Chapter 4 - Introduction to spatial variation

Principle of Mass Balance

rate of change = net movement or flux + net rate of production

4.1 Derivation of the reaction-diffusion equations

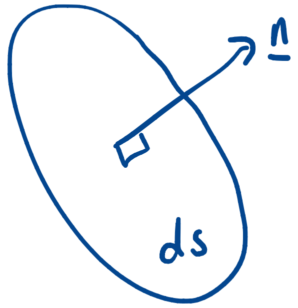
chemical species $C_1, \ldots, C_m$

concentrations $c_1, \ldots, c_m$

w/o diffusion : $\frac{dc_i}{dt} = \underbrace{R_i(c_1, \ldots, c_m)}_{\text{net production rate}}$ – per unit volume.

concentration $c_i(\underline{x}, t)$

Flux $\underline{q}_i(\underline{x}, t)$



flux : defined s.t.

amount of chemical flowing through dS in the infinitessimal time interval dt

$$= \underline{n} \cdot \underline{q} \, dS \, dt$$

Fick's law of diffusion : $\underline{q} = -\underbrace{D}_{\text{diffusion coeff.}} \nabla c$

For any closed volume $V \in D$ (fixed in time and space), with boundary ∂V

$$\frac{d}{dt}\underbrace{\int_V c_i \, dV}_{\text{total amount of } c_i \text{ in } V} = -\underbrace{\int_{\partial V} \underline{q}\cdot\underline{n}\, dS}_{\text{flux out through } \partial V} + \underbrace{\int_V R_i(c_1,\dots,c_m)\, dV}_{\text{net production}}$$

Divergence thm gives

$$\frac{d}{dt}\int_V c_i \, dV = -\int_V \nabla\cdot\underline{q}\, dV + \int_V R_i(c_1,\dots,c_m)\, dV$$

$$= \int_V \left\{\nabla\cdot(D_i \nabla c_i) + R_i(c_1,\dots,c_m)\right\} dV$$

For any closed volume $V \in D$ with boundary ∂V

$$\int_V \left\{ \frac{\partial c_i}{\partial t} - \nabla\cdot(D_i\nabla c_i) - R_i \right\} dV = 0$$

therefore $\boxed{\dfrac{\partial c_i}{\partial t} = \nabla\cdot(D_i\nabla c_i) + R_i}$ $\quad \underline{x} \in D.$

$i = 1, \dots, m$

System of reaction-diffusion eqns.

Require: ICs and BCs to close the system.

Think further about the step

suppose $\dfrac{\partial c_i}{\partial t} - \nabla\cdot(D_i\nabla c_i) - R_i \neq 0$ some $\underline{x}^* \in D$

WLOG suppose the above is positive at $\underline{x}^* \in D$.

Then $\exists\, \varepsilon > 0$ s.t. $\dfrac{\partial c_i}{\partial t} - \nabla\cdot(D_i \nabla c_i) - R_i > 0$

for $\underline{x} \in B_\varepsilon(\underline{x}^*)$.

In this case

$$\int_{B_\varepsilon(\underline{x}^*)} \left[\frac{\partial c_i}{\partial t} - \nabla\cdot(D_i \nabla c_i) - R_i \right] dV > 0$$

contradicts our original assumption, and so the RD eqns hold.

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① Single species, 1D, no reactions

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} \qquad \text{(diffusion eq}^{\underline{n}}\text{)}$$

Length scale L timescale $T = \dfrac{L^2}{D}$

Cell $L \sim 10^{-5}\,\text{m} = 10^{-3}\,\text{cm}$

$D \sim 10^{-7}\,\text{cm}^2\text{s}^{-1}$

Then $T \sim \dfrac{10^{-6}\,\text{cm}^2}{10^{-7}\,\text{cm}^2\text{s}^{-1}} \sim 10\,\text{s}$

