11/22/04

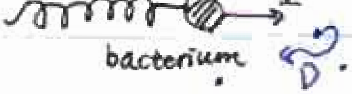
Convection / Diffusion Problems

(Mechanical / Chemical Subsystems) See Chapter 9 - Deen text

situations in which both fluid flow and molecular diffusion are present

Examples

a) bacterial movement in a nutrient environment.



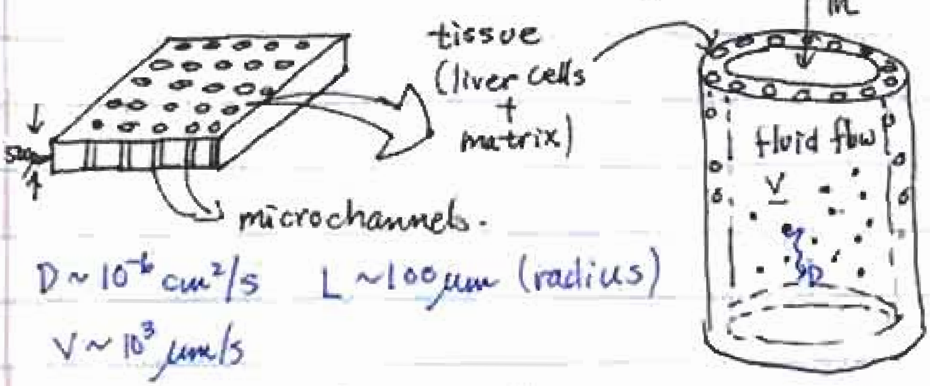

nutrient molecular species

What is effect of $\underline{V}$ on uptake of nutrient by bacteria? (None)

Redraw in bacterial frame of reference


$L \sim 1\mu m$
$V^* \sim 10\, \mu m/s$
$D \sim 10^{-5}\, cm^2/s$
$\Rightarrow Pe \approx 10^{-2}$

b) Perfused tissue bioreactor (e.g. liver biochip in Griffith lab)




How should channel be designed to get proper nutrient levels to cells?

$D \sim 10^{-6}\, cm^2/s$ $L \sim 100\,\mu m$ (radius)

$V \sim 10^3\, \mu m/s$

$Pe \approx 10^3$ (convection dominating in direction of moving fluid)

First, some scaling analysis

$$\frac{\partial c}{\partial t} = -\nabla \cdot J + R$$

nutrient Conc [moles/vol]; $J$: molecular flux; $R$: reaction in bulk fluid, $\to 0$, negligible in 2 cases

$$J = -D\nabla c + \underline{V}c$$

$$-\nabla \cdot J = D\nabla^2 c + \nabla D \cdot \nabla c - \underline{V}\cdot\nabla c - c(\nabla \cdot V)$$

$\nabla D \to 0$: $D$ is isotropic; $\nabla \cdot V = 0$: continuity.

$$\frac{\partial c}{\partial t} = D\nabla_x^2 c - \underline{V}\cdot\nabla_x c$$

$c(x,t)$

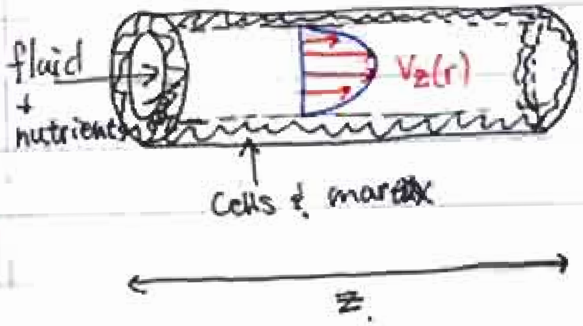
scaling: $\tau = \frac{t}{t^*}$, $\omega = \frac{c}{c^*}$, $\xi = \frac{x}{L}$, $\underline{u} = \frac{\underline{V}}{V^*}$

$L$ — relative distance; $V^*$ — max or avg. velocity.

$$\frac{\partial w}{\partial \tau} = \boxed{\frac{D t^*}{L^2}} \left[ \underbrace{\nabla_\xi^2 w}_{O(1)} - \left(\frac{v^* L}{D}\right) \underline{u} D_\xi w \right]$$

Peclet number $Pe = \frac{\text{convective transport}}{\text{diffusive transport}}$

overall rate of diffusion relative ~~to~~ problem time-scale




Under "fully-developed" conditions (i.e.) sufficently far along channel).

$V_z(r) = 2V_m \left[1 - \left(\frac{r}{R}\right)^2\right]$

maximum velocity $= \frac{-R^2}{8\mu} \nabla P$

See Deen section 6.5 "Entrance effects"

$L$"entrance" $\sim R[1 + 0.1 Re]$

99% of fully-developed profile

stringent because 99% fully developed flow.

@ 5%s ...

$\mu \sim 10^{-2}$ g/cm-sec

$\rho \sim 1$ g/cm$^3$

$Re \sim 10^{-1}$

neglect axial diffusion, relative to axial convection ($Pe \sim 10^3$)

$$\text{So, } \cancel{\frac{\partial c}{\partial t}} = D\left[\cancel{\frac{\partial^2 c}{\partial z^2}} + \frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial c}{\partial r}\right)\right] - 2V_m\left(1 - \left[\frac{r}{R}\right]^2\right)\frac{\partial c}{\partial z}$$

SS.

