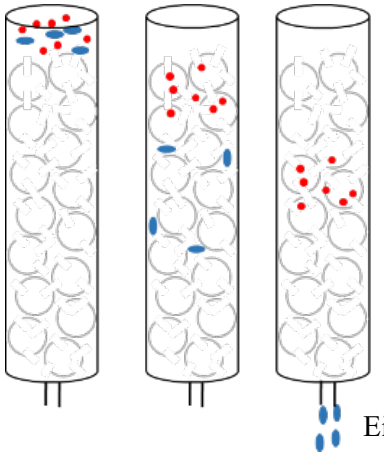
ChE 333 Transport Phenomena III, fundamentals of Mass Transfer
Studio Worksheet #4 Liquid diffusion

NAME_____

Studio Section	**Studio 12:00-12:50**	**Studio 13:00-13:50**	**Studio 14:00-14:50**	**Studio 15:00-15:50**

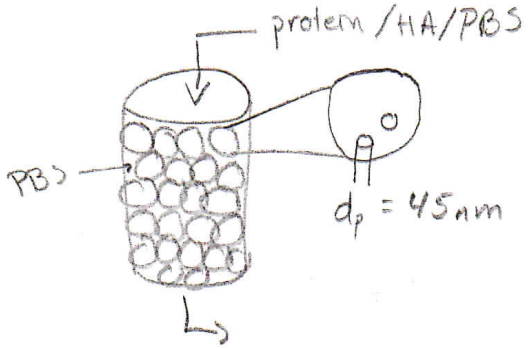
Instructions: Open book, notes, and homework. Make sure to write your name and studio on any additional sheet of paper with your solution. Show your calculation, and algebraic setup, and make sure to include units. Please turn in your studio at the end of class.

Characterization of Equine Synovial Fluid – Separation of Macromolecules
For several years the *CBEE Polymer Characterization Laboratory* has been involved with the Dr. Jill Parker of the *OSU School of Veterinary Medicine* on a project to characterize the molecular and rheological properties of equine synovial fluid. Synovial fluid is primarily responsible for the lubrication of most equine and human articular joints (knee and hip joints). Synovial fluid is composed of phosphate buffer solution (PBS), low molecular weight species (immunoglobulins), proteins, and a very large polymer molecule called *Hyaluronic Acid (HA)*, which is primarily responsible for lubrication. ***S**ize **E**xclusion **C**hromatography* (SEC) is used to characterize the molecular properties of synovial fluid and determine the size of the proteins and hyaluronic acid. SEC utilizes a packed column of semi-permeable gel particles (***G**el **P**ermeation **C**hromatography*) to separate macromolecules and here we are mainly interested in separating the *protein* and the *hyaluronic acid*.



As a first-pass approximation, you may assume that the gel particles have *cylindrical 45 nm pores*.
GPC is always run at *very dilute conditions.*
Temperature = 20 C (293 K)
Hyaluronic Acid (HA): Mw = 500,000 Daltons (g/gmole), d_s = 18nm
Protein (P): Mw = 80,000 Daltons, d_s = 8nm
Solvent: Phosphate Buffer Solution (PBS) (relative viscosity = 1.15 – compared to water at same T)
The viscosity of water = 9.90 x 10^{-4} Pa s or 0.990 cP
Boltzmann const: κ = 1.38 x 10^{-23} J/K, [1 J = 1 Pa-m^3 = 1 kg-m^2/sec^2]
Assumptions: Protein and HA may be considered rigid spheres at infinite dilution, and molecular diffusivity can be calculated using the Stokes-Einstein equation.

a) Sketch the process and state assumptions.



- assumptions
  - dilute solution
  - protein & HA rigid spheres
  - diffusion described by Stokes-Einstein
  - cylindrical pores
  - steady state
  - no reactions
  - liquid diffusion

ChE 333 Transport Phenomena III, fundamentals of Mass Transfer
Studio Worksheet #4 Liquid diffusion

b) Calculate the *molecular diffusion coefficients* for the protein (D_{AC}) and HA (D_{BC}) in PBS.

Stokes - Einstein eqn. $D_{AB} = \frac{kT}{6\pi r_A \mu_B}$

protein – PBS

$$D_{AC} = \frac{kT}{6\pi r_A \mu_c} = \frac{(1.38\times10^{-23}\ J/K)(293\ K)}{6\pi\,(4\times10^{-9}\ m)(1.14\times10^{-3}\ Pa\cdot s)} = 4.70\times10^{-11}\ m^2/s$$

$$= 4.70\times10^{-7}\ cm^2/s$$

check units: $\left[\frac{J}{K}K\frac{1}{m\cdot Pa\cdot s} = \frac{Pa\ m^3}{m\cdot Pa\cdot s} = \frac{m^2}{s}\right]$

HA – PBS

$$D_{BC} = \frac{kT}{6\pi r_B \mu_c} = \frac{(1.38\times10^{-23}\ J/K)(293)}{6\pi(9\times10^{-9}\ m)(1.14\times10^{-3}\ Pa\cdot s)} = 2.09\times10^{-11}\ m^2/s$$

$$= 2.09\times10^{-7}\ cm^2/s$$

c) Calculate the effective diffusivities (D_{Ae} and D_{Be}) due to *hindered diffusion* for the protein and HA in the porous gel particle.

$D_{Ae} = D_{AC} F_1(\varphi) F_2(\varphi)$ $\quad \varphi = d_A/d_{pore} = 8/45 = 0.18$

$F_1(0.18) = (1-0.18)^2 = 0.676$

$F_2(0.18) = 1 - 2.104(0.18) + 2.09(0.18)^3 - 0.95(0.18)^5 = 0.633$

$D_{Ae} = (4.70\times10^{-7}\ cm^2/s)(0.676)(0.633) = 2.01\times10^{-7}\ cm^2/s$

$D_{Be} = D_{BC} F_1(\varphi) F_2(\varphi)$ $\quad \varphi = d_B/d_{pore} = 18/45 = 0.4$

$F_1(0.4) = (1-0.4)^2 = 0.36$

$F_2(0.4) = 1 - 2.104(0.4) + 2.09(0.4)^3 - 0.95(0.4)^5 = 0.2824$

$D_{Be} = (2.09\times10^{-7}\ cm^2/s)(0.36)(0.2824) = 2.125\times10^{-8}\ cm^2/s$

ChE 333 Transport Phenomena III, fundamentals of Mass Transfer
Studio Worksheet #4 Liquid diffusion

d) Calculate the *separation factor* ($\alpha = D_{Ae}/D_{Be}$ and $\alpha^0 = D_{AC}/D_{BC}$) for the GPC column and the *enhancement* (α/α^0) compared to the molecular diffusivities at infinite dilution. Will using the GPC enhance the separation of the protein and the hyaluronic acid?

Separation factor:

$$\alpha = D_{Ae}/D_{Be} = \frac{2.01 \times 10^{-7}\ cm^2/s}{2.13 \times 10^{-8}\ cm^2/s} = 9.44$$

$$\alpha^0 = D_{AC}/D_{BC} = \frac{4.70 \times 10^{-7}\ cm^2/s}{2.09 \times 10^{-7}\ cm^2/s} = 2.25$$

enchancement

$$\frac{\alpha}{\alpha^0} = \frac{9.44}{2.25} = 4.20$$