BMOLE 452-689 – Transport

Chapter 8. Transport in Porous Media

Text Book: Transport Phenomena in Biological Systems
Authors: Truskey, Yuan, Katz
Focus on what is presented in class and problems…

Dr. Corey J. Bishop
Assistant Professor of Biomedical Engineering
Principal Investigator of the Pharmacoengineering Laboratory:
pharmacoengineering.com
Dwight Look College of Engineering
Texas A&M University
Emerging Technologies Building Room 5016
College Station, TX 77843
cbishop@tamu.edu

If I have seen further than other… was this humble or sticking it to them?

Describing Porosity, Tortuosity, and Available Volume Fraction to Characterize Porous Materials

Chapter 8, Section 2

Interface: border between solid and void spaces

$$Specific\ Surface = s = \frac{Total\ interface\ area}{Total\ volume}$$

Units = $\frac{1}{length}$

$$Porosity = \varepsilon = \frac{Void\ volume}{Total\ volume}$$

ε is dimensionless

Void volume: total volume of void space in a porous medium

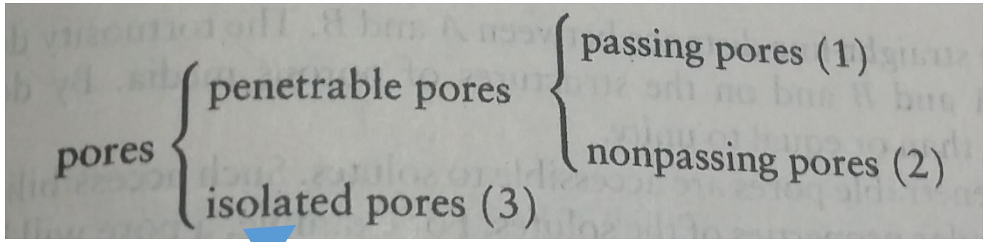
To give you an idea of values:

If total volume is based on interstitial space: ε is generally > 0.9
If ε is generally < 0.30, cells and vessels should be considered
Note: In some tumors, ε is as high as 0.6

Porosity (ε)

$$Porosity = \varepsilon = \frac{Void\ volume}{Total\ volume}$$

- Context: porous medium
  - Does not provide information on how pores are connected or number of pores available for water and solute transport



- pores
  - penetrable pores
    - passing pores (1)
    - nonpassing pores (2)
  - isolated pores (3)

$$\varepsilon = \varepsilon_i + \varepsilon_p + \varepsilon_n$$

Note: isolated pores are not accessible to external solvents and solutes: They can sometimes be considered part of the solid phase

Tortuosity (T)

- L_{min} is the shortest path length
- L is the straight-line distance between A and B

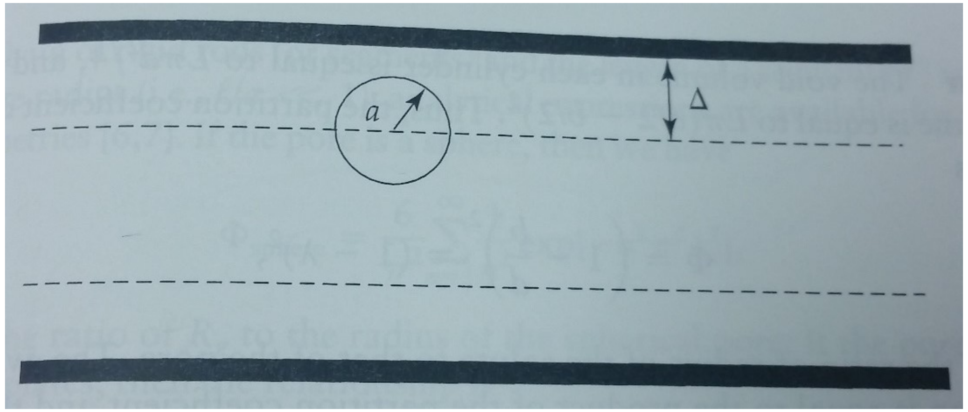
$$T = \left(\frac{L_{min}}{L}\right)^2$$

T is always greater than or equal to unity

Available Volume Fraction (K_{AV})

Available Volume: portion of accessible volume that can be occupied by the solute.
Not all penetrable pores are accessible to solutes

$$K_{AV} = \frac{Available\ volume}{Total\ volume}$$



$$K_{AV} = \frac{Available\ volume}{Total\ volume}$$

K_{AV} is molecule dependent and always smaller than porosity.

This can be caused by 3 scenarios:

1) Centers of the solute molecules cannot reach the solid surface in the void space
   Difference between total void volume and the available volume can be estimated as the product of the area of the surface and distance (Δ) between solute and surface
2) Some of the void space is smaller than the solute molecules
3) Inaccessibility of large penetrable pores surrounded by pores smaller than the solutes

Generally, K_{AV} decreases with size of solutes

- Partition Coefficient (Φ): ratio of available volume to void volume
  - Measure of solute partitioning at equilibrium between external solutions and void space in porous media

$$\Phi = \frac{K_{AV}}{\varepsilon}$$

Exclusion Volume

- Some porous media are fiber matrices: space inside and near surface of fibers not available to solutes
- Exclusion Volume: size of the space

$$Exclusion\ volume = \pi\left(r_f + r_s\right)^2 L$$

r_f and r_s are the radii of the fiber and solute
L is the length of the fiber
N is the number of the fibers

If minimum distance between fibers is larger than $2(r_f + r_s)$, such as when fiber density is very low or when fibers are parallel:

$$Exclusion\ volume\ fraction = \frac{\pi(r_f + r_s)^2 LN}{V} = \theta\left(\frac{r_s}{r_f} + 1\right)^2$$

θ is the volume fraction of fibers (ε=1- θ when θ is much less than unity)

$$K_{AV} = 1 - exclusion\ volume\ fraction = 1 - \theta\left(\frac{r_s}{r_f} + 1\right)^2$$

When $\theta\left(1+\frac{r_s}{r_f}\right)^2$ is much less than unity, Ogston Equation (eq. 8.2.24 in book) reduces to previous equation.

Porosity can be derived from the Ogston Equation by letting r_s=0

$$\varepsilon = \exp[-\theta]$$

When θ is much less than unity:

$$\varepsilon = 1 - \theta$$

Partition coefficient of solutes in liquid phase of fiber-matrix material:

$$\Phi = \frac{\exp\left[-\theta\left(1+\left(\frac{r_s}{r_f}\right)\right)^2\right]}{1-\theta}$$

Darcy’s Law

Darcy’s Law

- Flow rate is proportional to pressure gradient so rate = constant *grad(p)
- Valid in many porous media
- NOT valid for:
  - Non-Newtonian fluids (what is a Newtonian fluid?)
  - Newtonian liquids at high velocities
  - Gasses at very low and high velocities

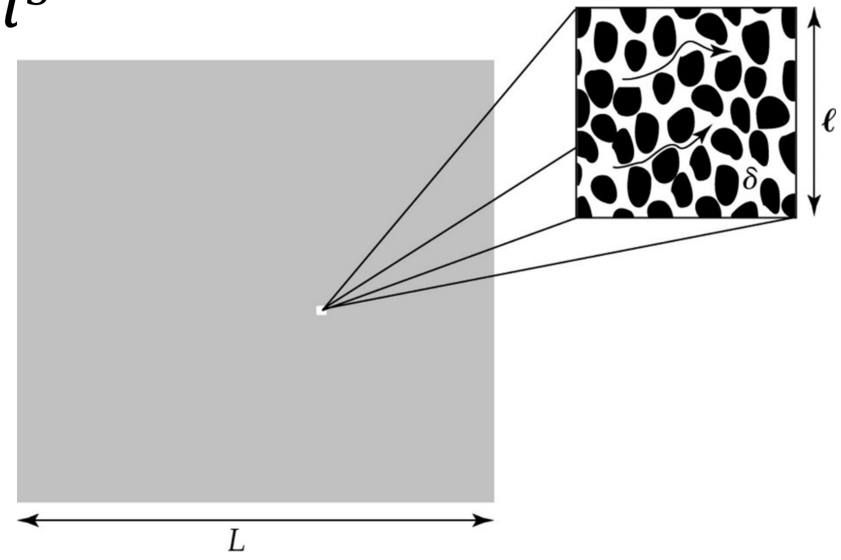
Darcy’s Law

Describing fluid flow in porous media

- Two Ways:
  - Numerically solve governing equations for fluid flow in individual pores if structure is known
  - Assume porous medium is a uniform material (Continuum Approach)

Three Length Scales

1. $\delta =$ average size of pores
2. L = distance which macroscopic changes of physical quantities must be considered (ie. Fluid velocity and pressure)
3. $l \Rightarrow$ a small volume with dimension l^3



Continuum Approach Requires:

- δ << l_0 << L

Darcy’s Law

- l_0 = Representative Elementary Volume from l_0^3 (REV)
  - $l_0 << L$
- Total volume of REV can give the averaging over a volume value
- V_f = fluid velocity of each fluid particle averaged in the volume of the fluid phase
- V = velocity of each fluid particle averaged in the REV
- $V = \varepsilon V_f$

Darcy’s Law

- Law of Mass Conservation
  - No Fluid Production = “Source”
  - Fluid Consumption = “Sink”

Mass Balance with velocities

- $\nabla * \mathrm{v} = \phi_B - \phi_L$
- $\nabla * \mathcal{E}v_f = \phi_B - \phi_L$

- Determined by Starling’s Law (more in chapter 9)
  - ϕ_B = volumetric flow from sources (units?)
  - ϕ_L = volumetric flow from sinks (L=lymphatic drainage)
- If volume of the system is not changing or if the flow in and flow out are balanced then?

Darcy’s Law

- Momentum Balance in Porous Media
  - v = -K $\nabla \mathrm{p}$

- $\nabla \mathrm{p} = \text{gradient of hydrostatic pressure}$
- K = hydraulic conductivity constant
- p = average quantity within the fluid phase in the REV

Darcy’s Law

- Substituting the Equations to form:
  - $\nabla * (-K \nabla p) = \phi_B - \phi_L$

- Steady State:
  - $\nabla^2 * p = 0$

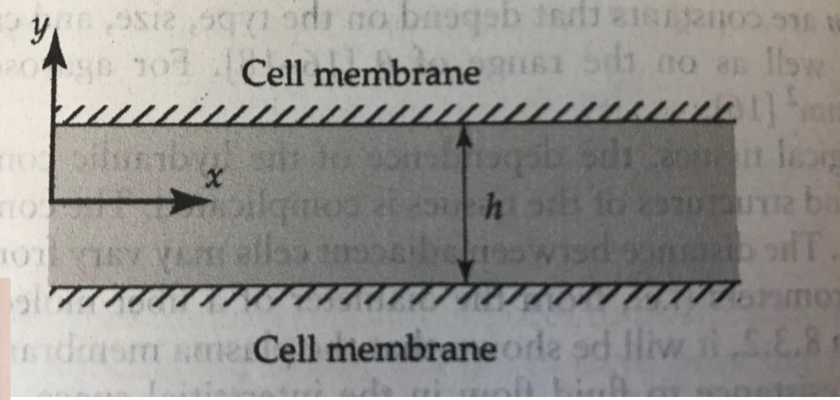
Brinkman Equation

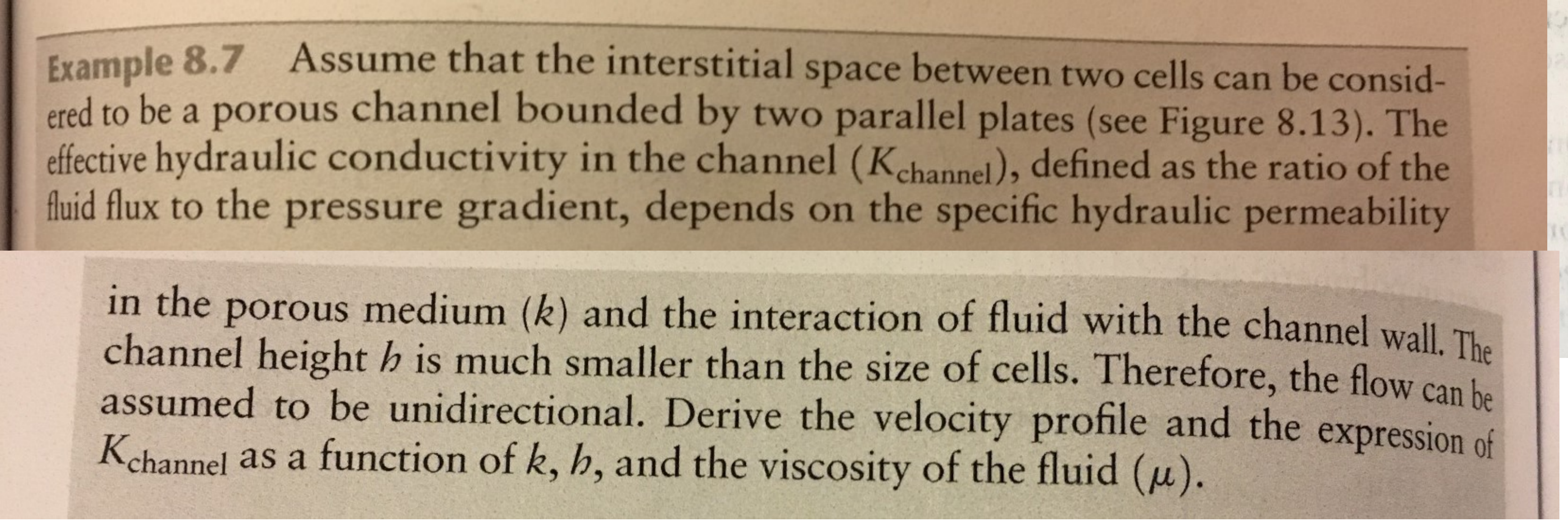
Brinkman Equation

- $k = K\mu$
  - k is the specific hydraulic permeability (usually units of nm^2)
  - Darcy's law is used when k is low: when k is much smaller than the square of L
  - When k is not low: Brinkman Equation
- $Brinkman\ Equation$:
  - $\mu\nabla^2 V - \frac{1}{K}V - \nabla p$=0
  - Darcy's Law is a special case of this equation when the first term = 0 ($V = -K\nabla p$)

The beginning of example 8.7

Example 8.7 Assume that the interstitial space between two cells can be considered to be a porous channel bounded by two parallel plates (see Figure 8.13). The effective hydraulic conductivity in the channel (K_{channel}), defined as the ratio of the fluid flux to the pressure gradient, depends on the specific hydraulic permeability in the porous medium (k) and the interaction of fluid with the channel wall. The channel height h is much smaller than the size of cells. Therefore, the flow can be assumed to be unidirectional. Derive the velocity profile and the expression of K_{channel} as a function of k, h, and the viscosity of the fluid (μ).





