Continuity eqn PDEs (1D)

$$\frac{\partial C}{\partial T} = -\frac{\partial J}{\partial X}$$

Diffusion eqn

$$\frac{\partial C}{\partial T} = D\frac{\partial^2 C}{\partial X^2} \rightsquigarrow J = -D\frac{\partial C}{\partial X}$$

Advection eqn

$$\frac{\partial C}{\partial T} = -\frac{\partial}{\partial X}(VC) \rightsquigarrow J = VC$$

Nondimensionalizing

Example

on $0 \leq X \leq L$

$$\frac{\partial C}{\partial T} = -\frac{\partial J}{\partial X} \quad \text{with} \quad J = V\sin\left(2\pi\frac{X}{L}\right)C - D\frac{\partial C}{\partial X}$$

independent variables: X, T

dependent variable: C

parameters: L, V, D

$$\frac{[C]}{[T]} \sim \frac{[J]}{[X]} \Rightarrow [J] \sim \frac{[C] \times \text{length}}{\text{time}}$$

$$[V][C] \sim [D]\frac{[C]}{[X]} \sim [J] \sim \frac{[C][X]}{[T]}$$

$$\Rightarrow [D] \sim [X^2]/[T], \quad [V] \sim [X]/[T]$$

suppose $VL > D$ $\rightsquigarrow$ advection dominated

$X = \frac{L}{2\pi} x \quad C = \bar{C} c$ ← no need to choose

$T = \frac{L/2\pi}{V} x$

$$\frac{\partial C}{\partial T} = -\frac{\partial J}{\partial X} = -\frac{\partial}{\partial X}\left(V \sin\left(2\pi \frac{X}{L}\right) C - D\frac{\partial C}{\partial X}\right)$$

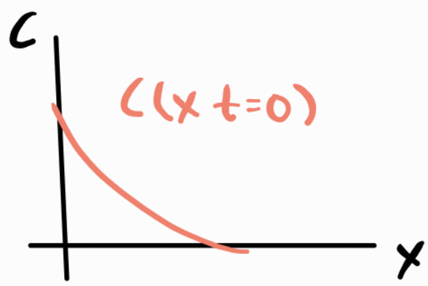
$$\frac{\bar{C}}{L/2\pi V} \frac{\partial c}{\partial t} = -\frac{2\pi}{L} \frac{\partial}{\partial x}\left(V \sin(x) \bar{C} c + \frac{2\pi D}{L} \bar{C} \frac{\partial c}{\partial x}\right)$$

$$\frac{\cancel{2\pi} \cancel{\bar{C}} V}{\cancel{L}} \frac{\partial c}{\partial t} = -\frac{\cancel{2\pi} V \cancel{\bar{C}}}{\cancel{L}} \frac{\partial}{\partial x}(\sin(x) c) + \frac{\cancel{\bar{C}} \cancel{2\pi} D}{L^{\cancel{2}}} \frac{\partial^2 c}{\partial x^2}$$

$$\boxed{\frac{\partial c}{\partial t} = -\frac{\partial}{\partial x}(\sin(x) c) + \frac{D}{VL} \frac{\partial^2 c}{\partial x^2}}$$

Stationary soln

$c^*(x)$ s.t. $\frac{\partial c}{\partial t} = 0$



Example

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} \rightsquigarrow D\frac{\partial^2 c}{\partial x^2} = 0$$

⊕ B.C. $c = 1$ at $x = 0$

$\frac{\partial c}{\partial x} = 0$ at $x = 1$

I.C. $c(x,0) = (x-1)^2$

[Matlab]

$\Rightarrow \frac{\partial c}{\partial x} = C_0$

$\Rightarrow c(x) = C_0 x + C_1$

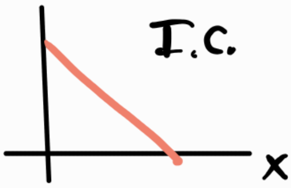
(apply B.C.