If $L \mapsto 10L$ $\quad T \mapsto 10^2 T$

$L \mapsto 100L$ $\quad T \to 10^4 T$

4.2 chemotaxis

chemotaxis – movements up chemical gradients

diffusive flux $J_D = -D_n \nabla n$

chemotactic flux $J_c = n\underline{\chi(c)}\nabla c = n\nabla \Phi(c)$

chemotactic coefficient

monotonic inc

eg $\chi(c) = \chi,\ \dfrac{\chi_0}{c},\ \dfrac{\chi_0}{(k+c)^2}$

Total flux: $J = J_D + J_c$

$= -D_n \nabla n + n\chi(c)\nabla c$

Typical model

$$\frac{\partial n}{\partial t} = \nabla \cdot (D_n \nabla n) - \nabla \cdot (n\chi(c)\nabla c) + f(n,c)$$

$$\frac{\partial c}{\partial t} = \nabla \cdot (D_c \nabla c) + \lambda n - \mu c$$

eg. logistic growth.

4.3 Positional information and pattern formation

Theories

① Positional information – Wolpert
"French Flag Model"

② Diffusion-driven instability – Turing (§6)

The French Flag Model

$$\frac{\partial m}{\partial t} = D\frac{\partial^2 m}{\partial x^2}$$

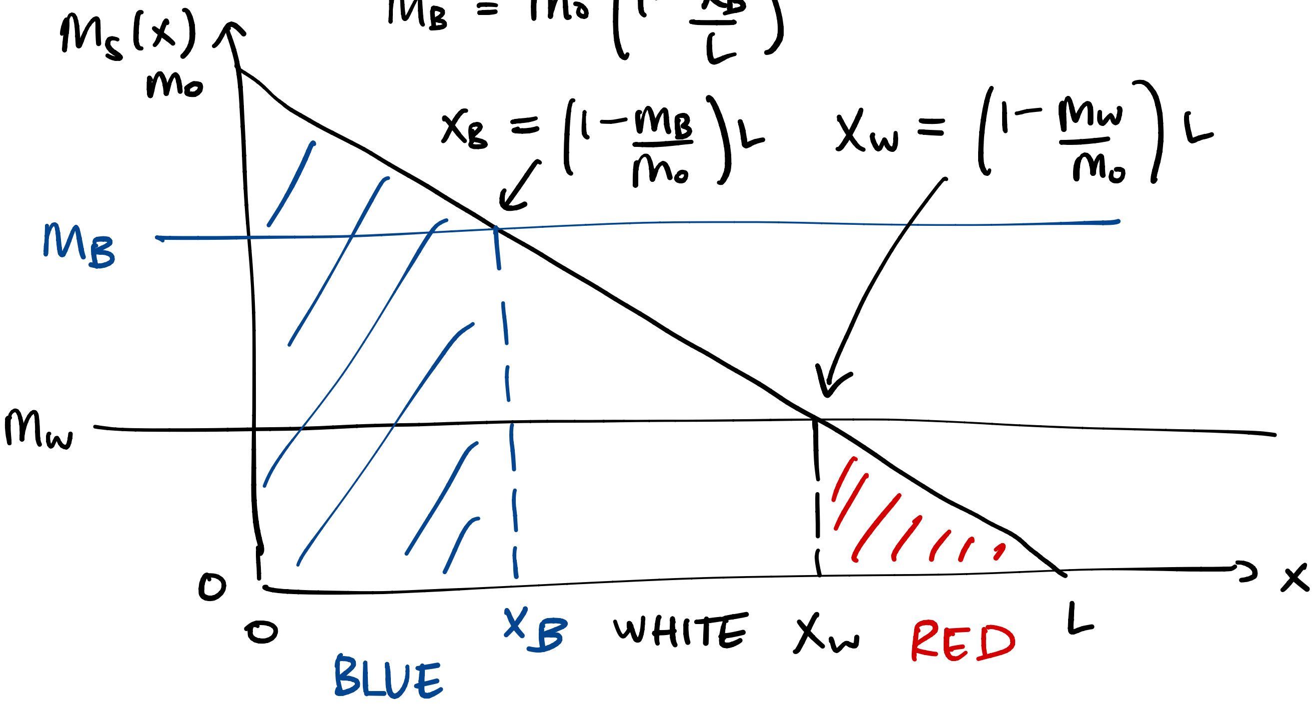
$$m(0,t) = m_0$$
$$m(L,t) = 0$$
$$m(x,0) = 0$$