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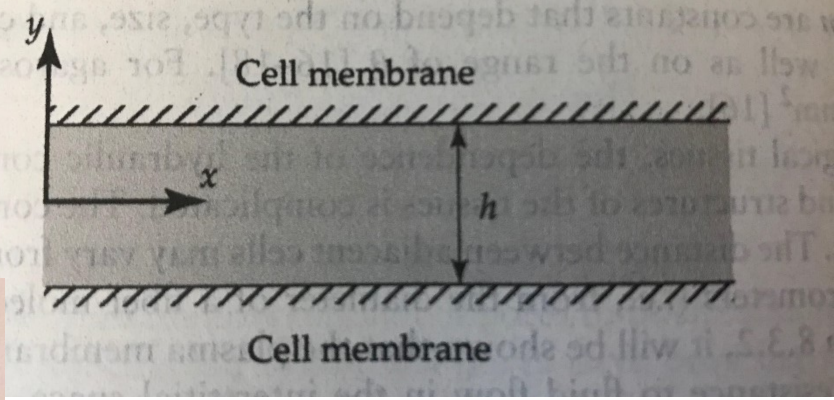
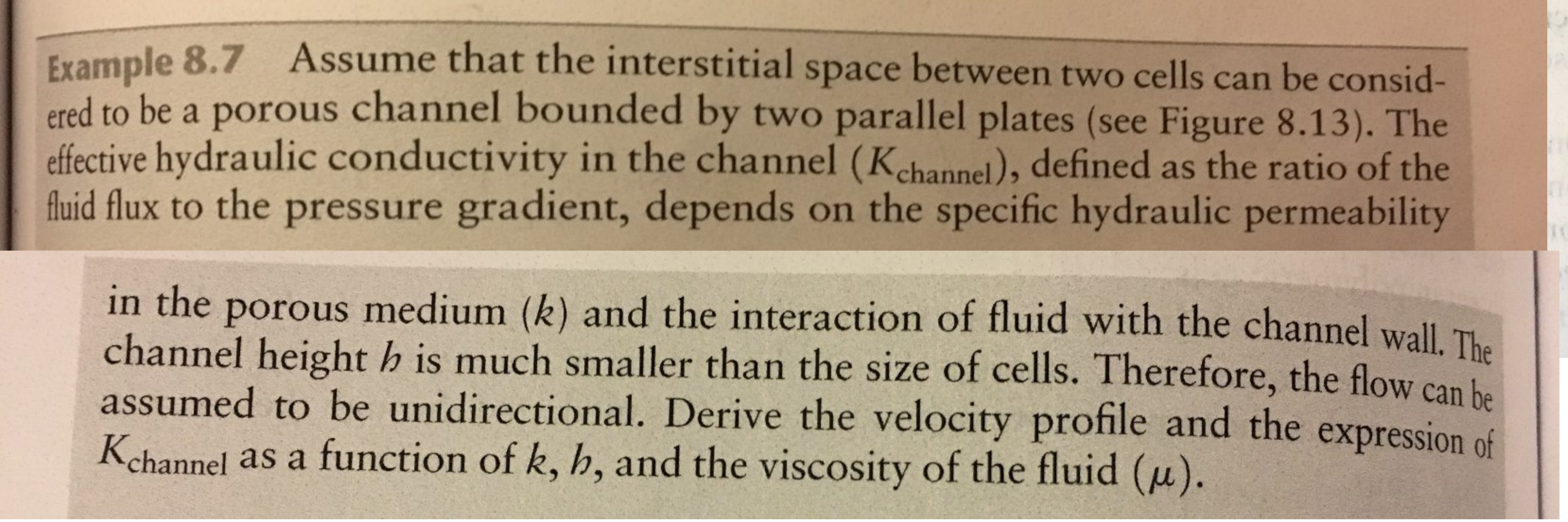


Flow is unidirectional in the channel and is governed by:
Mass balance
Brinkman equations

$$\mu\nabla^2 V - \frac{1}{K}V - \nabla p=0; \; k = K\mu$$



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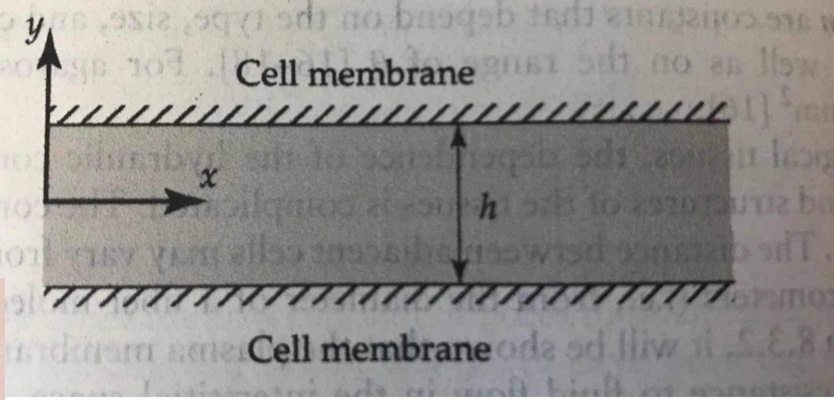

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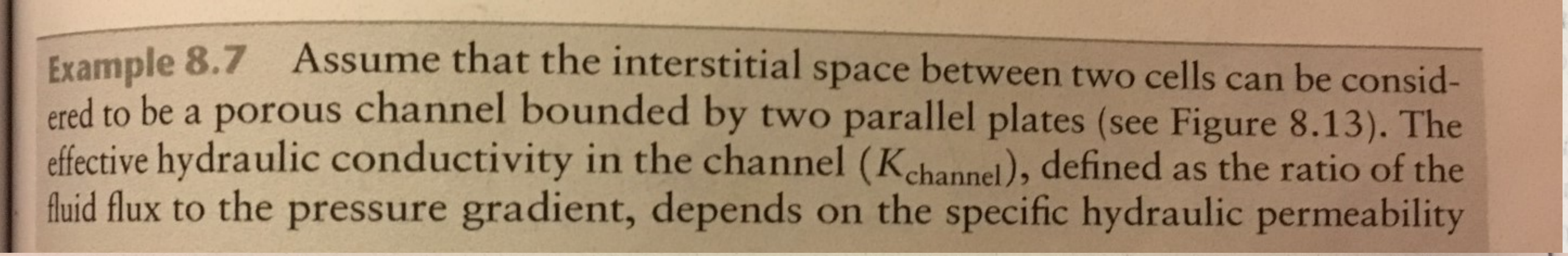

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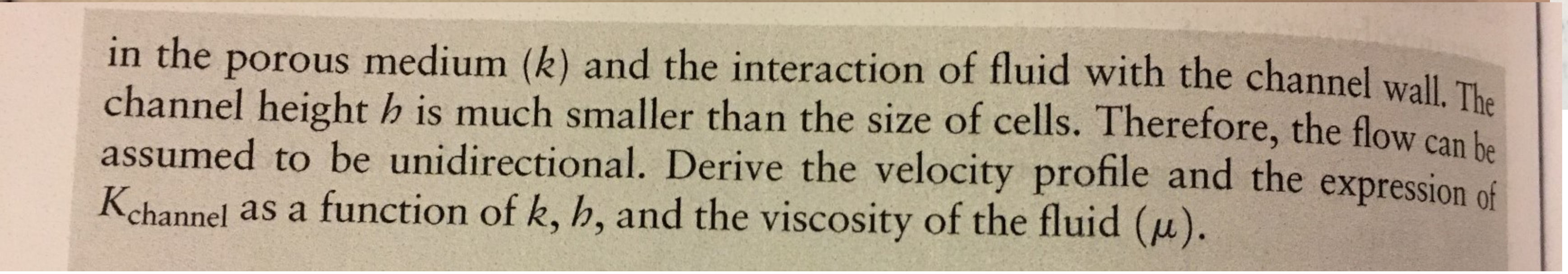
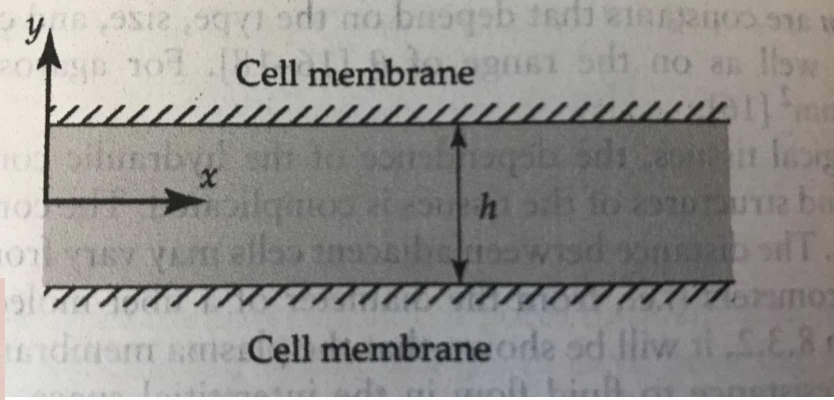


in the porous medium (k) and the interaction of fluid with the channel wall. The channel height h is much smaller than the size of cells. Therefore, the flow can be assumed to be unidirectional. Derive the velocity profile and the expression of K_{channel} as a function of k, h, and the viscosity of the fluid (μ).



