$\Rightarrow$ Deriving Standard diffusion curve equations as described in (Gleaves et al) TAP-2

$\bar{C}_A(\xi,\tau) \leftarrow$ Dimensionless concentration

$$\frac{\partial \bar{C}_A}{\partial \tau} = \frac{\partial^2 \bar{C}_A}{\partial \xi^2}$$

I.C. $0 \le \xi \le 1,\ t=0,\ \bar{C}_A = \delta_\xi$

B.C $\xi = 0 \quad \frac{\partial \bar{C}_A}{\partial \xi} = 0$

$\xi = 1 \quad \bar{C}_A = 0$

let $\bar{C}_A = u$

$\Rightarrow u_\tau = u_{\xi\xi}$

$u(\xi,0) = \delta_\xi \rightarrow$ dirac delta function of ξ $\quad \delta_\xi = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ip\xi}\,dp$

$\left.\frac{\partial u}{\partial \xi}\right|_{\xi=0} = 0$

$u(1,\tau) = 0$

Method of separation of variables

let: $u(\xi,\tau) = X(\xi)\,T(\tau)$

$\left.\begin{array}{l} u_\tau = XT' \\ u_{\xi\xi} = X''T \end{array}\right\}$ $u_\tau = u_{\xi\xi}$ $\therefore XT' = X''T \Rightarrow \frac{X''}{X} = \frac{T'}{T} = k \rightarrow$ constant that is not a function of ξ or τ

Therefore,

$$X'' - kX = 0 \ ; \ X'(0) = X(1) = 0$$
$$T' - kT = 0$$

Solving for X : $X'' - kX = 0$ (2^{nd} order ODE)

— case 1: let $k = \mu^2 > 0 \Rightarrow X'' - \mu^2 X = 0$

$r^2 - \mu^2 = 0 \Rightarrow r = \pm\mu$

$X = c_1 e^{\mu\xi} + c_2 e^{-\mu\xi} \Rightarrow X' = \mu c_1 e^{\mu\xi} - \mu c_2 e^{-\mu\xi}$

BCs:

- $X'(0) = \mu c_1 - \mu c_2 = 0 \Rightarrow c_1 = c_2$
- $X(1) = c_1 e^{\mu} + c_1 e^{-\mu} = 0 \Rightarrow$ since $\mu \neq 0 \therefore c_1 = 0$

$\therefore c_1 = c_2 =$

Gives trivial result $\therefore$ not acceptab

- Case 2: let $k=0 \Rightarrow X''=0$

$\therefore X = c_1\xi + c_2 \quad ; \quad X' = c_1$

BCs:

- $X'(0) = c_1 = 0$
- $X(1) = c_1 + c_2 = 0 + c_2 = 0 \qquad \therefore c_1 = c_2 = 0$

Gives trivial result $\therefore$ not acceptable

- Case 3: let $k=-\mu^2<0 \Rightarrow X''+\mu^2 X=0$

$r^2+\mu^2=0 \rightarrow r=\pm i\mu$

$\therefore X = c_1\cos(\mu\xi) + c_2\sin(\mu\xi) \quad ; \quad X' = -\mu c_1 \sin(\mu\xi) + \mu c_2\cos(\mu\xi)$

BCs:

- $X'(0) = \mu c_2 = 0 \Rightarrow c_2 = 0$
- $X(1) = c_1\cos(\mu) = 0$; To avoid trivial result c_1 can't be equal to zero, therefore, $\cos(\mu)=0$

Since $\cos(\mu)=0 \Rightarrow \underline{\mu_n=(n+0.5)\pi}$ for $(n \in \mathbb{N}\cup\{0\})$

$c_1 \rightarrow c_n$

$$\boxed{X_n = c_n \cdot \cos((n+0.5)\pi\xi)}$$

- Solving for T: $T' - kT = 0$

from before, $k = -\mu_n^2$

$$T' + \mu_n^2 T = 0 \Rightarrow T' = -\mu_n^2 T \Rightarrow \boxed{T = T_n = a_n e^{-\mu_n^2 \tau}}$$

- Combining the variables

$$u_n(\xi,\tau) = X_n(\xi)T_n(\tau) = \left(c_n\cos((n+0.5)\pi\xi)\right)\left(a_n e^{-([n+0.5]\pi)^2\tau}\right)$$

Applying principle of superposition | let $b_n = a_n \cdot c_n$ #A new constant

$$u(\xi,\tau) = \sum_{n=0}^{\infty} u_n(\xi,\tau) = \sum_{n=0}^{\infty} b_n \cos((n+0.5)\pi\xi)\, e^{-([n+0.5]\pi)^2\tau}$$

$\therefore$

$$u(\xi,\tau)=\sum_{n=0}^{\infty} b_n \cos\left((n+0.5)\pi\xi\right) e^{-([n+0.5]\pi)^2\tau}$$

$\Rightarrow$ Solving for b_n: | Note for $x=\sum_{i=0}^{n} a_i b_i \Rightarrow a_i=\dfrac{\langle b_i, x\rangle}{\langle b_i, b_i\rangle}$