Assume rapidly reaches steady state : $m_s(x)$

$$\frac{d^2 m_s}{dx^2} = 0 \Rightarrow m_s(x) = m_0\left(1-\frac{x}{L}\right)$$

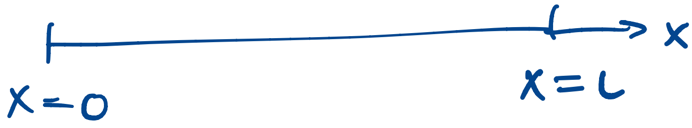
$$m_B = m_0\left(1-\frac{x_B}{L}\right)$$

$$x_B = \left(1-\frac{m_B}{m_0}\right)L \qquad x_W = \left(1-\frac{m_W}{m_0}\right)L$$



4.4 Minimum domains for spatial structure

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + f(u)$$



$$f(u) = ru\left(1-\frac{u}{q}\right) - \frac{u^2}{1+u^2}$$

Boundary conditions $u(0,t)=0$
$u(L,t)=0$

Q - If we start with a small initial distribution, will there be an outbreak, or will the pop^n die out?

Suppose $0 \le u(x,0) \ll 1$ $\quad f(u) \approx f'(0)u = ru$

Then $$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + \underbrace{f'(0)}_{=r}u$$

Seek a solution $$u(x,t) = \sum_{n=1}^{\infty} a_n(t)\sin\left(\frac{n\pi x}{L}\right)$$

then $$\frac{da_n}{dt} = \underbrace{\left[-\frac{Dn^2\pi^2}{L^2} + f'(0)\right]}_{\sigma_n} a_n$$

$$\Rightarrow \quad a_n(t) = a_n(0)e^{-\sigma_n t}$$

$$\therefore \quad u(x,t) = \sum_{n=1}^{\infty} a_n(0)e^{\underbrace{\left(f'(0)-\frac{Dn^2\pi^2}{L^2}\right)}_{+\sigma_n}t}\sin\left(\frac{n\pi x}{L}\right)$$

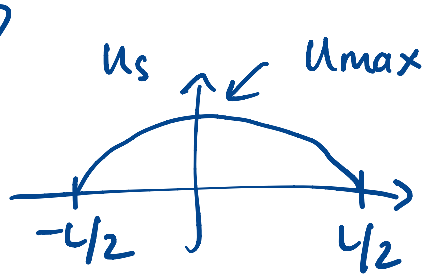
For the outbreak to die out : $\sigma_n < 0 \;\forall n$

$$f'(0) - \frac{Dn^2\pi^2}{L^2} < 0 \quad \forall n$$

ie $\boxed{L \leq \sqrt{\frac{D\pi^2}{f'(0)}} := L_{crit}}$

Q - how does the steady state pattern depend on the domain size?

shift coordinates



At steady state $\quad 0 = D\frac{\partial^2 u}{\partial x^2} + f(u)$

multiply by $\partial u/\partial x$, and integrate :

$$0 = \int D\left(\frac{\partial u}{\partial x}\right)\left(\frac{\partial^2 u}{\partial x^2}\right)dx + \int f(u)\frac{\partial u}{\partial x}\,dx$$

$$\frac{1}{2}D\left(\frac{\partial u}{\partial x}\right)^2 + F(u) = F(u_{max})$$

(for $x>0$, $\frac{\partial u}{\partial x} < 0$) $\qquad F(u) := \int_0^u f(y)\,dy$

$$F'(u) = f(u)$$

$$\frac{\partial u}{\partial x} = -\sqrt{\frac{2}{D}}\sqrt{F(u_{max}) - F(u)}$$

$$2\int_0^{L/2} dx = -\sqrt{2D}\int_{u_{max}}^{0} \frac{1}{\sqrt{F(u_{max}) - F(\bar{u})}}\,d\bar{u}$$

$$\frac{L}{\sqrt{2D}} = \int_0^{u_{max}} \frac{1}{\sqrt{F(u_{max}) - F(\bar{u})}} \, d\bar{u}$$