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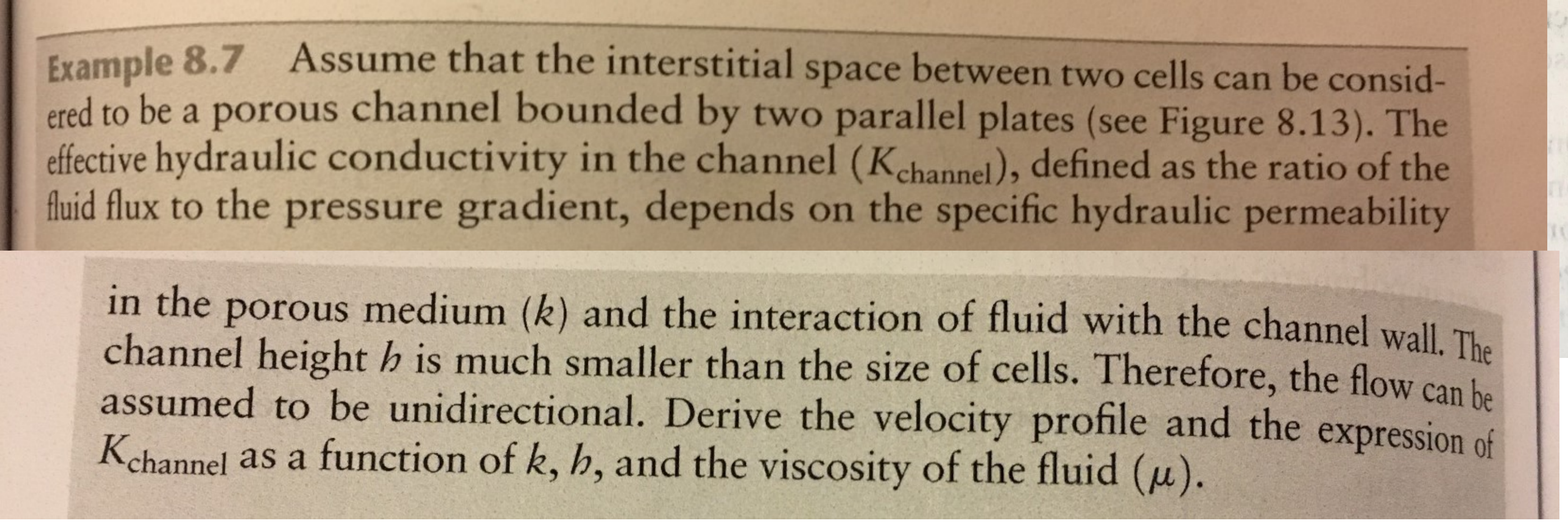

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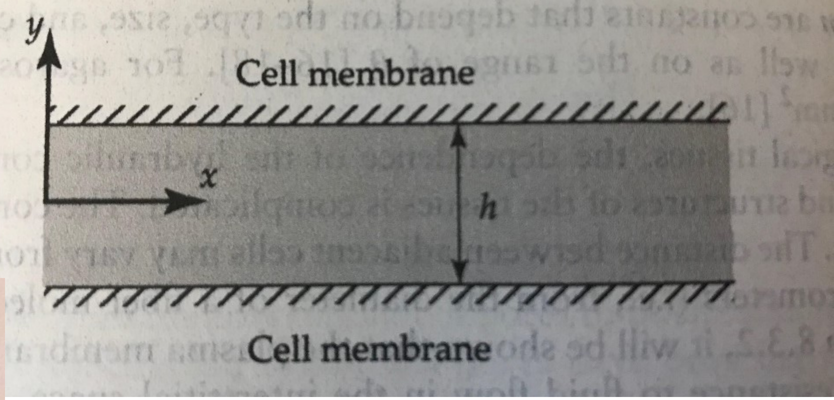

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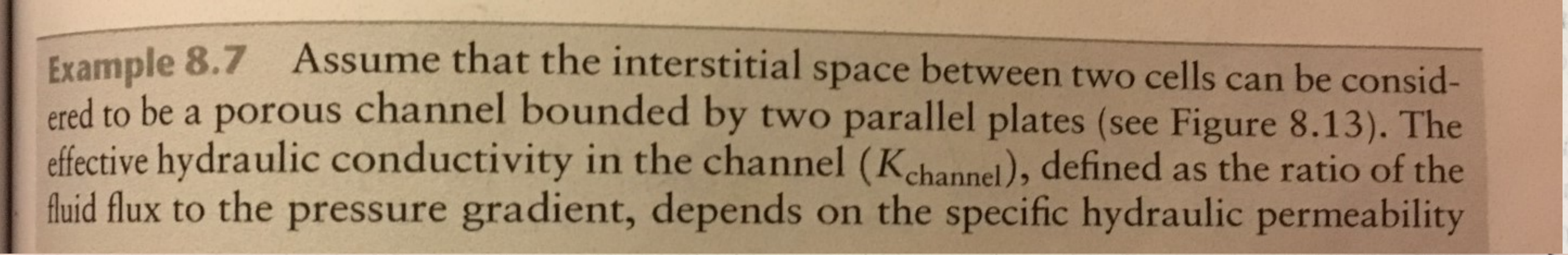

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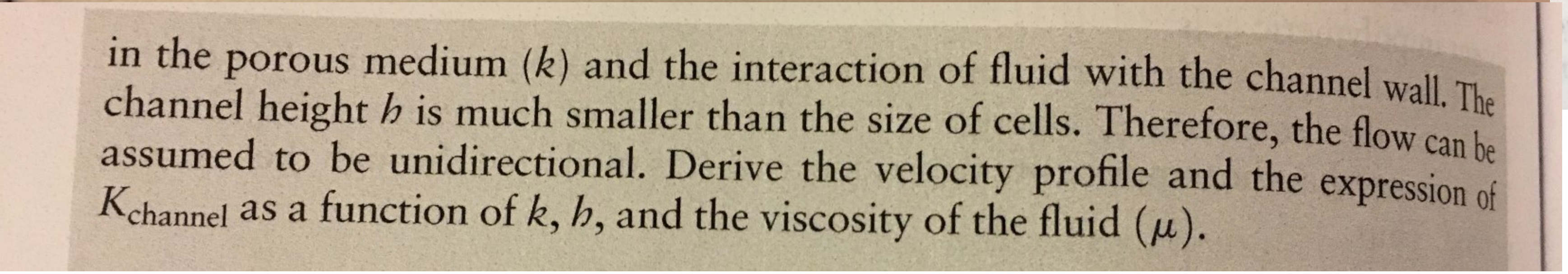

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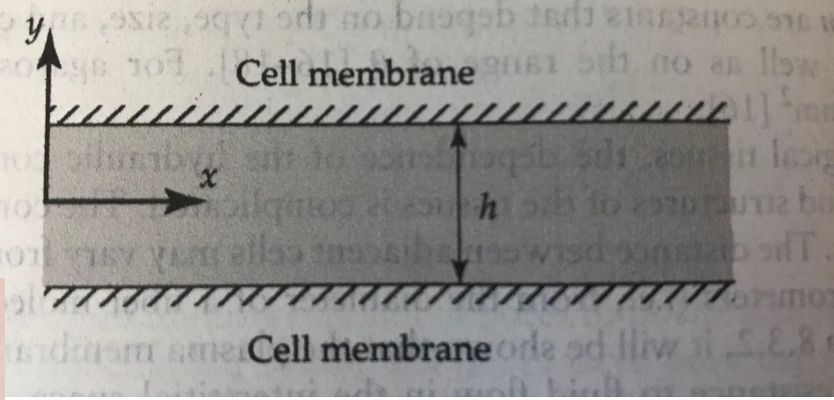

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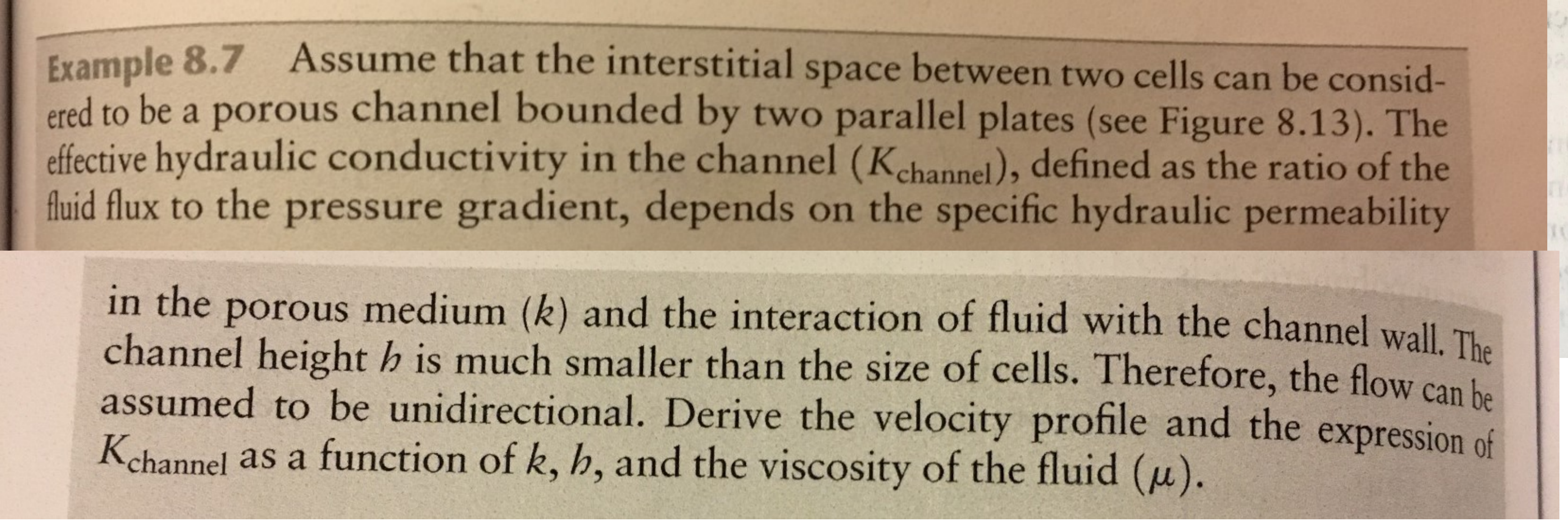
$$\nabla^2 V - \frac{V}{k} = \frac{\nabla p}{\mu}$$

$$\nabla^2 V_x - \frac{V_x}{k} = \frac{\nabla p}{\mu} = \mathrm{V}_x'' - \frac{\mathrm{V_x}}{\mathrm{k}}$$



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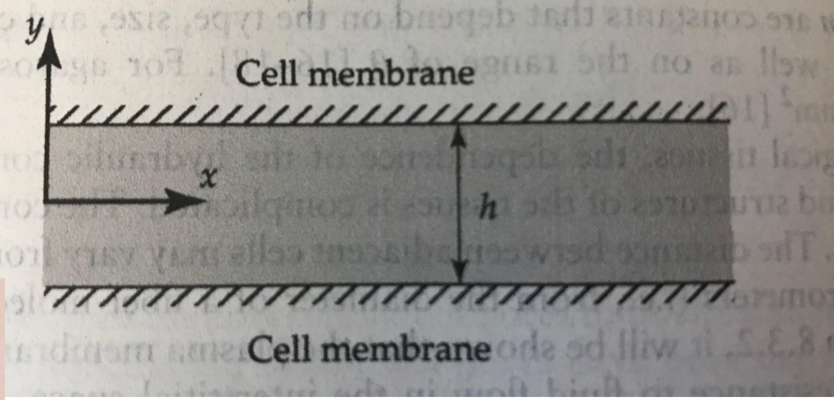

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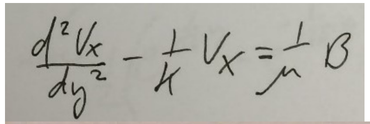
$$\nabla^2 V - \frac{V}{k} = \frac{\nabla p}{\mu}$$

$$\nabla^2 V_x - \frac{V_x}{k} = \frac{\nabla p}{\mu} = \mathrm{V}_\mathrm{x}'' - \frac{\mathrm{V}_\mathrm{x}}{\mathrm{k}}$$

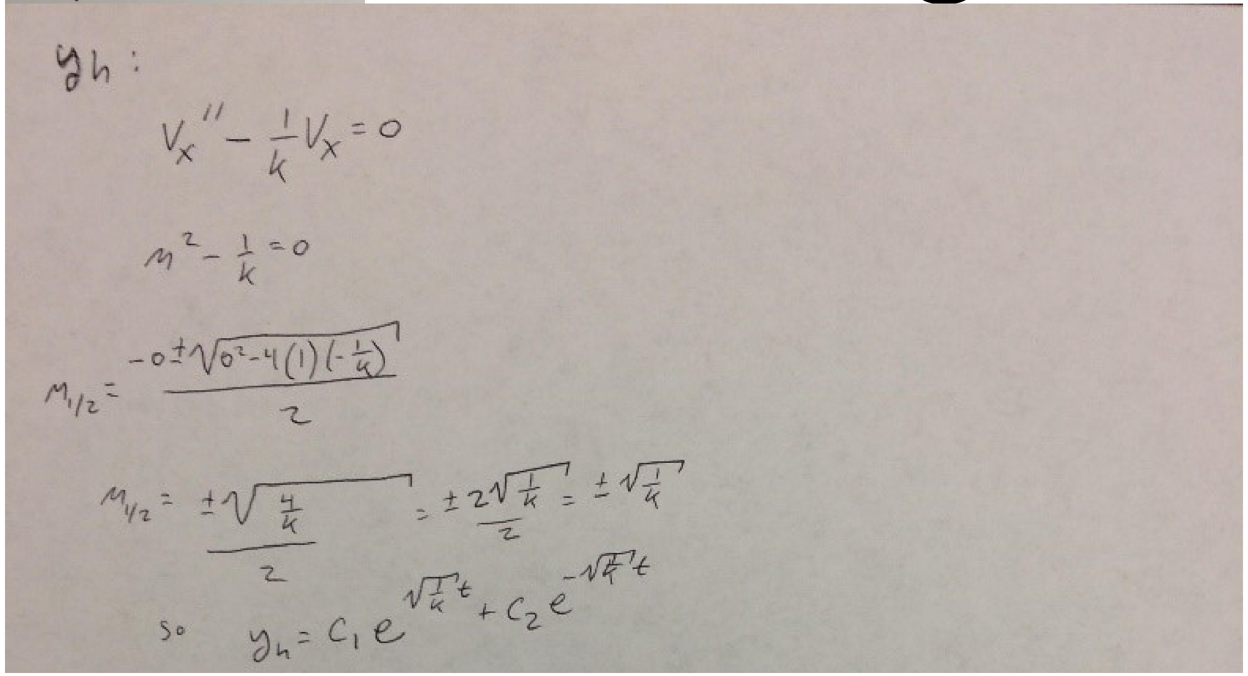
$$\frac{\nabla p}{\mu} = \mathrm{V}_\mathrm{x}'' - \frac{\mathrm{V}_\mathrm{x}}{\mathrm{k}}$$

How?

