = A J_p(ix) + B J_{-p}(ix)$ $\quad p \neq int$

or $\qquad y = A J_p(ix) + B I_p(ix)$ $\quad p = int$

$J_p(ix) \stackrel{\text{def}}{=} I_p(x)$ Modified Bessel Function of 1st Kind.

$I_p(ix) \stackrel{\text{def}}{=} K_p(x)$ Modified Bessel Function of 2nd Kind.

Main Properties of J_p, Y_p, I_p, K_p

$$J_0(0) = I_0(0) = 1$$

for $p>0$ (integer) $J_p(0) = I_p(0) = 0$

for $p>0$ (not-integer) $J_{-p}(0) = \pm I_{-p}(0) \to \begin{matrix} +\infty \\ -\infty \end{matrix}$

Since Y_p and K_p include a logarithmic term:

$$-Y_p(0) = K_p(0) \to \infty$$

In this case, only J and I are admissible.

Differential Properties:

$$\frac{d}{dx}\left[Z_p(\lambda x)\right] = \begin{cases} -\lambda Z_{p+1}(\lambda x) + \frac{p}{x} Z_p(\lambda x) & Z = J, Y, K \\ \lambda Z_{p+1}(\lambda x) + \frac{p}{x} Z_p(\lambda x) & Z = I \end{cases}$$

Integral Properties:

$$\int \lambda x^p J_{p-1}(\lambda x)\, dx = x^p J_p(\lambda x)$$

$$\int \lambda x^p I_{p-1}(\lambda x)\, dx = x^p I_p(\lambda x)$$

Continuation of the Coated Well Reactor Example:

Equation (5):

$$\xi^2 \frac{d R^2}{d\xi^2} + \xi \frac{dR}{d\xi} + \xi^2 R = 0 \qquad (5)$$

The solution is:

$$R = B J_0(\xi) + C Y_0(\xi) = B J_0(\alpha r) + C Y_0(\alpha r) \qquad (6)$$

or (2) $$C_A = A e^{-\frac{\alpha^2}{\beta} z}\left[B J_0(\alpha r) + C Y_0(\alpha r)\right] \qquad (7)$$

Since $Y(0) = \rightarrow \infty \Rightarrow C = 0$

Define $A \cdot B = E \Rightarrow$ $$C_A = E e^{-\frac{\alpha^2}{\beta} z} J_0(\alpha r) \qquad (8)$$

Boundary Condition:

$$-D_A \frac{\partial C_A}{\partial r}\bigg|_{r_0} = -D_A \cancel{E e^{-\frac{\alpha^2}{\beta} z}}\left[-\alpha J_1(\alpha r_0)\right] = K \cancel{E e^{-\frac{\alpha^2}{\beta} z}} J_0(\alpha r_0)$$

$$D_A \alpha J_1(\alpha r_0) - K J_0(\alpha r_0) = 0 \Rightarrow \text{infinite } \alpha\text{'s} \qquad (9)$$

This equation is solved numerically to give $\alpha_1, \alpha_2, \ldots \alpha_n$

Finally $$C_A(r, z) = \sum_{n=0}^{\infty} E_n e^{-\frac{\alpha_n^2}{\beta} z} J_0(\alpha_n r) \qquad (10)$$

Inlet condition $$C_A(r, 0) = C_{A0} = \sum_{n=0}^{\infty} E_n J_0(\alpha_n r) \qquad (11)$$

need Bessel-Fourier Series

Orthogonality Property.

if $$\int_a^b W(x)\, P_n(x)\, P_m(x)\, dx = 0 \quad \text{if } m \neq n$$

$P_n(x)$ and $P_m(x)$ are said to be orthogonal in $a \le x \le b$.

Examples:

$$\int_{-\pi}^{\pi} \sin(nx)\,\sin(mx)\,dx = \int_{-\pi}^{\pi} \frac{1}{2}\left[\cos(n-m)x - \cos(n+m)x\right]dx$$

$$= \begin{cases} 0 & n \neq m \\ \pi & n = m \end{cases}$$

Similar Properties apply to Bessel Functions

$$\int_0^1 x\, J_\nu(nx)\, J_\nu(mx)\, dx = 0 \qquad n \neq m$$

or for $n = m$

$$\int_0^1 x\, J_\nu^2(nx)\, dx = \frac{1}{2} J_{\nu+1}^2(n)$$

J_ν - Bessel function of Order ν.

