Problem I/ A) FALSE; $y_{reactant} = 0 \Rightarrow$ diffusion-limited

B) FALSE; Sc equivalent of Pr

C) TRUE; $Sc = \left(\frac{\delta}{\delta_c}\right)^{1/3}$

D) FALSE; cannot say $\frac{C_f}{2} = j_H$ or $\frac{C_f}{2} = j_D$ with form drag, but $j_H = j_D$

E) TRUE;

F) TRUE

G) TRUE

H) FALSE; $x \uparrow \Rightarrow \delta_c, \delta_t \uparrow \Rightarrow k, h \downarrow$

Problem II/ A) * At interface $N_{org}|_{r=R} = N_{bulk}|_{r=R}$

$$\Rightarrow D_{org} \frac{dc_{O_2}}{dr}\Big|_{r=R,org} = D_{bulk} \frac{dc_{O_2}}{dr}\Big|_{r=R,bulk}$$

$\Rightarrow$ b/c $D_{org} < D_{bulk}$, concentration gradient must be <u>steeper</u> inside organism $\Rightarrow$ <u>curve I</u>

B) * All kinds of organelles and stuff inside cell, which makes fluid more viscous and hinders transport

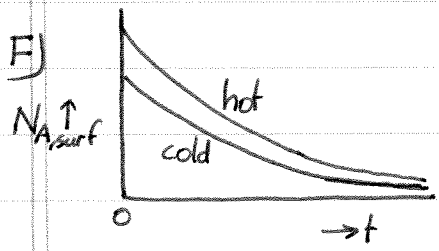
C) * Yes, "pseudo steady state" is appropriate; Mylar skin is thin and balloon fairly large, so during time it takes for H_2 molecule to diffuse through skin, pressure (and C_{H_2}) inside balloon remain essentially constant

D) * $D \sim \frac{L^2}{t} \Rightarrow t \sim \frac{L^2}{D}$

Diffusion coefficient remains same (same material) $\Rightarrow t \sim L^2$

$\Rightarrow$ Doubling thickness to 2 mm will increase time by factor 4

E) * Chemical engineers are often interested in <u>molar</u> fluxes ($\vec{N}, \vec{J}$) b/c chemical reactions, and usually prefer to know how transport occurs relative to lab coordinates ($\vec{N}$) rather than in relation to average bulk motion ($\vec{J}$)

F) 

- $N_A|_{surf} \sim \frac{1}{\sqrt{t}}$ for both cases (max at $t=0$, 0 for $t \to \infty$)
- $T\uparrow \Rightarrow D\uparrow \Rightarrow$ greater flux $N_A|_{surf}$
- Note: if supply of insecticide is limited (small spill), then $N_{A,hot}$ will drop below $N_{A,cold}$ after some time.

Problem III/ A) * y_{H_2O} small everywhere $\Rightarrow D_{H_2,mix} = D_{H_2,O_2}$

* Note: in table of handout, only D_{O_2,H_2} given: 0.697 cm²/s at 1 atm, 273 K
$\Rightarrow$ according to Hirschfelder equation $D_{AB} = D_{BA}$ (dilute solute)
so can use the table data with correction for P & T

$$D_{H_2O_2} = 0.697 \cdot \left(\frac{1}{1.5}\right) \cdot \left(\frac{373}{273}\right)^{1.75} = 0.802 \text{ cm}^2/\text{s}$$

* Direct use of Hirschfelder: $D_{H_2,O_2} = \dfrac{0.001858 \cdot T^{3/2}\left[\frac{1}{M_A} + \frac{1}{M_B}\right]^{1/2}}{P\,\sigma_{AB}^2\,\Omega_D}$

$\sigma_{H_2} = 2.968\,\text{Å}$, $\sigma_{O_2} = 3.433\,\text{Å} \Rightarrow \sigma_{AB} = \frac{\sigma_{H_2}+\sigma_{O_2}}{2} = 3.201\,\text{Å}$

$\frac{\varepsilon_{H_2}}{\kappa} = 33.3$, $\frac{\varepsilon_{O_2}}{\kappa} = 113 \Rightarrow \varepsilon_{AB}/\kappa = \sqrt{33.3 \cdot 113} = 61.3\,\text{K} \Rightarrow \frac{\kappa T}{\varepsilon_{AB}} = \frac{373}{61.3} = 6.08$