Solving for Example 8.7



$$\frac{d^2V_x}{dy^2} - \frac{1}{k}V_x = \frac{1}{\mu}B$$



y_h:

$$V_x'' - \frac{1}{k}V_x = 0$$

$$m^2 - \frac{1}{k} = 0$$

$$m_{1/2} = \frac{-0 \pm \sqrt{0^2 - 4(1)(-\frac{1}{k})}}{2}$$

$$m_{1/2} = \frac{\pm\sqrt{\frac{4}{k}}}{2} = \frac{\pm 2\sqrt{\frac{1}{k}}}{2} = \pm\sqrt{\frac{1}{k}}$$

so $y_h = C_1 e^{\sqrt{\frac{1}{k}}t} + C_2 e^{-\sqrt{\frac{1}{k}}t}$

Consider using

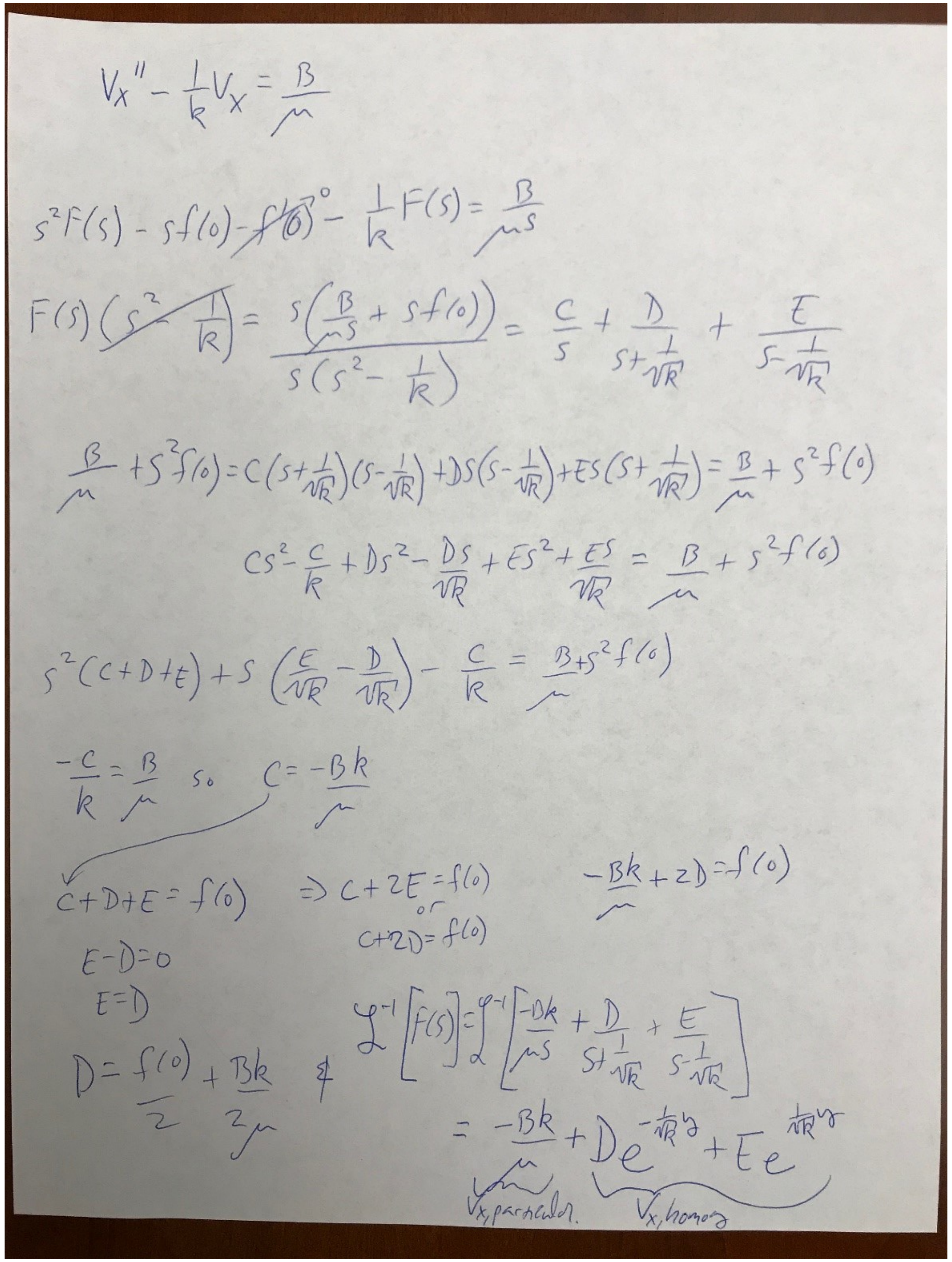
- Laplace
- Undetermined coefficients

Laplace Transformation

ransforms

	$f(t)=\mathfrak{L}^{-1}\{F(s)\}$	$F(s)=\mathfrak{L}\{f(t)\}$
1.	1	$\frac{1}{s}$
3.	$t^n, \quad n=1,2,3,\ldots$	$\frac{n!}{s^{n+1}}$
5.	$\sqrt{t}$	$\frac{\sqrt{\pi}}{2s^{\frac{3}{2}}}$
7.	$\sin(at)$	$\frac{a}{s^2+a^2}$
9.	$t\sin(at)$	$\frac{2as}{(s^2+a^2)^2}$
11.	$\sin(at)-at\cos(at)$	$\frac{2a^3}{(s^2+a^2)^2}$
13.	$\cos(at)-at\sin(at)$	$\frac{s(s^2-a^2)}{(s^2+a^2)^2}$
15.	$\sin(at+b)$	$\frac{s\sin(b)+a\cos(b)}{s^2+a^2}$
17.	$\sinh(at)$	$\frac{a}{s^2-a^2}$
19.	$\mathbf{e}^{at}\sin(bt)$	$\frac{b}{(s-a)^2+b^2}$
21.	$\mathbf{e}^{at}\sinh(bt)$	$\frac{b}{(s-a)^2-b^2}$
23.	$t^n\mathbf{e}^{at}, \quad n=1,2,3,\ldots$	$\frac{n!}{(s-a)^{n+1}}$
25.	$u_c(t)=u(t-c)$ **Heaviside Function**	$\frac{\mathbf{e}^{-cs}}{s}$
27.	$u_c(t)f(t-c)$	$\mathbf{e}^{-cs}F(s)$
29.	$\mathbf{e}^{ct}f(t)$	$F(s-c)$
31.	$\frac{1}{t}f(t)$	$\int_s^\infty F(u)\,du$
33.	$\int_0^t f(t-\tau)g(\tau)\,d\tau$	$F(s)G(s)$
35.	$f'(t)$	$sF(s)-f(0)$
37.	$f^{(n)}(t)$	$s^nF(s)-s^{n-1}f(0)-s^{n-2}f'(0)\cdots-sf^{(n-2)}(0)-f^{(n-1)}(0)$

	$f(t)=\mathfrak{L}^{-1}\{F(s)\}$	$F(s)=\mathfrak{L}\{f(t)\}$
2.	$\mathbf{e}^{at}$	$\frac{1}{s-a}$
4.	$t^p, p>-1$	$\frac{\Gamma(p+1)}{s^{p+1}}$
6.	$t^{n-\frac{1}{2}}, \quad n=1,2,3,\ldots$	$\frac{1\cdot3\cdot5\cdots(2n-1)\sqrt{\pi}}{2^n s^{n+\frac{1}{2}}}$
8.	$\cos(at)$	$\frac{s}{s^2+a^2}$
10.	$t\cos(at)$	$\frac{s^2-a^2}{(s^2+a^2)^2}$
12.	$\sin(at)+at\cos(at)$	$\frac{2as^2}{(s^2+a^2)^2}$
14.	$\cos(at)+at\sin(at)$	$\frac{s(s^2+3a^2)}{(s^2+a^2)^2}$
16.	$\cos(at+b)$	$\frac{s\cos(b)-a\sin(b)}{s^2+a^2}$
18.	$\cosh(at)$	$\frac{s}{s^2-a^2}$
20.	$\mathbf{e}^{at}\cos(bt)$	$\frac{s-a}{(s-a)^2+b^2}$
22.	$\mathbf{e}^{at}\cosh(bt)$	$\frac{s-a}{(s-a)^2-b^2}$
24.	$f(ct)$	$\frac{1}{c}F\left(\frac{s}{c}\right)$
26.	$\delta(t-c)$ **Dirac Delta Function**	$\mathbf{e}^{-cs}$
28.	$u_c(t)g(t)$	$\mathbf{e}^{-cs}\mathfrak{L}\{g(t+c)\}$
30.	$t^nf(t), \quad n=1,2,3,\ldots$	$(-1)^nF^{(n)}(s)$
32.	$\int_0^t f(v)\,dv$	$\frac{F(s)}{s}$
34.	$f(t+T)=f(t)$	$\frac{\int_0^T \mathbf{e}^{-st}f(t)\,dt}{1-\mathbf{e}^{-sT}}$
36.	$f''(t)$	$s^2F(s)-sf(0)-f'(0)$



$$V_x'' - \frac{1}{k}V_x = \frac{B}{\mu}$$

$$s^2F(s) - sf(0) - \cancelto{0}{f'(0)} - \frac{1}{k}F(s) = \frac{B}{\mu s}$$

$$F(s)\cancel{\left(s^2 - \frac{1}{k}\right)} = \frac{s\left(\frac{B}{\mu s} + sf(0)\right)}{s\left(s^2 - \frac{1}{k}\right)} = \frac{C}{s} + \frac{D}{s+\frac{1}{\sqrt{k}}} + \frac{E}{s-\frac{1}{\sqrt{k}}}$$

$$\frac{B}{\mu} + s^2f(0) = C\left(s+\frac{1}{\sqrt{k}}\right)\left(s-\frac{1}{\sqrt{k}}\right) + Ds\left(s-\frac{1}{\sqrt{k}}\right) + Es\left(s+\frac{1}{\sqrt{k}}\right) = \frac{B}{\mu} + s^2f(0)$$

$$Cs^2 - \frac{C}{k} + Ds^2 - \frac{Ds}{\sqrt{k}} + Es^2 + \frac{Es}{\sqrt{k}} = \frac{B}{\mu} + s^2f(0)$$

$$s^2(C+D+E) + s\left(\frac{E}{\sqrt{k}} - \frac{D}{\sqrt{k}}\right) - \frac{C}{k} = \frac{B}{\mu} + s^2f(0)$$

$-\frac{C}{k} = \frac{B}{\mu}$ so $C = -\frac{Bk}{\mu}$

$C+D+E = f(0)$ $\Rightarrow C + 2E = f(0)$ or $C+2D = f(0)$ $\quad -\frac{Bk}{\mu} + 2D = f(0)$

$E - D = 0$

$E = D$

$D = \frac{f(0)}{2} + \frac{Bk}{2\mu}$ \& $\mathcal{L}^{-1}\left[F(s)\right] = \mathcal{L}^{-1}\left[\frac{-Bk}{\mu s} + \frac{D}{s+\frac{1}{\sqrt{k}}} + \frac{E}{s-\frac{1}{\sqrt{k}}}\right]$

$$= \underbrace{\frac{-Bk}{\mu}}_{V_{x,\text{particular}}} + \underbrace{De^{-\frac{1}{\sqrt{k}}y} + Ee^{\frac{1}{\sqrt{k}}y}}_{V_{x,\text{homog}}}$$

Laplace gives you both the homog. and particular solns.