B.C. $z = 0 \quad c(r) \equiv c_i$

~~$z = L$~~ a) exptl design? b) self consistent condition from overall balance

don't need.

c) $\frac{\partial c}{\partial z} = 0$

$r = 0 \quad \frac{\partial c}{\partial r} = 0$

$r = R - \quad -D\frac{\partial c}{\partial r}$ ~~= 0~~ $\quad -D\frac{\partial c}{\partial r} = R \equiv [kC]\, n\delta$

moles/area

moles/vol

time$^{-1}$ (cells/vol)$^{-1}$

# cells/vol

thickness of tissue layers.

Scaling: $\eta = \frac{r}{R}$ $\xi = \frac{z}{L}$ $\theta = \frac{c}{c_i}$ $\Rightarrow$ $\boxed{\begin{array}{l} Pe \frac{\partial \theta}{\partial \xi} = \frac{1}{(1-\eta^2)\eta} \frac{\partial}{\partial \eta}\left(\eta \frac{\partial \theta}{\partial \eta}\right) \\ Pe \equiv \frac{2 V_m L}{D^2}\left(\frac{R^2}{L^2}\right) \end{array}}$

B.C. $\xi = 0$ $\theta = 1$

$\eta = 0$ $\frac{\partial \theta}{\partial \eta} = \cancel{\theta} = 0$

$\eta = 1$ $-\left[\frac{D}{KRS_n}\right]\frac{\partial \theta}{\partial \eta} = \theta$

$\ll P \frac{\text{diff}}{\text{reaction @ wall}} \Rightarrow \eta = 1,\ \theta = 0$

Can solve by separation of variables, Sturm-Liouville Linear Op, $\boxed{\text{FFT}}$ (can see chap 4 Deen and example 9.5-1) assume an eigenfunction expansion for $\theta(\eta, \xi)$

FFT of $\theta$

$$\theta(\eta, \xi) = \sum_{j=1}^{\infty} \bar{\theta}_j(\xi)\, \Phi_j(\eta)$$

infinite set of eigenfunctions,

$$\boxed{\mathcal{L} = \frac{1}{(1-\eta^2)\eta} \frac{\partial}{\partial \eta}\left(\eta \frac{\partial}{\partial \eta}\right)}$$

self-adjoint. Liouville-Sturm Operator

+ associated B.C.

$$\left.\begin{array}{l} \eta = 0,\ \frac{\partial \Phi_j}{\partial \eta} = 0 \\ \eta = 1,\ \Phi_j = 0 \end{array}\right\} \mathcal{L}\Phi_j = -\lambda_j^2 \Phi_j \quad j = 1, 2, \ldots$$

$$\bar{\theta}_j(\xi) = \int_0^1 \underbrace{\Phi_j(\eta)}_{\text{eigen-vector}} \underbrace{(1-\eta^2)\eta}_{\text{operator}} [\theta(\eta, \xi)]\, \underbrace{d\eta}_{\text{domain}}$$

How do we get $\Phi_j(\eta), \lambda_j$? Solve Eqns, get $j = 1, 2, \ldots$ solution Confluent hypergeometric functions; also called "Cylindrical Graeta functions"

Now, in FFT method, take FFT of PDE

LHS $\int_0^1 \Phi_j(\eta)(1-\eta^2)\eta\left[Pe\frac{\partial\theta}{\partial\xi}\right]d\eta = Pe\frac{d\bar{\theta}}{d\xi}$

RHS $\int_0^1 \Phi_j(\eta)(1-\eta^2)\eta\left[\frac{1}{(1-\eta^2)\eta}\frac{\partial}{\partial\eta}\left(\eta\frac{\partial\theta}{\partial\eta}\right)\right]d\eta$

RHS Integrate by parts twice:

$$= \underbrace{\left[\eta\Phi_j(\eta)\frac{\partial\theta}{\partial\eta}\right]_0^1}_{0} - \underbrace{\left[\eta\frac{d\Phi_j}{d\eta}\theta\right]_0^1}_{0} + \boxed{\int_0^1\left(\eta\frac{d^2\Phi_j}{d\eta^2}+\frac{d\Phi_j}{d\eta}\right)\theta\,d\eta}$$

$$= \int_0^1 \underline{\frac{1}{(1-\eta^2)\eta}\frac{\partial}{\partial\eta}\left(\eta\frac{\partial\Phi_j}{\partial\eta}\right)}\theta(1-\eta^2)\eta\,d\eta$$

$$= \int_0^1 -\lambda_j^2\Phi_j\,\theta(1-\eta^2)\eta\,d\eta = -\lambda_j^2\bar{\theta}_j$$

So, we get $Pe\frac{d\bar{\theta}_j}{d\xi} = -\lambda_j^2\bar{\theta}_j$ w/ IC $\bar{\theta}_j(0) = \int_0^1\Phi_j(\eta)(1-\eta^2)\eta\cdot 1\cdot d\eta$.

$= b_j$ can calculate for each $j=1, 2, \pm 3, \pm 4 \dots \pm n$.

$$\bar{\theta}_j(\xi) = b_j e^{-\frac{1}{Pe}\lambda_j^2\xi}$$

$$\theta(\eta,\xi) = \sum_{j=1}^{\infty} b_j\,\Phi_j(\eta)e^{-\frac{1}{Pe}\lambda_j^2\xi}$$

eigenvalues ~~from~~ for eigenvectors eqn.

integral.

eigenvectors for eigenvalue eqn.