HW5

① (i) $\frac{\delta c_1}{\delta t} = D\nabla^2 c_1 - r$

$\frac{\delta c_2}{\delta t} = D\nabla^2 c_2 - r$

$\frac{\delta c_3}{\delta t} = r$

$u = c_1 - c_2 \Rightarrow \frac{\delta u}{\delta t} = D\frac{\delta^2 u}{\delta x^2}$ $\qquad c_1 c_2 = K$

(ii) $r = -\frac{\delta c_1}{\delta t} + D\frac{\delta^2 c_1}{\delta x^2}$

$= -\frac{\delta c_1}{\delta u}\frac{\delta u}{\delta t} + D\frac{\delta}{\delta x}\left(\frac{\delta c_1}{\delta u}\frac{\delta u}{\delta x}\right)$

$= -\frac{\delta c_1}{\delta u}\frac{\delta u}{\delta t} + \frac{\delta c_1}{\delta u}D\frac{\delta^2 u}{\delta x^2} + D\frac{\delta u}{\delta x}\frac{\delta}{\delta x}\left(\frac{\delta c_1}{\delta u}\right)$

$= -\frac{\delta c_1}{\delta u}\underbrace{\left(\frac{\delta u}{\delta t} - D\frac{\delta^2 u}{\delta x^2}\right)}_{0} + D\frac{\delta u}{\delta x}\frac{\delta\left(\frac{\delta c_1}{\delta u}\right)}{\delta u}\frac{\delta u}{\delta x}$

$= \underbrace{D\frac{\delta u}{\delta x}\frac{\delta u}{\delta x}}_{\text{mixing}}\underbrace{\frac{\delta^2 c_1}{\delta u^2}}_{\text{speciation}}$

(iii) For $u(t=0) = \delta(x) \Rightarrow u = \frac{1}{(4\pi Dt)^{1/2}} e^{-x^2/4Dt}$

$\Rightarrow \frac{\delta u}{\delta x} = \frac{-2x}{(4\pi Dt)^{1/2}\, 4Dt} e^{-x^2/4Dt}$

$\left.\begin{array}{l} u = c_1 - c_2 \\ c_1 c_2 = K \end{array}\right\} \Rightarrow c_1^2 - u c_1 - K = 0 \Rightarrow c_1 = \frac{u}{2} \pm \frac{\sqrt{u^2+4K}}{2}$

Only one physical root $\Rightarrow c_1 = \frac{u}{2} + \frac{\sqrt{u^2+4K}}{2}$

$\downarrow$

$c_1 > 0$

Differentiating twice $\Rightarrow$ $$\frac{d^2c_1}{du^2} = \frac{1}{2(4K+u^2)^{1/2}} - \frac{u^2}{2(4K+u^2)^{3/2}}$$

Now $r = D\left(\frac{\delta u}{\delta x}\right)^2 \frac{d^2c_1}{du^2}$ and $u = \frac{1}{(4\pi Dt)^{1/2}} e^{-x^2/4Dt}$

$$\therefore r = D\left(\frac{-2x}{(4\pi Dt)^{1/2}\,4Dt} e^{-x^2/4Dt}\right)^2 \left[\frac{1}{2\left(4K + \frac{1}{4\pi Dt} e^{-x^2/2Dt}\right)^{1/2}} + \frac{\frac{1}{4\pi Dt} e^{-x^2/2Dt}}{2\left(4K + \frac{1}{4\pi Dt} e^{-x^2/2Dt}\right)^{3/2}}\right]$$

plot this

When u is small $\frac{d^2c_1}{du^2} \approx$ constant $\rightarrow$ Therefore if all u are small it is a reasonable approximation

Use $u = \frac{1}{(4\pi Dt)^{1/2}}$ as max u to assess <u>this</u>

(iv), (v) + (vi) Create plots using above expressions

A few things to note • r is always 0 at $x = 0$ $\left(\frac{\delta u}{\delta x} = 0\right)$

• Bigger D means lower values locally, but could have bigger total reaction

(vii) A uniform advection just moves everything along at a velocity v shifting by a distance vt, but does not change values of r.

Because c_2 is immobile it's ultimate distribution will change

(2) $$C = \frac{1}{(4\pi D t)^{1/2}} e^{-x^2/4Dt}$$

$$\Rightarrow \frac{\partial C}{\partial x} = \frac{-2x}{(4\pi D t)^{1/2}\, 4Dt} e^{-x^2/4Dt}$$

$$\left(\frac{\partial C}{\partial x}\right)^2 = \frac{4x^2}{16 D^2 t^2 (4\pi D t)} e^{-x^2/2Dt}$$

$$\Rightarrow D \int_{-\infty}^{\infty} \left(\frac{\partial C}{\partial x}\right)^2 dx = \frac{1}{8(2\pi D)^{1/2}} t^{-3/2}$$

$$\int C^2 dx = \int_{-\infty}^{\infty} \frac{1}{(4\pi D t)} e^{-\frac{x^2}{2Dt}} dx = \frac{1}{2(2\pi D)^{1/2}} t^{-1/2}$$

$$-\frac{1}{2}\frac{d}{dt}\int C^2 dx = \frac{1}{8(2\pi D)^{1/2}} t^{-3/2}$$

$$\therefore D \int_{\Omega} \left(\frac{\partial C}{\partial x}\right)^2 dx = -\frac{d}{dt}\int_{\Omega} C^2 dx \qquad \text{Q.E.D.}$$

(ii) Faster - more interfacial area for mixing

(iii) 2d $C = \frac{1}{4\pi D t} e^{\frac{-x^2-y^2}{4Dt}}$

$$\int C^2 \, dx\, dy = \frac{1}{8\pi D} t^{-1}$$

$$-\frac{1}{2}\frac{d}{dt}\int C^2 \, dx\, dy = \frac{1}{16\pi D} t^{-2}$$

" 3d $C = \frac{1}{(4\pi D t)^{3/2}} e^{\frac{-x^2-y^2-z^2}{4Dt}} = \frac{1}{16(2\pi D)^{3/2}} t^{-3/2}$

$$-\frac{1}{2}\frac{d}{dt}\int C^2 \, dx\, dy = \frac{3}{64(2\pi D)^{3/2}} t^{-5/2}$$

1 d $\Rightarrow t^{-3/2}$; 2d $\Rightarrow t^{-2}$; 3d $\Rightarrow t^{-3/2}$

$\therefore \quad M \sim t^{-\frac{1+d}{2}}$ where d is number of spatial dimensions

(iv) In dilution index calculation each dimension acts seperately and so gives the multiplicative behaviour

$$E \simeq (4\pi D t)^{d/2} e^{d/2} \sim t^{d/2}$$

(v) $E \uparrow$ for greater mixing and depends directly on d

$M \downarrow$ " " " , but also depends directly on d

Product $EM \sim t^{-1/2}$

OR $EMt^{1/2}$ is **flat**