Undetermined Coefficients

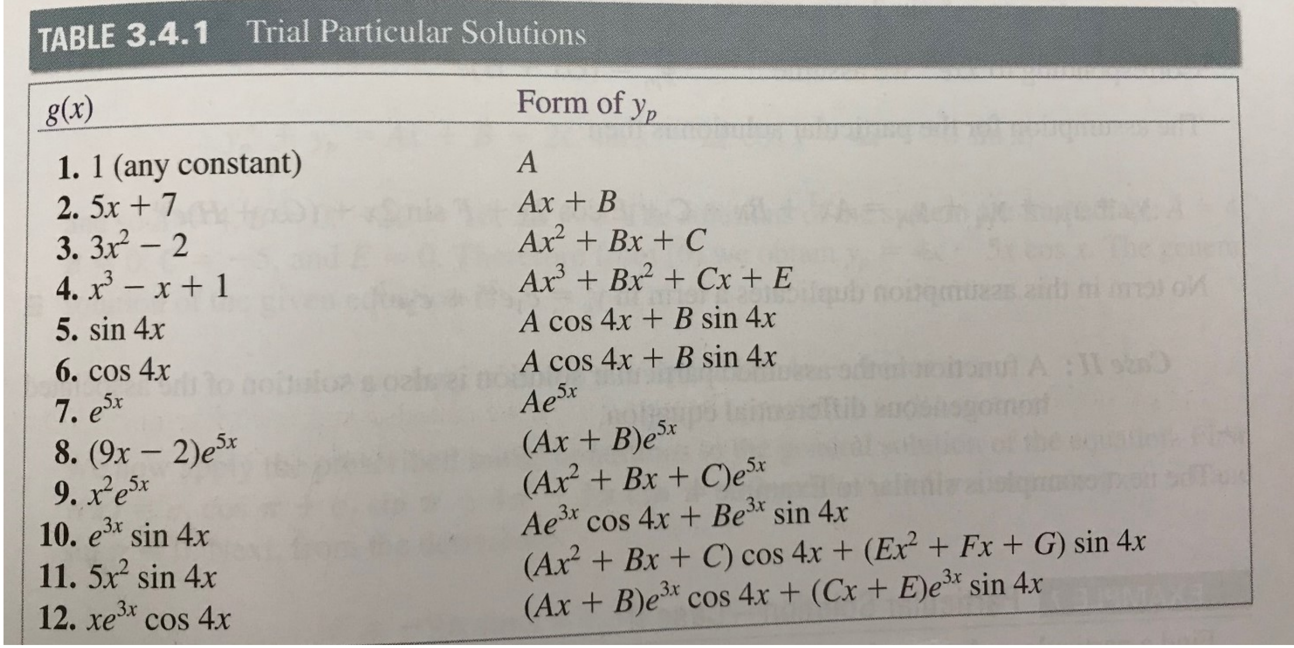
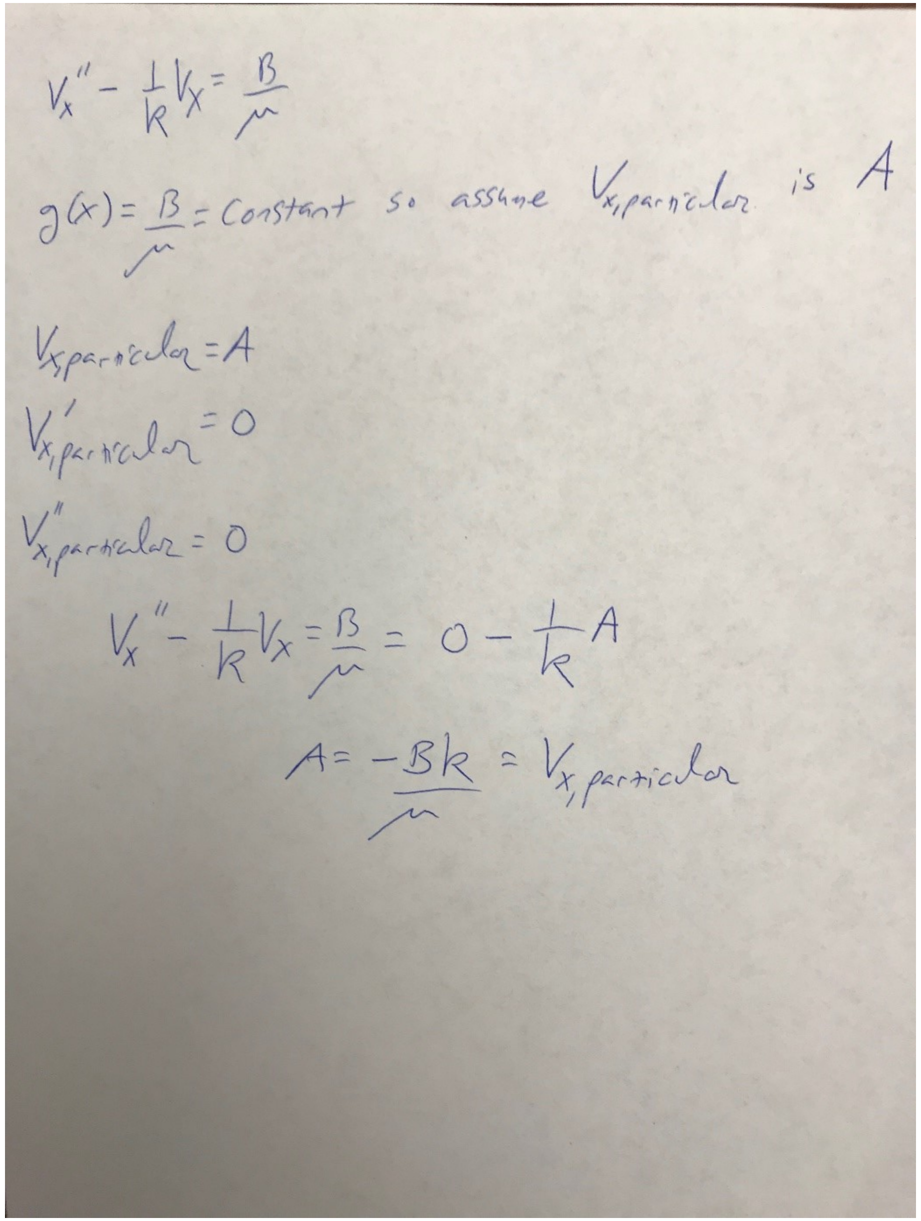


TABLE 3.4.1 Trial Particular Solutions

$g(x)$	Form of y_p
1. 1 (any constant)	A
2. $5x + 7$	$Ax + B$
3. $3x^2 - 2$	$Ax^2 + Bx + C$
4. $x^3 - x + 1$	$Ax^3 + Bx^2 + Cx + E$
5. $\sin 4x$	$A \cos 4x + B \sin 4x$
6. $\cos 4x$	$A \cos 4x + B \sin 4x$
7. e^{5x}	Ae^{5x}
8. $(9x - 2)e^{5x}$	$(Ax + B)e^{5x}$
9. x^2e^{5x}	$(Ax^2 + Bx + C)e^{5x}$
10. $e^{3x} \sin 4x$	$Ae^{3x} \cos 4x + Be^{3x} \sin 4x$
11. $5x^2 \sin 4x$	$(Ax^2 + Bx + C) \cos 4x + (Ex^2 + Fx + G) \sin 4x$
12. $xe^{3x} \cos 4x$	$(Ax + B)e^{3x} \cos 4x + (Cx + E)e^{3x} \sin 4x$



$$V_x'' - \frac{1}{k}V_x = \frac{B}{\mu}$$

$g(x) = \frac{B}{\mu}$ = Constant so assume $V_{x,\text{particular}}$ is A

$$V_{x,\text{particular}} = A$$

$$V'_{x,\text{particular}} = 0$$

$$V''_{x,\text{particular}} = 0$$

$$V_x'' - \frac{1}{k}V_x = \frac{B}{\mu} = 0 - \frac{1}{k}A$$

$$A = -\frac{Bk}{\mu} = V_{x,\text{particular}}$$

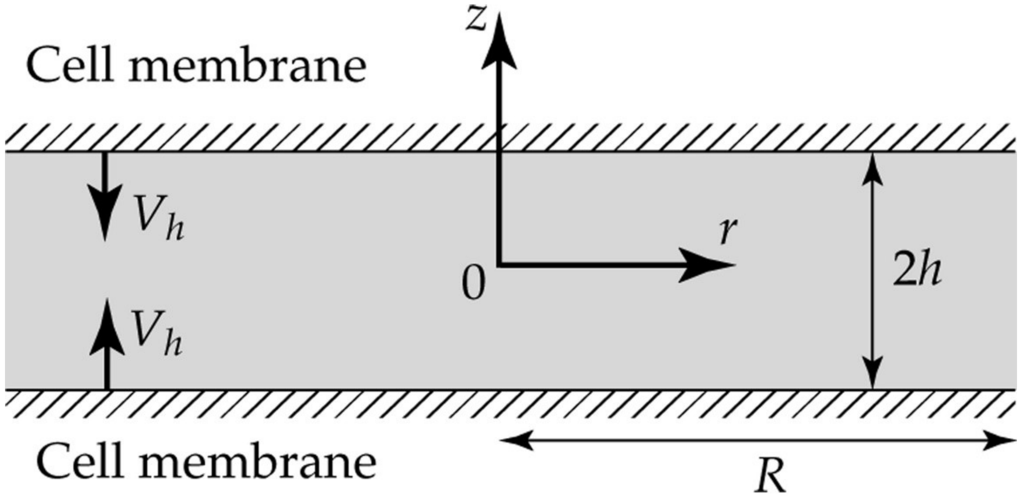
This method is only for calculating the particular solution

This is the end of example 8.7

Squeeze Flow

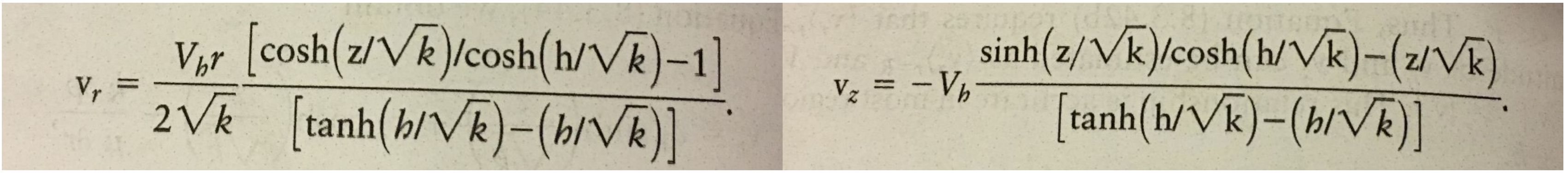
- Squeeze flow is the fluid flow caused by the relative movement of solid boundaries towards each other
- Tissue deformation causes change in volume fraction of the interstitial space
    - Leads to fluid flow

Squeeze Flow



- Vh is the velocity of cell membrane movement
- R is the radius of the plate
- z and r are cylindrical coordinates
- Vr is velocity in the r direction
- Vz is velocity in the z direction

- These equations will be more useful and will make more sense in later discussions The derivation of them is in 8.3.3
- Velocity profiles:



$$v_r = \frac{V_h r}{2\sqrt{k}} \frac{\left[\cosh(z/\sqrt{k})/\cosh(h/\sqrt{k}) - 1\right]}{\left[\tanh(h/\sqrt{k}) - (h/\sqrt{k})\right]}.$$

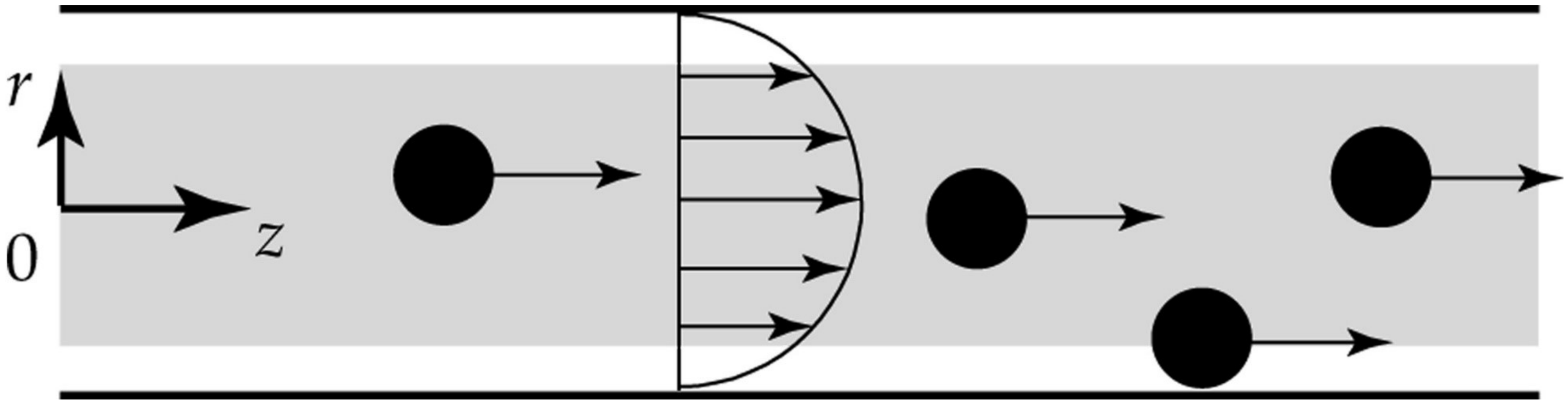
$$v_z = -V_h \frac{\sinh(z/\sqrt{k})/\cosh(h/\sqrt{k}) - (z/\sqrt{k})}{\left[\tanh(h/\sqrt{k}) - (h/\sqrt{k})\right]}.$$

8.4 Solute Transport in Porous Media

8.4.1-8.4.2

8.4.1 General Considerations

- Solute Transport in Porous Media



8.4.1 General Considerations

- There are 4 general problems using the continuum approach(Darcy’s Law) for analyzing transport of solutes through porous media