See Proof in the next page

Proof of Orthogonality of Bessel's Functions

Bessel Equation $x\frac{d}{dx}\left(x\frac{du}{dx}\right)+(m^2x^2-\nu^2)u=0$ (1)

The solution to this equation is: $u=J_\nu(mx)$.

$J_\nu(mx)$ - Bessel function of order ν-th

Is $J_\nu(mx)$ orthogonal with $J_\nu(nx)$?

For $x(xu')'+(m^2x^2-\nu^2)u=0$ $u=J_\nu(mx)$ (2)

and $x(xv')'+(n^2x^2-\nu^2)v=0$ $=J_\nu(nx)$ (3)

Assume that the integration limits are zeros of $J_\nu(mx)$, $J_\nu(nx)$

@ $x=0,1 \Rightarrow J_\nu(0)=J_\nu(n)=J_\nu(m)=0$

Multiply (2) by v and (3) by u and subtract:

$$(m^2-n^2)\,xuv=\frac{d}{dx}(vxu'-uxv')$$

$$\Rightarrow (m^2-n^2)\int_0^1 xuv=\underbrace{(vxu'-uxv')\Big|_0^1}_{u(0)=u(1)=v(0)=v(1)=0}=0 \quad \therefore$$

Thus, for $m\neq n$ $\int_0^1 xuv=0 \Rightarrow \int_0^1 x\,J_\nu(mx)J_\nu(nx)\,dx=0$

Repeat (11) from before

$$C_{A_0} = \sum_{n=0}^{\infty} E_n J_0(\alpha_n r) \qquad (11)$$

Multiply by $J_0(\alpha_m r)$ and integrate from $0 \to r_0$

$$\int_0^{r_0} C_{A_0} r\, J_0(\alpha_m r)\, dr = \sum_{n=0}^{\infty} E_n \int_0^{r_0} r\, J_0(\alpha_n r) J_0(\alpha_m r)\, dr$$

Orthogonality $\int_0^{r_0} r\, J_0(\alpha_n r) J_0(\alpha_m r)\, dr = 0 \quad n \neq m$

$$\Rightarrow \quad \int_0^{r_0} C_{A_0} r\, J_0(\alpha_m r)\, dr = E_n \int_0^{r_0} r\, J_0^2(\alpha_m r)\, dr$$

$$\Rightarrow \quad E_n = \frac{\int_0^{r_0} C_{A_0} r\, J_0(\alpha_m r)\, dr}{\int_0^{r_0} r\, J_0^2(\alpha_m r)\, dr} \qquad (12)$$

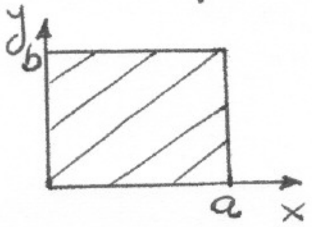
The final solution is, from (12) and (10):

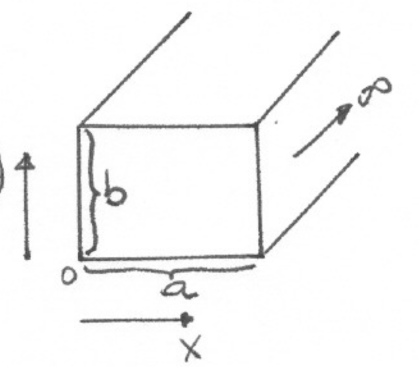
$$C(r,z) = \sum_{m=0}^{\infty} \frac{\int_0^{r_0} C_{A_0} r\, J_0(\alpha_m r)\, dr}{\int_0^{r_0} r\, J_0^2(\alpha_m r)\, dr} \cdot e^{-\frac{\alpha_m^2 z}{\beta}} J_0(\alpha_m r)$$

2-D Steady State Conduction/Diffussion

Example: A bar with rectangular crossection (very long)

Solve the temperature $T(x,y)$





The general heat transfer equation (or mass diffussion):

$$\underbrace{\rho c \cancel{\frac{\partial T}{\partial t}}^{\,0}}_{\text{steady state}} + \underbrace{\rho c u \cancel{\frac{\partial T}{\partial x}}^{\,0} + \rho c v \cancel{\frac{\partial T}{\partial y}}^{\,0} + \rho c w \cancel{\frac{\partial T}{\partial z}}^{\,0}}_{\text{no convection (solid)}} = k\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \underbrace{\cancel{\frac{\partial^2 T}{\partial z^2}}^{\,0}}_{\text{very long in } z}\right) \qquad (1)$$

$$\Rightarrow \quad \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0 \qquad (2)$$