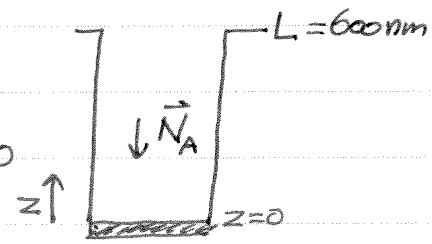
$\Rightarrow \Omega_D \approx 0.81$

$$\Rightarrow D_{H_2O_2} = \frac{0.001858 \cdot (373)^{3/2} \cdot \left[\frac{1}{2} + \frac{1}{32}\right]^{1/2}}{1.5 \cdot (3.201)^2 \cdot 0.81} = 0.784 \text{ cm}^2/\text{s}$$

B) - $\underbrace{\vec{\nabla} \cdot \vec{N}_A}_{\text{1D, z only}} + \underbrace{\cancel{\frac{\partial c_A}{\partial t}}}_{\text{steady}} - \underbrace{\cancel{R_A}}_{\text{no bulk reaction}} = 0 \Rightarrow \frac{dN_A}{dz} = 0$

$\Rightarrow N_{A,z} = \text{constant}$

A: H_2
B: O_2
C: H_2O



- $\vec{N}_A = -c D_{A,mix} \vec{\nabla} y_A + \cancel{y_A \sum \vec{N}_i}$ $\hookrightarrow$ $y_A \ll 1$ ($y_{A,max} = 0.01$ at top of well)

$\overset{\text{1D}}{\Rightarrow} N_{A,z} = -c D_{A,mix} \frac{dy_A}{dz}$

C) - Combine equations from B): $\frac{d}{dz}\left(\overbrace{-c D_{A,mix}}^{\text{constant}} \frac{dy_A}{dz}\right) = 0 \Rightarrow \frac{d^2 y_A}{dz^2} = 0$

BC: 1) $y_A = 0$ @ $z = 0$ (diffusion limited)

2) $y_A = 0.01$ @ $z = L = 600$ nm

D) - Solving DE from C): $\frac{dy_A}{dz} = C_1 \Rightarrow y_A = C_1 \cdot z + C_2$

- BC 1) $\Rightarrow C_2 = 0$
- BC 2) $\Rightarrow C_1 = \frac{y_{A,L}}{L}$

$\Rightarrow y_A = \frac{y_{A,L}}{L} z$

$N_{A,z} = -c D_{A,mix} \frac{y_{A,L}}{L} = -\frac{P}{RT} D_{A,mix} \frac{y_{A,L}}{L}$

* Rate of H_2O generation is equal to hydrogen flux towards surface
* $N_{A,z} = \frac{1.5\ \text{atm}}{8.206\cdot10^{-5}\frac{m^3\,atm}{mol\cdot K}\cdot 373\,K} \cdot 0.784\cdot10^{-4}\,m^2/s \cdot \frac{0.01}{600\cdot10^{-9}\,m} = 64.0\ mol/m^2\cdot s$
  $= $ rate of H_2O generation

E) * $N_{A,z} \sim P\cdot D_{A,mix}$ with $D_{A,mix} \sim \frac{1}{P}$ (see A))
$\Rightarrow N_{A,z}$ not function of $P \Rightarrow$ hydrogen conversion not changed

Problem IV/ A) * For 1 m of pipe, salt volume is: $V_{salt} = \overbrace{\pi\cdot d}^{\text{circumference}}\cdot\delta\cdot L$ (essentially flat b/c $\delta \ll d$)
$= \pi\cdot 0.02\cdot 0.1\cdot 10^{-3}\cdot 1 = 6.28\cdot10^{-6}\,m^3$

$\Rightarrow$ # moles per m pipe $= \frac{V_{salt}\cdot\rho_{salt}}{M_W} = \frac{6.28\cdot10^{-6}\cdot 2500\,kg/m^3}{0.100\,kg/mol} = 0.157$ mol