1)D_{eff}

2) Solute velocity

3) Dispersion

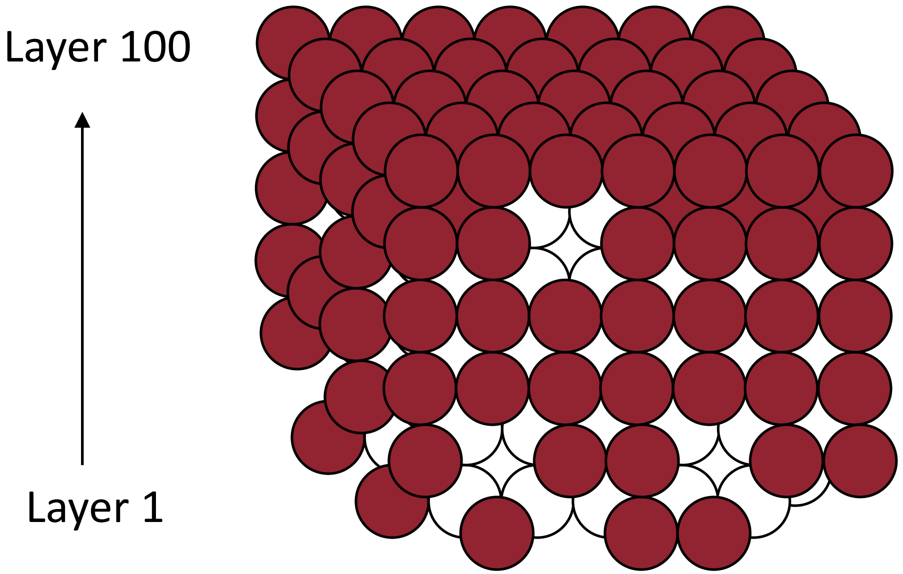
4) Boundary Conditions

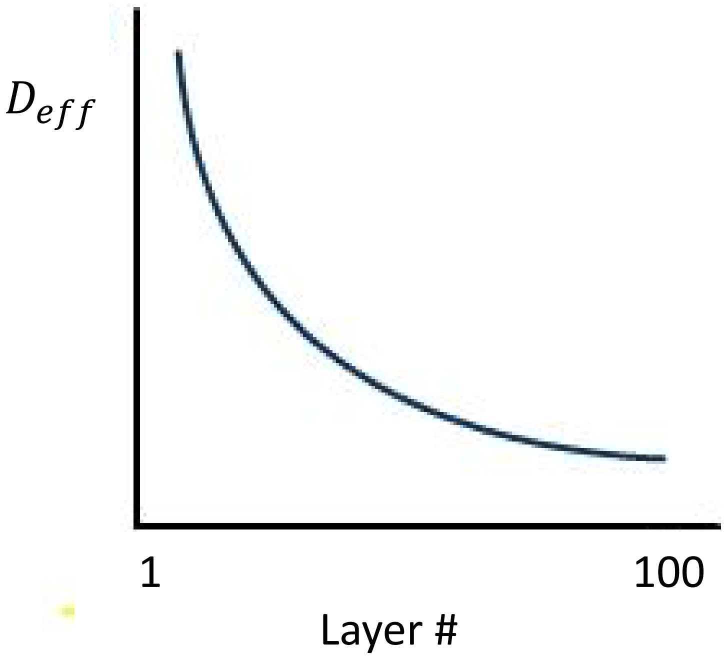
1) D_{eff}

- Diffusion of solutes is characterized by the effective diffusion coefficient: D_{eff}
- D_{eff} in porous media < D_{eff} in solutions Why?...

1) D_{eff} cont.

- Factor effecting Diffusion in Porous Media:
  - Connectedness of Pores





As we near layer 100, available space for diffusion and D_{eff} decrease exponentially

2) Solute Velocity

- Convective velocities ≠ Solvent velocities
  - Solutes are hindered by porous structures
    - Ex: filtering coffee grounds

$$f = \frac{v_s}{v_f} = \frac{solute\ velocity}{solvent\ velocity}$$

f is retardation coefficient

2) Solvent Velocity cont.

- $\sigma = 1 - f$: reflection coefficient
  - Characterizes the hindrance of convective transport across a membrane

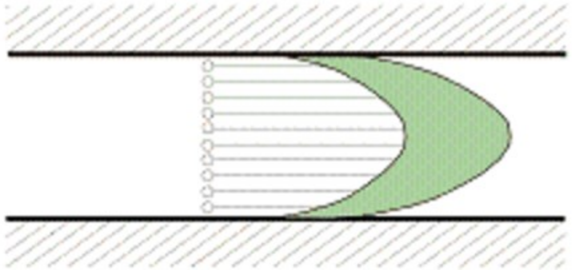
- f is dependent on:
  - Fluid velocity
  - Solute size
  - Pore Structure

- Flux of Convective transport across tissue:

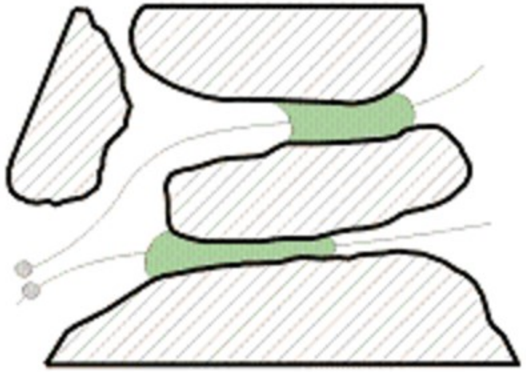
$$N_s = v_s C = f v_f C$$

Where v_s is solute velocity and C is local concentration of solutes

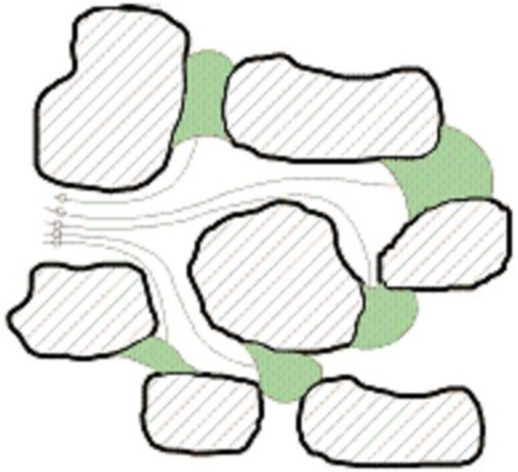
3) Dispersion of Solutes



(a) Velocity variation inside pore



(b) Variation of pore diameter



(c) Variation of direction of pore

4) Boundary Conditions

- Concentrations of solutes can be discontinuous at interfases between solutions and porous media
  - Thus, for two regions, 1 and 2

$$N_1 = N_2$$

N = flux

and

$$\frac{C_1}{K_{AA1}} = \frac{C_2}{K_{AA2}}$$

K_{AA} = area fraction available at interphase for solute transport

When all 4 are considered…

Governing Equation for Transport of neutral molecule through porous media:

$$\frac{\partial C}{\partial t} + \underbrace{\nabla\left(f v_f C\right)}_{\text{Flux of Convective Transport}} = \underbrace{D_{eff}}_{\substack{\text{Isotropic, uniform}\\ \text{and dispersion}\\ \text{coefficient is}\\ \text{negligible}}} \nabla^2 C + \underbrace{\phi_B - \phi_L}_{\text{Solute vel.}} + \underbrace{Q}_{\text{Reaction}}$$

negligible → If we do consider dispersion coefficient:
Deff = Deff + Disp. Coeff.

Governing Equation cont.

$$\frac{\partial C}{\partial t} + \nabla\left(f v_f C\right) = D_{eff}\nabla^2 C + \phi_B - \phi_L + Q$$

$$C, \phi_B, \phi_L, Q: \frac{avg.quantity}{unit\ tissue\ volume}$$

$$f, v_f, D_{eff}: \frac{avg.quantity}{unit\ volume\ of\ fluid\ phase}$$

8.4.2 Effective Diffusion Coefficient in Hydrogels

- 3 Factors effecting D_{eff} of uncharged solutes in hydrogels:
  - 1) Diffusion coefficient of solutes in WATER (D_0)
  - 2) **Hydrodynamic Interactions** between solute and surrounding solvent molecules, F
  - 3) **Tortuosity** of diffusion pathways due to the steric exclusion of solutes in the matrix, S

$$D_{eff} = D_0 F S$$

So, how do we solve for F and S?

Hydrodynamic Interactions, F

F is a ratio:

$$F = \frac{friction\ coeff.of\ solute\ in\ porous\ media}{friction\ coeff.of\ solute\ in\ water}$$

→Friction coeff. in water = $6\pi\mu r_s$

$$\mu = viscocity$$
$$r_s = radius\ of\ molecule$$

F measures the enhancement of drag on solute molecule due to presence of polymeric fibers in water

Hydrodynamic Interactions, F cont.

Two approaches to determining F:

1) Effective-medium or Brinkman-medium

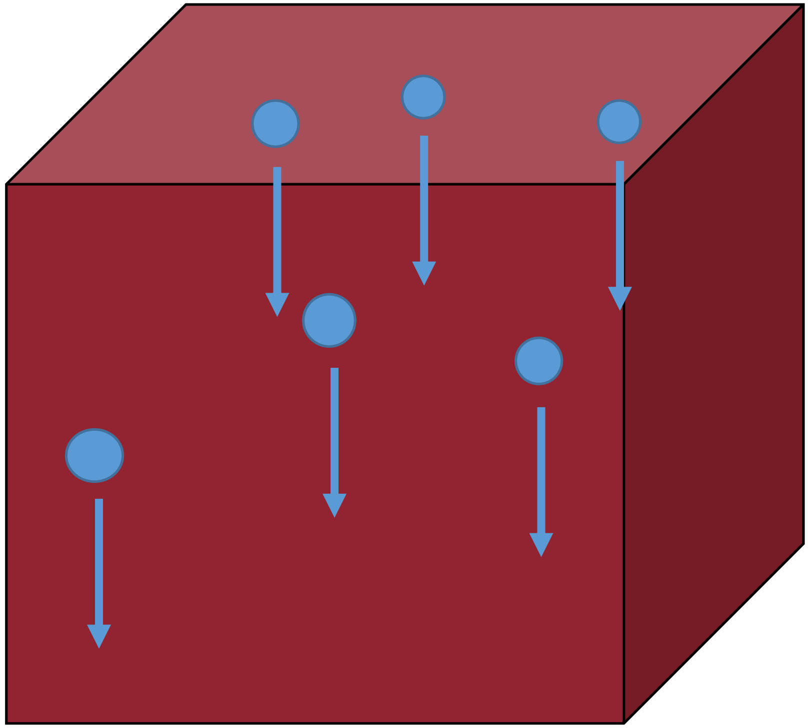
2) 3-D space with cylindrical fibers model

1) Effective-Medium or Brinkman-Medium

- Assumptions:
  - Hydrogel is a uniform medium
  - Spherical solute molecule
  - Constant velocity
  - Movement governed by Brinkman Equation

$$F = \left[1 + \frac{r_s}{\sqrt{k}} + \frac{1}{9}\left(\frac{r_s}{\sqrt{k}}\right)^2\right]^{-1}$$

where $\phi_B = \phi_L = 0$

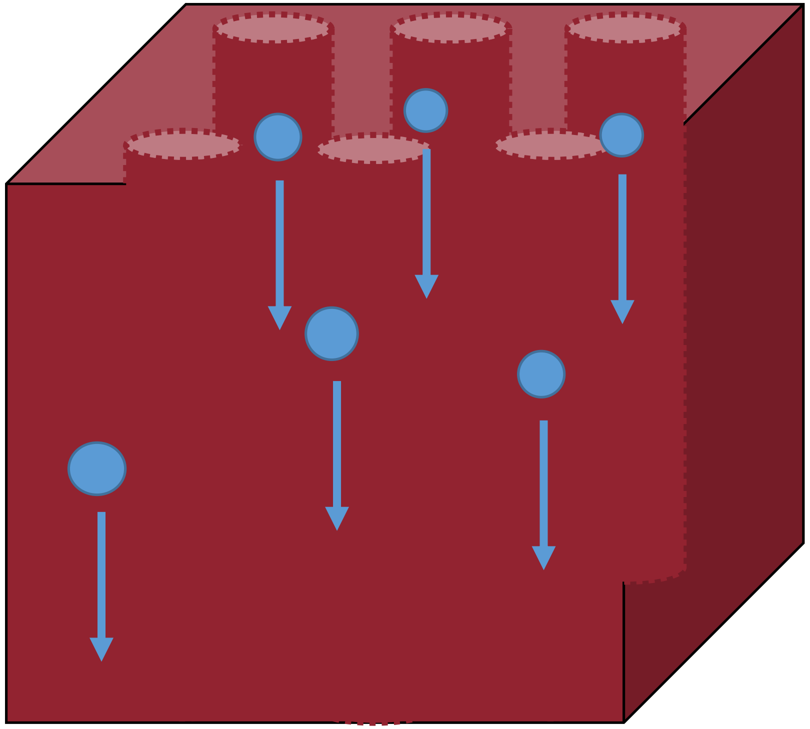


2) 3-D space with cylindrical fibers model

- Assumptions:
  - Hydrogel is modeled as 3-D spaces filled with water and randomly placed cylindrical fibers
  - Movement of spherical particles is determined by Stokes-Einstein Equation