$\Rightarrow c(x) = 1$

Example $\frac{\partial C}{\partial T} = -\frac{\partial}{\partial X}(VXC)$

$$\frac{\partial c}{\partial t} = -\frac{\partial}{\partial x}(xc)$$

$\oplus$ B.C. $\frac{\partial c}{\partial x} = -1$ at $x=1$



I.C. $c = 1-x$ at $t=0$

$$-\frac{\partial}{\partial x}(xc) = 0$$

$$\Rightarrow xc(x) = c_0$$

$$\Rightarrow c(x) = c_0/x$$

apply B.C.:

$$\frac{\partial c}{\partial x} = -\frac{c_0}{x^2}$$

$$\frac{\partial c}{\partial x}(1) = -c_0 = -1$$

$$c(x) = 1/x$$

put back into dimensions:

$$C = \bar{C}c, \quad T = \frac{X}{V}t, \quad X = Lx$$

$$C(X)/\bar{C} = 1/X/L \Rightarrow \underline{\underline{C(X) = \bar{C}L/X}}$$

Remarks:

I.C. & B.C. must be consistent

$\Rightarrow$ if I.C. does not satisfy the B.C., problem is ill-posed

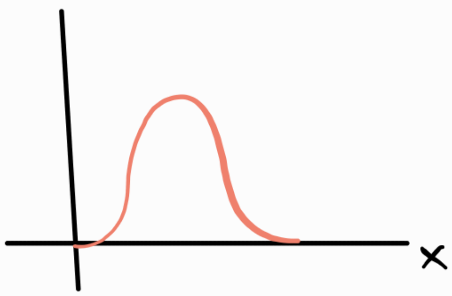
Example

$$\frac{\partial c}{\partial t} = -\frac{\partial}{\partial x}(\sin(2\pi x)c) + d\frac{\partial^2 c}{\partial x^2}$$

$\oplus$ I.C. $c = \sin(\pi x)^4$

B.C. $c = 0$ at $x = 0$

$c = 0$ at $x = 1$



Hard to solve $\frac{\partial c}{\partial t}$ analytically $\Rightarrow$ [Matlab]

Example

$$\underbrace{\frac{\partial c}{\partial t}}_{=0} = -\frac{\partial c}{\partial x} + d\frac{\partial^2 c}{\partial x^2}$$

$$d\frac{d^2c}{dx^2} = \frac{dc}{dx}$$

integrate

$$d\frac{dc}{dx} = c + c_0$$

$$\frac{dc}{c+c_0} = \frac{1}{d}dx$$

integrate

$$\ln(c+c_0) = \frac{x}{d} + c_1$$

$$c + c_0 = c_2 \exp(x/d)$$

$$c(x) = c_0 + c_2 \exp(x/d)$$

$\oplus$ B.C. $c=0$ at $x=0$

$\frac{\partial c}{\partial x} = 1$ at $x=1$

<u>apply B.C.:</u>

① $c(0) = c_0 + c_2 = 0$

$$\Rightarrow c_2 = -c_0$$

$$c(x) = c_0(1-\exp(x/d))$$

② $\frac{\partial c}{\partial x} = c_0\left(1 - \frac{1}{d}\exp(x/d)\right)$

$$\frac{\partial c}{\partial x}(1) = c_0\left(1 - \frac{1}{d}\exp\left(\frac{1}{d}\right)\right) = 1$$

$$\Rightarrow c_0 = \frac{1}{1-\frac{1}{d}\exp(1/d)}$$

$$\boxed{c(x) = \frac{1}{1-\frac{1}{d}\exp\left(\frac{1}{d}\right)}\left(1-\exp(x/d)\right)}$$

Example (Homework)

"reaction" part

$$\frac{\partial C}{\partial T} = D\frac{\partial^2 C}{\partial X^2} + S \quad \text{on } 0 \le X \le L$$

nondimensionalize

$$[D] \sim \frac{[X]^2}{[T]} \Rightarrow T \sim [X]^2/[D]$$

$$[S] \sim [C]/[T]$$

$$\begin{cases} X = Lx \\ T = \frac{L^2}{D}t \\ C = \frac{L^2 S}{D}c \end{cases}$$

$$\Rightarrow \frac{\cancel{L^2}S/\cancel{D}}{\cancel{L^2}/\cancel{D}}\frac{\partial c}{\partial t} = \frac{\cancel{D}}{\cancel{L^2}}\frac{\cancel{L^2}S}{\cancel{D}}\frac{\partial^2 c}{\partial x^2} + S \qquad \boxed{\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial x^2} + 1}$$

