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## CHEMICAL ENGINEERING 179 Exam 2 Monday, April 8 2013 Closed Book with 3x5 Card

 $k_{B} = 1.381 \text{ x } 10^{-23} \text{ J K}^{-1}; R = 8.314 \text{ J (mole K)}^{-1} = 1.987 \text{ cal (mole K)}^{-1}; N_{A} = 6.022 \text{ x } 10^{23} \text{ (mole)}^{-1}; e = 1.602 \text{ x } 10^{-19} \text{ C}; m_{p} = 1.673 \text{ x } 10^{-27} \text{ kg} = 1.007 \text{ amu}; 1 \text{ liter} = 1000 \text{ cm}^{3}; \text{ STP} = 273 \text{ K}, 760 \text{ torr (1 atm)}; 1 \text{ atm} = 1.013 \text{ x } 10^{5} \text{ Pa}; 1 \text{ Pa} = 1 \text{ J/m}^{3}; 1 \text{ eV} = 1.602 \text{ x } 10^{-19} \text{ J}$ 

## Short Answer. 5 pts. each.

1.Estimate the mean thermal speed (m/s) for Ar (40 amu) at 300K.

 $v = (8kT/\pi/m)^{0.5} = 397 m/s$ 

2. Estimate the viscosity of  $H_2$  (amu 2) at 300K if the collision cross section is  $10^{-15}$  cm<sup>2</sup>.

$$\mu \sim \rho v = \rho * \left(\frac{1}{3} \lambda v\right) = \frac{PM}{kT} * \left[\frac{1}{3} \left(\frac{1}{N\sigma}\right) v\right] = \frac{PM}{kT} * \left[\frac{1}{3} \left(\frac{kT}{P\sigma}\right) v\right] = \left(\frac{M}{3\sigma}\right) \left(\frac{8kT}{\pi m}\right)^{0.5}$$
$$= 1.97 * 10^{-5} \frac{kg}{ms}$$

3. What is the approximate collisional mean free path at  $10^{-3}$  torr and 300K?

$$PV = nRT \rightarrow \frac{n}{V} = 3.2 * 10^{13} \frac{molecules}{cm^3}$$
$$\lambda = \frac{1}{N\sigma} = \frac{1}{[(3.2 * 10^{13} cm^{-3}) x \ 10^{-15} cm^2]} = 31.08 \ cm$$

4. If a tube diameter is 1 cm and the mean free path is 1 cm, what is the name for the type of flow that occurs inside the tube?

*Transition flow or transition regime flow – between free molecular flow and continuum flow.* 

5. For cylindrical, isothermal LPCVD (low pressure CVD) reactors with multiple wafers and flow in the annular region, what is the expected axial profile (that is, along the <u>length</u> of the reactor) in reactant concentration?

Concentration should vary exponentially: e.g.  $C_A(z) \sim exp [-\alpha z]$ 

6. What is the definition of the effectiveness factor (in terms of a ratio of reaction rates)?

*Ratio of actual integrated rate divided by the maximum rate unhindered by mass transfer limitation.* 

7. For best growth rate uniformity results, should the LPCVD reactor be operated in the reaction rate limited or mass transfer limited regimes? Why?

*Reaction rate limited since we want no concentration gradients to induce non-uniform film thickness profiles.* 

8. Why do most low-pressure CVD reactors have multiple regions of temperature control down the length of the reactor?

To counteract the decrease in reactant concentration temperature increases down the length of the reactor can keep the reaction rates and therefore the film growth rates, approximately equal as a function of position.

9. Approximately how long does it take for a gas at  $10^{-6}$  torr and 300K to cover a surface to one monolayer if every collision sticks at the surface?

About 1 second. This can be estimated from  $[10^{15} \text{ sites } \text{cm}^{-2}]/[1/4 \text{ N v } \text{cm}^2/\text{s}] \sim 1$  second. For  $N_2$ :  $N = P/RT = 3.2 * 10^{10} \text{ cm}^2 - 3$ ; V = 480 m/s;  $\tau = 2.6 \text{ sec}$ For Ar:  $N = P/RT = 3.2 * 10^{10} \text{ cm}^2 - 3$ ; V = 397 m/s;  $\tau = 3.15 \text{ sec}$ 

10. Write and name the (1-D) equation that governs electrostatics in plasmas in terms of potential (V), position x, charge density  $N_+$  and negative charge density  $N_-$ .

This is the Poisson equation:  $\frac{d^2 V}{dx^2} = -\frac{e}{\varepsilon_0}(N_+ - N_-)$ 

## Problem.

(50) 1. Consider a tube of length L and diameter D with a mixture of gases flowing at volumetric flowrate Q ( $m^3/s$ ) down the tube. A reactant (concentration  $C_A$  moles/ $m^3$ ) is present at very low concentration in excess inert gas and this species reacts at the tube inside surface (only) with first order rate kinetics ( $r_A = -k_sC_A$ ; moles/ $m^2/s$ ). The reacting component enters the reactor at concentration  $C_{A0}$ . The film formed has molar volume  $V_m$  ( $m^3/mole$ )

40 (a) If you assume isobaric, isothermal plug flow, derive the expression for growth rate (m/s) down the length of the tube in terms Q, D,  $C_{A0}$ , and  $k_s$ .

10 (b) If Q=10<sup>-6</sup> m<sup>3</sup>/s; D=0.01 m; k<sub>s</sub>=0.01 m/s;  $C_{A0} = 10^{-4}$  moles/m<sup>3</sup>, and  $V_m = 12.1 \times 10^{-6}$  m<sup>3</sup>/mole what is the thickness of the film (in meters) after reacting for 10 minutes, at x=1m down the tube?

Solution:

(a) The 'plug flow' gas velocity in the tube  $v = Q/(\pi D^2/4)$ . Then we can write the solution in terms of the velocity v. The expression for the concentration can be shown to be:

$$v \frac{\mathrm{dC}_{\mathrm{A}}}{\mathrm{dx}} = -\mathrm{k}_{\mathrm{s}}\mathrm{C}_{\mathrm{A}} * \left(\frac{\mathrm{area}}{\mathrm{volume}}\right) = -\mathrm{k}_{\mathrm{s}}\mathrm{C}_{\mathrm{A}}\frac{4}{\mathrm{D}}$$

The solution is easily found to be

$$\frac{C_A(x)}{C_{Ao}} = \exp\left(-\frac{(4k_s)/D}{v}x\right)$$
  
Then growth rate = k<sub>s</sub>C<sub>A</sub>(x)V<sub>m</sub>

(b) Plugging in the numbers:

$$v = \left(10^{-6} \frac{m^3}{s}\right) / \left(\frac{\pi * 10^{-4} m^2}{4}\right) = 1.27 * 10^{-2} m/s$$

Then the argument in the exponential is

$$\frac{(4k_s)/D}{v} * x = \left[ \frac{4\left(1\frac{1}{s}\right)}{1.27 * 10^{-2}\frac{m}{s}} \right] * x = 314\frac{1}{m} x$$

 $C_A (x=1m) = (10^{-4} \text{ moles/m}^3) x \exp(-314) \sim 0$ 

Film thickness = 0