$F(\alpha, \theta) = \exp(-a_1 \theta^{a_2})$ pg. 426

→done after normalization of $6\pi\mu r_s$



2) 3-D space with cylindrical fibers model cont.

$$F(\alpha, \theta) = \exp(-a_1 \theta^{a_2})$$

Depends on:

$$\alpha = \frac{fiber\ radii}{solute\ radii}$$

$$\theta = \frac{fiber\ volume}{hydrogel\ volume}$$

Where: $a_1 = 3.272 \ - 2.460\alpha + 0.822\alpha^2$

$a_2 = 0.358 + 0.366\alpha - 0.0939\alpha^2$

Tortuosity Factor, S

- Depends on f_a

$$f_a = (1 + \frac{1}{\alpha})^2$$

- f_a is the excluded volume fraction of solute in hydrogel if:
  - Low fiber density
  - Fibers arranged in parallel manner
  - If $f_a < 0.7$

$$S(\alpha, \theta) = exp\left[-0.84 {f_a}^{1.09}\right]$$

Effective Diffusion Coefficient: In Liquid-Filled Pore and Biological Tissue

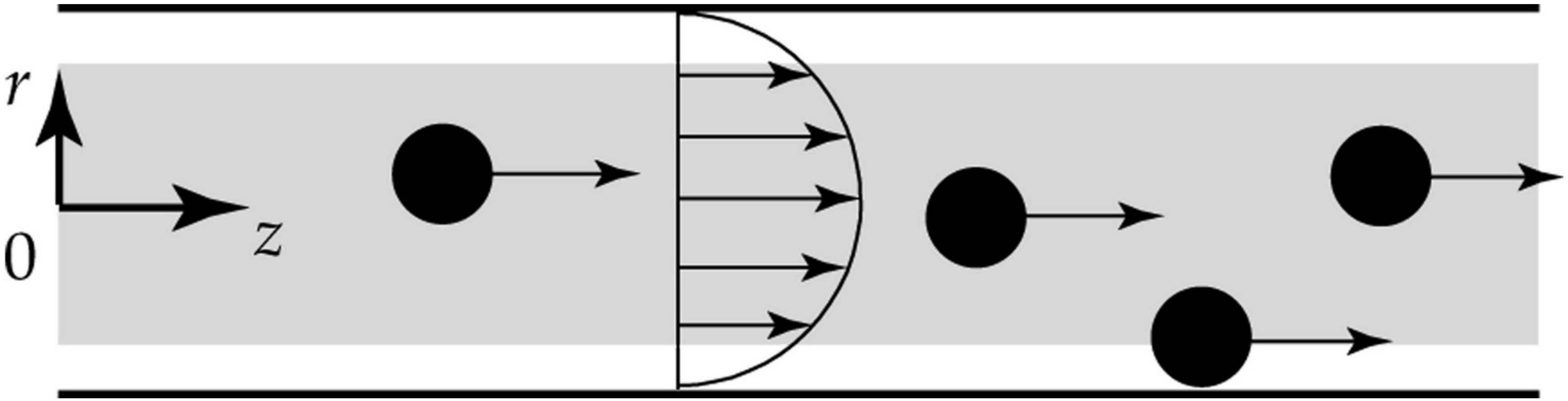
Chapter 8: Section 4.3-4.4

Effective Diffusion Coefficient in a Liquid-Filled Pore

- Depends on diffusion coefficient D_0 of solutes in water, hydrodynamic interactions between solute and solvent molecules, and steric exclusion of solutes near the walls of pores
- Assume entrance effect is negligible:

$$v_z = 2v_m(1 - \frac{r}{R})^2$$

v_z is the axial fluid velocity
v_m is the mean velocity in the pore
r is the radial coordinate
R is the radii of the cylinder



- Assume the volume fraction of spherical solutes is less than $\frac{2\lambda}{3}$

$$\lambda = \frac{a}{R}$$

a is the radii of the solute
R is the radii of the cylinder

- Solute-Solute interactions become negligible
- When λ ->0, solute-pore interactions are negligible

$$N_z = -D_0 \frac{\partial C}{\partial z} + C v_z$$

N_z is the flux
D_0 is the diffusion coefficient
C is the solute concentration
z is the axial coordinate

$$C = \begin{cases} C(z) & 0 \leq r \leq R - a \\ 0 & R - a < r \leq R \end{cases}$$

When λ does not approach 0:

$$N_s = -\frac{D_0}{K}\frac{dC}{dz} + GCv_z$$

K is the enhanced friction coefficient
G is the lag coefficient
K and G are functions of λ and r/R

Flux averaged over the entire cross-sectional area:

$$\overline{N}_s = \frac{2}{R^2}\int_0^R N_s r dr$$

Integrating the top flux equation:

$$\overline{N}_s = -HD_0\frac{dC}{dz} + WCv_m$$

H and W are called hydrodynamic resistance coefficients

$$H = \frac{2}{R^2} \int_0^{R-a} \frac{1}{K} r dr$$

$$W = \frac{4}{R^2} \int_0^{R-a} G \left[1 - \left(\frac{r}{R} \right)^2 \right] r dr$$

$$D_{eff} = H D_0$$

Centerline approximation: assume all spheres are distributed on the centerline position in the pore
For $\lambda < 0.4$:

$$K^{-1}(\lambda, 0) = 1 - 2.1044\lambda + 2.089\lambda^3 - 0.948\lambda^5$$

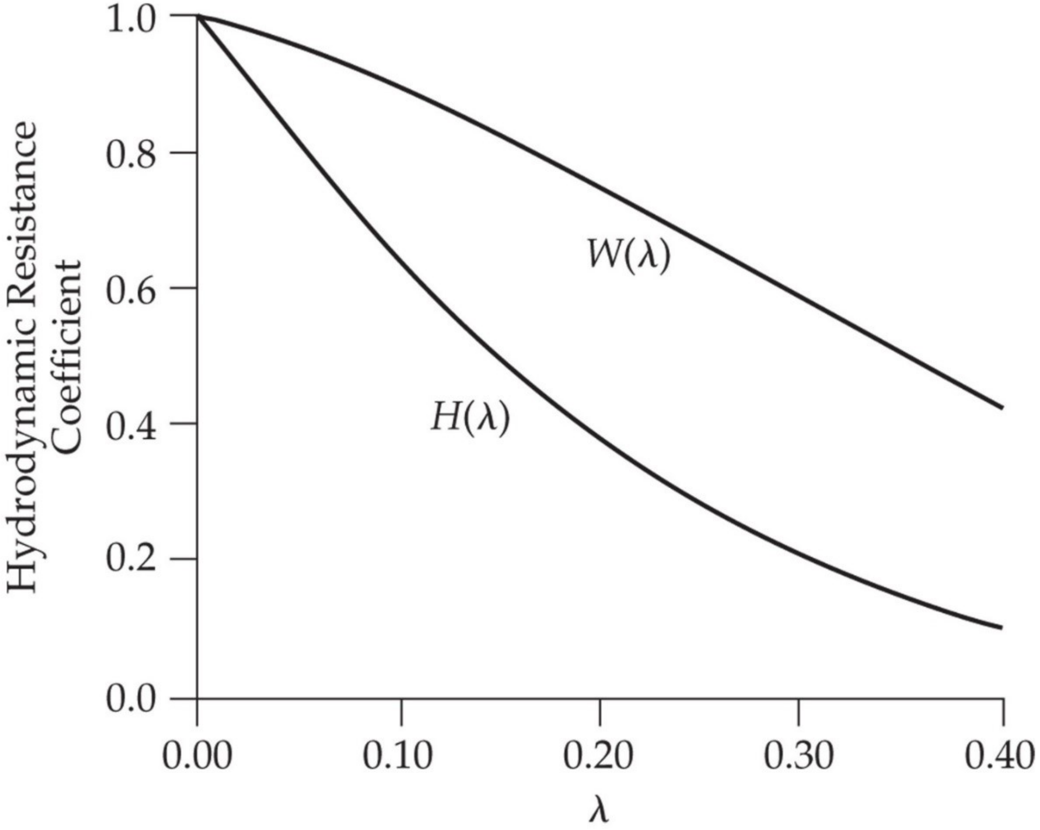
$$G(\lambda, 0) = 1 - \frac{2}{3}\lambda^2 - 0.163\lambda^3$$

$$H(\lambda) = \Phi(1 - 2.1044\lambda + 2.089\lambda^3 - 0.948\lambda^5)$$

$$W(\lambda) = \Phi(2 - \Phi)\left(1 - \frac{2}{3}\lambda^2 - 0.163\lambda^3\right)$$

Partition coefficient of solute in the pore: $\Phi = (1 - \lambda)^2$

For $\lambda > 0.4$:



Diffusion of spherical molecules between parallel plates:

$$\bar{N}_s = -HD_0 \frac{dC}{dz} + WCv_m$$

$$\bar{N}_s = \frac{1}{h}\int_0^h N_s dy$$

$$H = \frac{1}{h}\int_0^{h-a} \frac{1}{K} dy$$

h is the half-width of the slit

$$W = \frac{3}{2h}\int_0^{h-a} G\left[1-\left(\frac{y}{h}\right)^2\right] dy$$

$$D_{eff} = HD_0$$

K and G depend on λ and y/h

$$H(\lambda) = \Phi[1 - 1.004\lambda + 0.418\lambda^3 + 0.21\lambda^4 - 0.169\lambda^5 + O\lambda^6]$$

$$\Phi = 1 - \lambda$$

$$W(\lambda) = \frac{\Phi}{2}(3-\Phi^2)\left[1-\frac{1}{3}\lambda^2 + O\lambda^3\right]$$

Effective Diffusion Coefficient in Biological Tissues

$$D_{eff} = b_1(M_r)^{-b_2}$$

M_r is the molecular weight of the solutes
b_1 and b_2 are functions of charge and shape of solutes, and structures of tissues

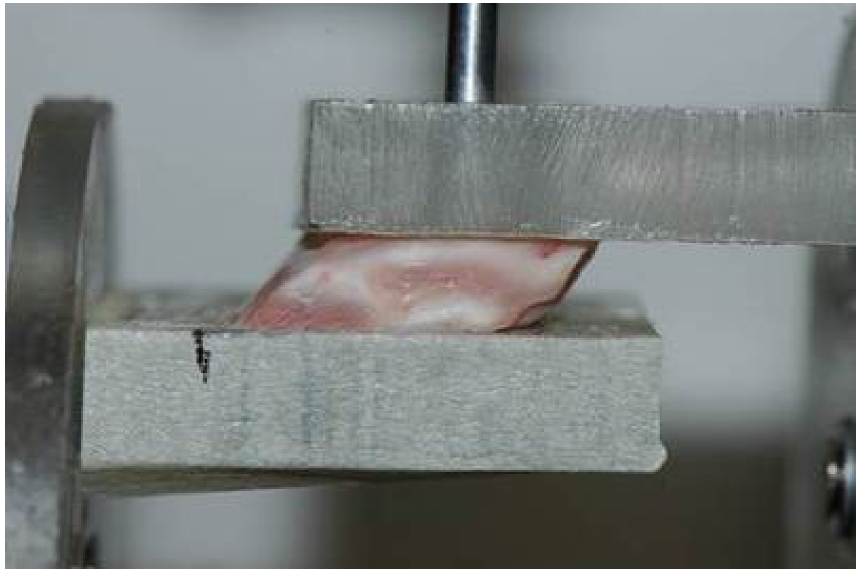
The effects of tissue structures on D_{eff} increases with the size of solutes

Fluid Transport in Poroelastic Materials

Section 8.5

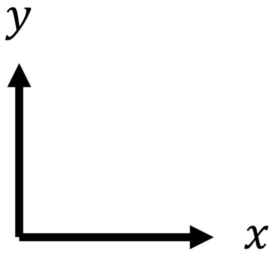
Biological Tissues:

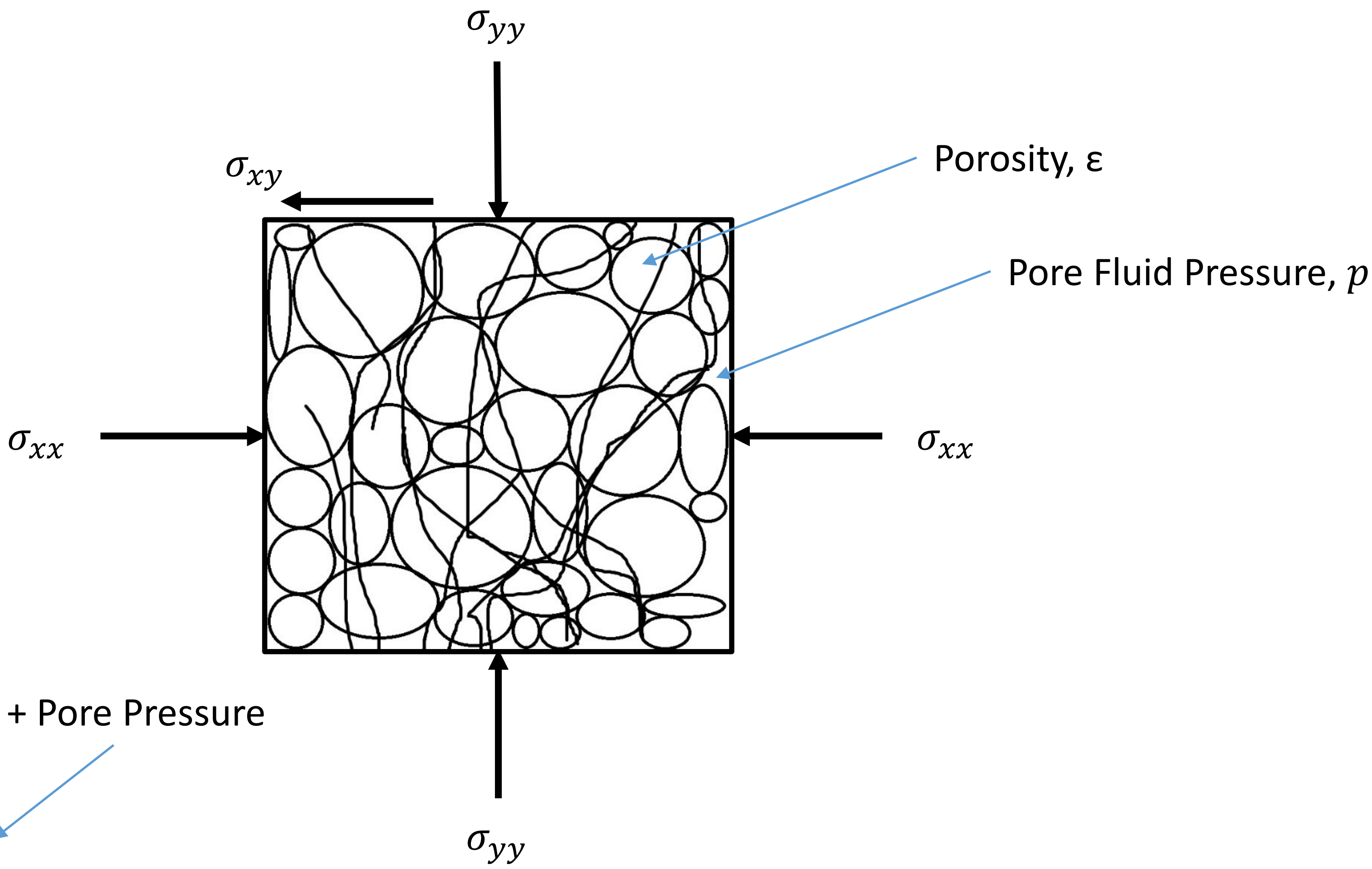
- Deformable
- Deformation can be linear or nonlinear



"*Extreme softness of brain matter in simple shear*"”

Poroelastic Response





Total Stress = Effective Stress + Pore Pressure

$$\boldsymbol{\sigma} = \boldsymbol{\tau} + p\boldsymbol{I}$$

Understanding the linear function of Stress

If,

$$\boldsymbol{I} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

then,

$$\boldsymbol{\sigma} = \begin{bmatrix} \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \tau_{zz} \end{bmatrix} + \begin{bmatrix} p & 0 & 0 \\ 0 & p & 0 \\ 0 & 0 & p \end{bmatrix} = \overbrace{\underbrace{2\mu_G \boldsymbol{E} + \mu_\lambda e\boldsymbol{I}}_{\text{Must be describing stresses that are NOT pore pressure related}}}^{} + p\boldsymbol{I}$$

Understanding the linear Function of Stress

$$\boldsymbol{\sigma} = \underbrace{2\mu_G \boldsymbol{E} + \mu_\lambda e\boldsymbol{I}} + p\boldsymbol{I}$$

We know this is pore pressure, and this is the only force happening INTERNALLY, right?

Then, these two terms must be describing the forces EXTERNALLY. How many external forces are there? Shear and Normal. Which term is which?

We must look at the *Lamé constants*…

LamÉ Constants

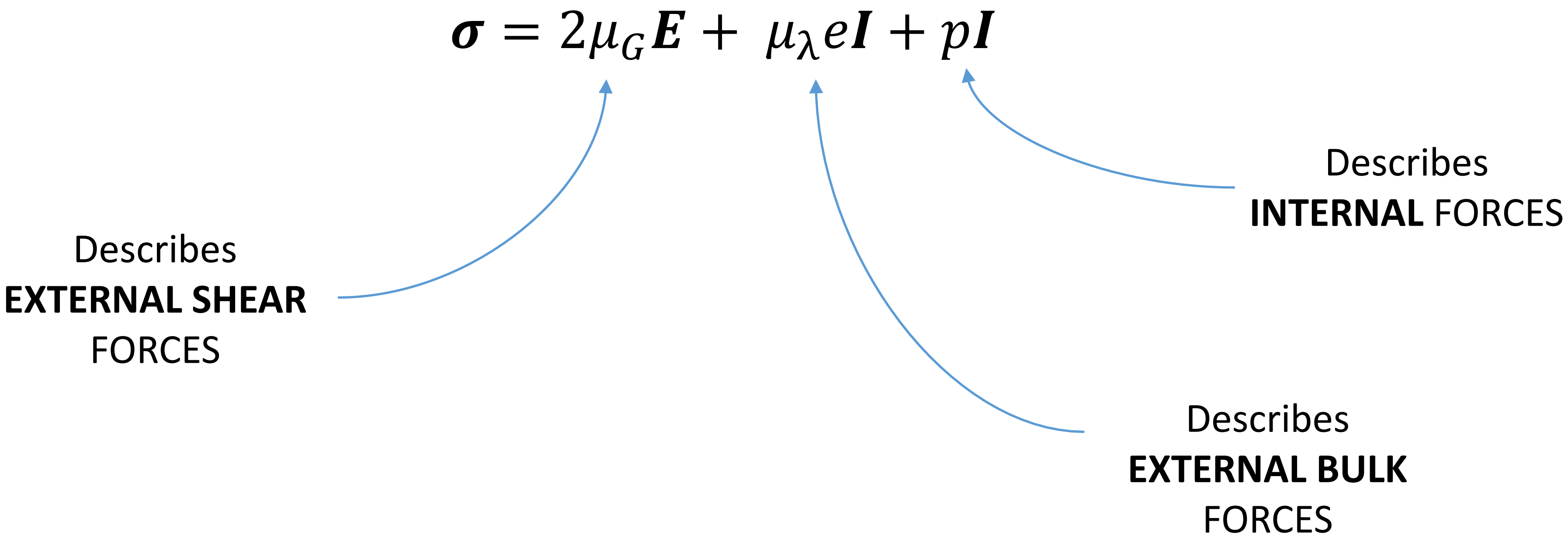
- Named after French Mathematician, Gabriel Lamé
- Two constants which relate stress to strain in isotropic, elastic material
- Depend on the material and its temperature

$$\mu_\lambda = K - {}^{2}/_{3}\, \mu_G$$

μ_λ : first parameter (related to bulk modulus)
μ_G : second parameter (related to shear modulus)

$$\mu_G = \frac{\tau}{\gamma} = \frac{\frac{\Delta F}{A}}{\frac{\Delta L}{L}}$$

Understanding the linear Function of Stress



$$\boldsymbol{\sigma} = 2\mu_G \boldsymbol{E} + \mu_\lambda e\boldsymbol{I} + p\boldsymbol{I}$$

Describes
EXTERNAL SHEAR
FORCES

Describes
EXTERNAL BULK
FORCES

Describes
INTERNAL FORCES

Now we need to understand E
and e…

Understanding the linear Function of Stress

- E = strain tensor (vector gradient) $E = \frac{1}{2}[\nabla u + (\nabla u)^T]$

$$\nabla u = \left(\frac{\partial u_x}{\partial x}, \frac{\partial u_y}{\partial y}, \frac{\partial u_z}{\partial z}\right)$$

$$(\nabla u)^T = \begin{pmatrix} \frac{\partial u_x}{\partial x} \\ \frac{\partial u_y}{\partial y} \\ \frac{\partial u_z}{\partial z} \end{pmatrix}$$

$$\longrightarrow$$

$$E = \frac{1}{2}\begin{bmatrix} 2\frac{\partial u_x}{\partial x} & \frac{\partial u_y}{\partial y} + \frac{\partial u_x}{\partial x} & \frac{\partial u_z}{\partial z} + \frac{\partial u_x}{\partial x} \\ \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} & 2\frac{\partial u_y}{\partial y} & \frac{\partial u_z}{\partial z} + \frac{\partial u_y}{\partial y} \\ \frac{\partial u_x}{\partial x} + \frac{\partial u_z}{\partial z} & \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} & 2\frac{\partial u_z}{\partial z} \end{bmatrix}$$

- e = volume dilation (scalar divergence)

$$e = Tr(E) = \nabla \cdot u$$

$$e = \nabla \cdot u = \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z}$$

Understanding the linear Function of Stress

- So now we understand this:

$$\boldsymbol{\sigma} = 2\mu_G \boldsymbol{E} + \ \mu_\lambda e\boldsymbol{I} + p\boldsymbol{I}$$

A tensor that's in units of stress

A scalar quantity that's multiplied by the identify matrix to make a tensor in units of pressure

A scalar quantity that's multiplied by the identify matrix to make a tensor in units of stress

Now we can reduce mass conservation equations to get an equation we can use to solve problems like these! ☺

Deriving mass and Momentum equations

mass conservation in the fluid phase is this:

$$\frac{\partial(\rho_f \varepsilon)}{\partial t} + \nabla \cdot \left(\rho_f \varepsilon v_f\right) = \rho_f(\phi_B - \phi_L)$$

mass conservation in the solid phase is this:

$$\frac{\partial[\rho_s(1-\varepsilon)]}{\partial t} + \nabla \cdot \left(\rho_s(1-\varepsilon)\frac{\partial \boldsymbol{u}}{\partial t}\right) = 0$$

Deriving mass and Momentum equations

Summing the two equations together:

$$\frac{\partial(\rho_f \varepsilon)}{\partial t} + \nabla \cdot \left(\rho_f \varepsilon v_f\right) - \rho_f(\phi_B - \phi_L) = \frac{\partial[\rho_s(1-\varepsilon)]}{\partial t} + \nabla \cdot \left(\rho_s(1-\varepsilon)\frac{\partial \boldsymbol{u}}{\partial t}\right)$$

$$\cancel{\frac{\partial(\rho_f \varepsilon)}{\partial t}} + \nabla \cdot \left(\cancel{\rho_f} \varepsilon v_f\right) - \nabla \cdot \left(\cancel{\rho_s}(1-\varepsilon)\frac{\partial \boldsymbol{u}}{\partial t}\right) = \cancel{\frac{\partial[\rho_s(1-\varepsilon)]}{\partial t}} + \cancel{\rho_f}(\phi_B - \phi_L)$$

$$\boxed{\nabla \cdot \left(\left(\varepsilon v_f\right) - \left((1-\varepsilon)\frac{\partial \boldsymbol{u}}{\partial t}\right)\right) = (\phi_B - \phi_L)}$$

Biot Law

- According to a paper written in 1984 (that I do not have access too):

$$\boxed{\varepsilon\left(\left(v_f\right) - \left(\frac{\partial \boldsymbol{u}}{\partial t}\right)\right) = -K\nabla p}$$

$$\boxed{\nabla \cdot \boldsymbol{\sigma} = 0}$$

- Zienkiewicz, O. C., and T. Shiomi. "Dynamic behaviour of saturated porous media; the generalized Biot formulation and its numerical solution." *International journal for numerical and analytical methods in geomechanics* 8.1 (1984): 71-96.

Using BIOTS law to substitute…

$$\boldsymbol{\nabla} \cdot \boldsymbol{\sigma} = \mu_G \nabla^2 \boldsymbol{u} + \ (\mu_G + \mu_\lambda)\nabla e + \nabla p = \mathbf{0}$$

$$\boxed{(2\mu_G + \mu_\lambda)\nabla^2 e = \nabla^2 p}$$

If volume dilation and hydraulic conductivity are homogenous

$$\varepsilon\left((\nabla\cdot v_f)-\left(\frac{\partial \boldsymbol{e}}{\partial t}\right)\right)=-K\nabla^2 p$$

$$\frac{\partial \boldsymbol{e}}{\partial t}=\underbrace{K\nabla^2 p}+(\phi_B-\phi_L)$$

$$\boxed{\frac{\partial \boldsymbol{e}}{\partial t}=\underbrace{K(2\mu_G+\mu_\lambda)}_{\text{Coefficient of consolidation}}\nabla^2 e+(\phi_B-\phi_L)}$$