stationary soln $\oplus$ B.C. $c(0,t) = 0$ absorbing

$D\frac{\partial c}{\partial x}(1,t) = 0$ no flux

$$\frac{\partial^2 c}{\partial x^2} = -1$$

$$\frac{\partial c}{\partial x} = -x + c_0$$

$$c(x) = -\frac{x^2}{2} + c_0 x + c_1$$

$$c(0) = c_1 = 0$$

$$\frac{\partial c}{\partial x}(1) = -1 + c_0 = 0$$

$$\Rightarrow c_0 = 1$$

$$\Rightarrow \boxed{c(x) = -\frac{x^2}{2} + x}$$

[Matlab]

in dimensions

$$\frac{D}{L^2 S}C(X) = -\frac{X^2}{2L^2} + \frac{X}{L} \Rightarrow \boxed{C(X) = -\frac{S}{D}X\left(\frac{X}{2} - L\right)}$$

Quiz

Consider the reaction-diffusion eqn:

$$\star \quad \frac{\partial C}{\partial T} = D\frac{\partial^2 C}{\partial X^2} + AX^2 - B \quad \text{on } 0 \le X \le L$$

with boundary conditions:

$$\frac{\partial C}{\partial X}(0) = 0 \quad \text{and} \quad C(L) = 0$$

Assume the density is measured in mM (millimolar).

A) Interpret the terms in $\star$ right hand side

first term is diffusion, second is a spatial-dependent source, third is a constant sink

B) Choose the scales & nondimensionalize

$[A] \sim [C] / [T][X]^2$ $\qquad X = Lx$ (natural choice)

$[B] \sim [C]/[T]$ $\qquad T = \frac{L^2}{D} t$ (straightforward choice)

$[D] \sim [X]^2/[T]$

<u>option 1</u>: $C = \frac{AL^4}{D} c$

$$\frac{AL^4/\cancel{D}}{L^2/\cancel{D}} \frac{\partial c}{\partial t} = \frac{\cancel{D}AL^4}{\cancel{D}L^2} \frac{\partial^2 c}{\partial x^2} + AL^2x^2 - B$$

$$\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial x^2} + x^2 - \left(\frac{B}{AL^2}\right) b$$

option 2: $C = \frac{BL^2}{D} c$

$$\frac{\cancel{BL^2/D}}{\cancel{L^2/D}} \frac{\partial c}{\partial t} = \frac{\cancel{D}\cancel{BL^2}}{\cancel{D}\cancel{L^2}} \frac{\partial^2 c}{\partial x^2} + AL^2x^2 - B$$

$$\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial x^2} + \underbrace{\frac{AL^2}{B}}_{a} x^2 - 1$$

c) Find the stationary non-dimensional soln for this eqn

if option 1, $a = 1$

if option 2, $b = 1$

$$\frac{\partial^2 c}{\partial x^2} + ax^2 - b = 0$$

$$\frac{\partial^2 c}{\partial x^2} = b - ax^2$$

$$\frac{\partial c}{\partial x} = bx - \frac{ax^3}{3} + C_0$$

$$C(x) = \frac{bx^2}{2} - \frac{ax^4}{12} + C_0 x + C_1$$

apply B.C.: $\frac{\partial c}{\partial x}(0) = 0$, $c(1) = 0$

① $\frac{\partial c}{\partial x}(0) = C_0 = 0$

② $c(1) = \frac{b}{2} - \frac{a}{12} + c_1 = 0 \Rightarrow c_1 = \frac{a}{12} - \frac{b}{2}$

$$C(x) = \frac{b}{2}x^2 - \frac{ax^4}{12} + \frac{a}{12} - \frac{b}{2}$$

D) Find the Stationary dimensional soln

option 1: $a=1$, $b=B/AL^2$

$$\frac{DC(X)}{AL^4} = \frac{B}{2AL^2}\frac{X^2}{L^2} - \frac{X^4}{12L^4} + \frac{1}{6} - \frac{B}{2AL^2}$$

$$C(X) = \frac{B}{2D}X^2 - \frac{A}{12D}X^4 + \frac{AL^4}{12D} - \frac{BL^2}{2D}$$

(same answer if option 2)

$$C(X) = \frac{B}{2D}(X^2 - L^2) - \frac{A}{12D}(X^4 - L^4)$$