Solve with Boundary Conditions:

$$T(0,y) = 0 \qquad T(a,y) = 0 \qquad T(x,0) = 0 \qquad T(x,b) = h(x) \qquad (3)$$

Let

$$T(x,y) = f(x)\, g(y) \qquad (4)$$

Substitute (4) into (2)

$$g f'' + f g'' = 0 \qquad (5)$$

Divide (5) by $f \cdot g$

$$\frac{f''}{f} + \frac{g''}{g} = 0 \Rightarrow \frac{f''}{f} = -\frac{g''}{g} = K \qquad (6)$$

if $K = p^2$ (positive number)

From (6)

$$f'' - p^2 f = 0 \Rightarrow f = Ae^{-px} + Be^{px} \qquad (7)$$

$$g'' + p^2 g = 0 \Rightarrow g = C\cos(py) + D\sin(py) \qquad (8)$$

$$\Rightarrow T(x,y) = (Ae^{-px} + Be^{px})(C\cos py + D\sin py) \qquad (9)$$

@ $y = b$ $\quad T(x,b) = h(x) = (Ae^{-px} + Be^{px})(C\cos pb + D\sin pb)$

<u>Impossible to satisfy</u>!! An arbitrary function of $h(x)$ cannot be equated to exponentials of x.

Exponential is not an orthogonal function, thus, we cannot construct a Fourier series with exponentials.

$\Rightarrow$ try $K = -p^2$ (negative value) (10)

Why? This will give trigonometric functions in x $\Rightarrow$ we can use Fourier series:

From (6) and (10)

$$f'' + p^2 f = 0 \qquad f = A\cos px + B\sin px$$

$$g'' - p^2 g = 0 \qquad g = Ce^{py} + De^{-py}$$

$$\Rightarrow T(x,y) = (A\cos px + B\sin px)(Ce^{py} + De^{-py}) \quad (11)$$

Let substitute all boundery conditions into (11):

$$T(0,y) = 0 \Rightarrow A(Ce^{py} + De^{-py}) = 0 \Rightarrow A = 0 \quad (12)$$

$$T(a,y) = 0 \Rightarrow B\sin pa\,(Ce^{py} + De^{-py}) = 0$$
$$B \neq 0 \Rightarrow \sin(pa) = 0 \Rightarrow p_n = \frac{n\pi}{a} \quad (13)$$

$$T(x,0) = 0 \Rightarrow B\sin(px)(C+D) = 0 \Rightarrow C = -D \quad (14)$$

From (11), (12), (13) and (14):

$$T(x,t) = \sum_{n=0}^{\infty} B_n \sin(p_n x)\left[C_n e^{p_n y} - C_n e^{-p_n y}\right] \quad (15)$$

Let $2 \cdot B_n \cdot C_n \triangleq E_n$ and remember $\sinh(p_n y) = \frac{e^{p_n y} - e^{-p_n y}}{2}$

$$\Rightarrow \text{from (15)} \quad T(x,t) = \sum_{n=0}^{\infty} E_n \sin(p_n x)\sinh(p_n y) \quad (16)$$

From boundary condition at $y = b$ into (16):

$$T(x,b) = \sum_{n=0}^{\infty} E_n \sin(p_n x)\sinh(p_n b) = h(x) \quad (17)$$

To compute E_n, expand $h(x)$ with Fourier Series:

$$h(x) = \sum_{n=0}^{\infty} F_n \sin(p_n x) \Rightarrow F_n = \frac{2}{a}\int_0^a h(x)\sin(p_n x)\,dx \quad (18)$$

From (17) and (18):

$$\sum_{n=0}^{\infty} E_n \sinh(p_n b) \sin(p_n x) = \sum_{n=0}^{\infty} \left(\frac{2}{a} \int_0^a h(x) \sin(p_n x)\, dx \right) \sin(p_n x) \quad (19)$$

From (19), equating terms:

$$E_n \sinh(p_n b) = \frac{2}{a} \int_0^a h(x) \sin(p_n x)\, dx \quad (20)$$

From (20)

$$E_n = \frac{2}{a \sinh(p_n b)} \int_0^a h(x) \sin(p_n x)\, dx \quad (21)$$

From (21) into (16)

$$T(x,t) = \sum_{n=0}^{\infty} \left(\frac{2}{a \sinh(p_n b)} \int_0^a h(x) \sin(p_n x)\, dx \right) \sin(p_n x) \sinh(p_n y) \quad (22)$$

$$p_n = \frac{n\pi}{a} \qquad n = 0, 1, 2, \ldots\ldots$$