$\boxed{0}$ Using initial condition:

$$u(\xi,0)=\delta_\xi=\sum_{n=0}^{\infty} b_n \cos\left((n+0.5)\pi\xi\right)$$

$$\therefore b_n = \frac{\langle\cos((n+0.5)\pi\xi)\rangle\langle\delta_\xi\rangle}{\langle\cos((n+0.5)\pi\xi)\rangle\langle\cos((n+0.5)\pi\xi)\rangle}$$

$$\therefore b_n = \frac{1}{\langle\cos((n+0.5)\pi\xi)\rangle\langle\cos((n+0.5)\pi\xi)\rangle}\int_0^1 \delta_\xi \cos\left((n+0.5)\pi\xi\right) d\xi$$

$$= \frac{1}{\int_0^1 \cos((n+0.5)\pi\xi)\cos((n+0.5)\pi\xi)\, d\xi}\int_0^1 \delta_\xi \cos\left((n+0.5)\pi\xi\right) d\xi$$

$$b_n = \underbrace{\frac{1}{\int_0^1 \cos^2((n+0.5)\pi\xi)\, d\xi}}_{\text{I}}\ \underbrace{\int_0^1 \delta_\xi \cos\left((n+0.5)\pi\xi\right) d\xi}_{\text{II}}$$

Solving I

u-substitution : $u=(n+0.5)\pi\xi$ | $du=(n+0.5)\pi\, d\xi$

$$\int_0^1 \cos^2((n+0.5)\pi\xi)\, d\xi \Rightarrow \int_0^{(n+0.5)\pi} \frac{1}{(n+0.5)\pi}\cos^2(u)\, du = \frac{1}{(n+0.5)\pi}\int_0^{(n+0.5)\pi} \cos^2(u)\, du$$

$$\Rightarrow \frac{1}{(n+0.5)\pi}\left[\frac{1}{2}u+\frac{\sin(u)\cos(u)}{2}\right]_0^{(n+0.5)\pi} = \frac{1}{(n+0.5)\pi}\left[\frac{(n+0.5)\pi}{2}\right] = \frac{1}{2}$$

$$\therefore \int_0^1 \cos^2\left((n+0.5)\pi\xi\right) d\xi = \frac{1}{2}$$

Solving II

$$\int_0^1 \delta_\xi \cos\left((n+0.5)\pi\xi\right) d\xi \; ; \; \text{let } s = (n+0.5)\pi \text{ \# a constant}$$

$\therefore$ Need to solve $\int_0^1 \delta_\xi \cos(s\xi)\, d\xi$

also Note: $\int \delta(x-a) f(x)\, dx = f(a)$

↳ Applying it to the problem:

$$\therefore \int_0^1 \delta_\xi \cos(s\xi)\, d\xi = \int_0^1 \delta(\xi - 0)\cos(s\xi)\, d\xi = \cos(0) = \underline{\underline{1}}$$

Therefore:

$$b_n = \frac{1}{(1/2)} \cdot 1 = 2 \quad \Rightarrow \boxed{b_n = 2}$$

As a result:

$$\boxed{\bar{C}_A(\xi, \tau) = \sum_{n=0}^{\infty} 2 \cdot \cos\left((n+0.5)\pi\xi\right) e^{-([n+0.5]\pi)^2 \tau}}$$

Note: dimensionless flow $\bar{F}_A$

$$\bar{F}_A(\xi, \tau) = -\frac{\partial \bar{C}_A}{\partial \xi} = \sum_{n=0}^{\infty} -2e^{-([n+0.5]\pi)^2\tau} \cdot \frac{d}{d\xi}\left(\cos\left((n+0.5)\pi\xi\right)\right)$$

$$= \sum_{n=0}^{\infty} -2e^{-([n+0.5]\pi)^2\tau} \cdot \left[-\pi(n+0.5)\sin\left((n+0.5)\pi\xi\right)\right]$$

$$\bar{F}_A = \pi \sum_{n=0}^{\infty} (2n+1) \sin\left((n+0.5)\pi\xi\right) e^{-([n+0.5]\pi)^2\tau}$$

Standard Diffusion Curve eqn (SDC) $\xi = 1$ $\Rightarrow$

$$\boxed{\bar{F}_A = \pi \sum_{n=0}^{\infty} (-1)^n (2n+1)\, e^{-([n+0.5]\pi)^2\tau}}$$

Note as defined in (Gleaves et. al) $\bar{F}_A = F_A \dfrac{\varepsilon_b L^2}{N_{pA} D_{eA}}$

$$\therefore \frac{F_A}{N_{pA}} = \frac{D_{eA}}{\varepsilon_b L^2} \bar{F}_A$$

$$\boxed{\frac{F_A}{N_{pA}} = \frac{D_{eA}}{\varepsilon_b L^2} \pi \sum_{n=0}^{\infty} (2n+1) \sin\left((n+0.5)\pi \xi\right) e^{-\left([n+0.5]\pi\right)^2 \tau}}$$