B) * For salt in liquid: $D \sim \frac{T}{\mu_L}$
$\Rightarrow D_{22°C} = D_{60°C}\cdot\frac{\mu_{water,60°C}}{\mu_{water,22°C}}\cdot\frac{T_{22°C}}{T_{60°C}} = 2.4\cdot10^{-9}\cdot\frac{471\cdot10^{-6}}{959\cdot10^{-6}}\cdot\frac{295}{333} = 1.044\cdot10^{-9}\,m^2/s$

C) * Transient diffusion into finite medium (salt from pipe wall into water)
$\Rightarrow$ Heissler charts for cylinder!
* $m \approx 0$ (no resistance getting salt to cylinder surface; $C_{surf} = C_{sat}$)
  $n = 0$ (center)
  $Y = \frac{C_{surf} - C}{C_{surf} - C_0} = \frac{C_{sat} - 0.99\cdot C_{sat}}{C_{sat} - 0} = 0.01$

chart $\Rightarrow X = 0.8$ (bottom graph) [or 0.9 (top graph)] $= \frac{D\cdot t}{(d/2)^2} \Rightarrow t = \frac{d^2 X}{4D} = \frac{0.8\cdot(0.02)^2}{4\cdot 1.04\cdot10^{-9}}$
$= 7.66\cdot10^4\,s \approx 21.3$ hr

D) * Once batch is complete, $C_{ave} \approx C_{sat} = 100\ mol/m^3$ in water
$\Rightarrow$ 1 m of pipe contains: $C_{sat}\cdot\frac{\pi}{4}d^2\cdot L = 100\cdot\frac{\pi}{4}(0.02)^2\cdot 1 = 0.0314$ mol
$\Rightarrow$ # flushes needed $= \frac{\text{total salt}}{\text{salt per flush}} = \frac{0.157}{0.0314} = 5.0 = 5$
$\Rightarrow$ total time: $5\cdot 21.3$ hr $= 106.5$ hr

E) * Can speed process up by not waiting until center reaches 99% of C_{sat}
* For example, if you wait half as long ($X = 0.4$) then $C_{center} \approx 0.90\cdot C_{sat}$ and C_{ave} pretty much unchanged $\Rightarrow$ extra wait has poor ROI

F) * Chilton-Colburn ($Pr \neq 1$ for water $\Rightarrow$ Reynolds not useful)

$$\frac{C_f}{2} = \frac{f_f}{2} = \frac{k_c}{V_\infty}\left(\frac{\nu}{D}\right)^{2/3} \Rightarrow k_c = \frac{f_f}{2}\cdot V_\infty\left(\frac{D}{\nu}\right)^{2/3}$$

* Find f_f: $Re = \frac{V_\infty \cdot d}{\nu} = \frac{0.1\cdot 0.02}{9.61\cdot 10^{-7}} = 2082$

$\left(\nu = \frac{\mu}{\rho} = \mu\cdot v_f = 9.59\cdot 10^{-6}\ Pa.s\cdot 1.002\cdot 10^{-3}\ \frac{m^3}{kg} = 9.61\cdot 10^{-7}\ m^2/s\right)$

$\Rightarrow$ Moody plot: $f_f = 0.0085$ [also: $f_f = \frac{16}{Re} = 0.0077$ for laminar]

$$\Rightarrow k_c = \frac{0.0085}{2}\cdot 0.1\left(\frac{1.04\cdot 10^{-9}}{9.61\cdot 10^{-7}}\right)^{2/3} = 4.49\cdot 10^{-6}\ m/s$$

G) * $N_A = k_c\,(C_{sat} - 0) = 4.49\cdot 10^{-6}\ m/s \cdot 100\ mol/m^3 = 4.49\cdot 10^{-4}\ mol/m^3\cdot s$

* Area of 1m pipe: $\pi dL = \pi\cdot 0.02\cdot 1 = 0.0628\ m^2$

$\Rightarrow$ dissolution rate: $N_A\cdot A = 4.49\cdot 10^{-4}\cdot 0.0628 = 2.82\cdot 10^{-5}\ mol/s$

$\Rightarrow$ time needed to dissolve 0.157 mole: $\frac{0.157}{2.82\cdot 10^{-5}} = 5568\ s = 1.54\ hr$

H) * Batch process: slow!

* Continuous process: creating lots of waste water with low C_{salt}