University of Calgary
Department of Chemical & Petroleum Engineering

ENCH 501: Mathematical Methods in Chemical Engineering

Final Examination, Fall 2003

Time: 8 - 11 am **Friday, December 12, 2003**

Instructions: **Attempt All Questions.**
Use of Electronic Calculators allowed.
Open Notes, Open Book Examination.

Problem #1 (20 points)

(a) Surface tension effects are important in the imbibition of liquids into porous media. Examples are the use of paper towels to mop up liquid spills, and the instability (formation of fingers) which develops when oil is displaced by water in reservoirs. The height $\boldsymbol{h}$ to which a liquid rises in capillary spaces depends on the capillary diameter $\boldsymbol{d}$, gravity $\boldsymbol{g}$, liquid density ρ, the surface tension σ, and the contact angle θ.

Determine the dimensionless variables for this system. Show your steps.

(b) At an amusement park, a water slide consists of a metal slab inclined at an angle of 30° to the horizontal. If the thickness of the water must be at least 5mm so that people sliding do not get a "burn" on the back side, at what flow rate must water be supplied to the top of the slide of a width of 1.4m? What is the velocity of the surface of the film? What assumptions have you made and are they valid?

Given for water: ρ = 998 kg/m^3; μ = 1.1 mPa.s

Problem #2 (30 points)

In solid catalyzed reactions or systems in which one of the reactants is a solid (such as for the combustion of coal), conversion rates are considerably enhanced because the reactions occur within porous structures which have large surface areas. The surface area within the pores may be up to 10,000 times the external surface area. Pellets are sintered from ceramic and metal powders for use as catalysts in the chemical process industry. The porosity and permeability of reservoir formations can be increased by injecting acids into the formation to react with and dissolve components of the medium. Chemicals enter into the structures and reaction products diffuse outwards. It is required that you analyze one of such systems.

A porous spherical pellet is a catalyst suspended in a rapidly flowing gas mixture. The mixture consists of 30 % (molar basis) of compound A which can react, in the presence of a catalyst, to form compound B. One mole of B is formed from each mole of A. The balance of the gas mixture (70%) is nitrogen which is inert. Species A diffuses into the pellet and undergoes a first order *reversible* reaction, viz:

A $\rightleftharpoons$ **B** with rate of reaction of A given as: $-R_A = k_1c_A - k_2c_B$ where k_1 and k_2 are the rate constants per unit volume of the pellet. The equilibrium constant, k_1/k_2, equal 5.

If species B, as soon as it diffuses out of the pellet, is very rapidly diluted that y_B at the surface of the pellet is effectively zero, and both temperature and pressure are constant for the system:

(a) Derive an expression for the concentration of reactant A versus radial position at steady state.

(b) What is the steady state rate of conversion of A? Show your steps and explain.

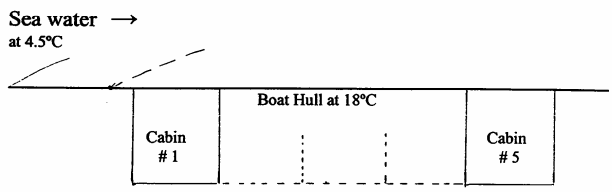
(c) Obtain an expression for the effectiveness factor η of the pellet.

Problem #3 (30 points)

An ocean liner, such as a cruise ship, typically has 8 to 10 levels above the water line and three below the water surface. Below the water line, cabins for crew are lined up along the wall. Each cabin is 2.5m wide (along the length of the boat) and 2.2m tall. This is the surface area exposed to sea water. The hull of the boat is made of a metal and it is assume that the wall is maintained at a constant temperature of 18°C. The sea water is at a temperature of 4.5°C. For the purpose of the current analysis, assume that the rooms are lined up against a flat wall, and the first room starts from a distance of 10m from the leading edge. Furthermore, the first 8m of the hull is unheated and is therefore at the temperature of the water.

You, as the boat engineer, are required to estimate and compare the heating requirement for cabins 1 and 5 from the leading edge. It may be assumed that all the heat loss from each cabin has been from the wall into the sea. The relative velocity between the water and the boat is 12 knots and, because of a special micro-sculpturing of the boat hull, the boundary layer is laminar along the entire length of the boat. Use the integral method.

Data:
1 knot (kn) is equal 0.51444 m/s.
Properties of sea water: ρ = 1028.6 kg/m^3; μ = 1.61 mPa.s; **k** = 0.57 W/mK; c_p = 3.915 kJ/kg K



The hull of the boat approximated as a flat plate.

Problem #4 (20 points)

Chloroform, discovered in 1831, had been used as an anesthetic but it is now used as a solvent.

The diffusion coefficient of chloroform vapor ($CHCl_3$)in air is to be determined. Liquid chloroform is poured into the bottom of a flat bottomed, uniform cross-section test tube. The level of the liquid at the start was 2cm above the base. The test tube is 9cm long. The test tube mouth was covered with a wire mesh so that there were no convection currents inside the tube. Air free of chloroform is blown over the mouth of the tube at a rate that the concentration of the chloroform may be assumed negligible at the rim or mouth. The tube and contents were maintained at a constant temperature of 30°C. After 19 hours, the level of the liquid is observed to have dropped to 0.8cm above the base.

(a) Estimate the diffusion coefficient for chloroform in air.

(b) Calculate the time it will take for all the liquid to disappear, i.e. complete evaporation.

Data:
Vapor Pressures of Chloroform

Temperature, °C	Vapor Pressure, mm Hg
20	158.4
25	198

Density of liquid Chloroform at 30°C = 1,470.4 kg/m^3
Molar Mass of Chloroform 119.38 g/mol
The room pressure is given as 692 mm Hg
The Universal Gas Constant R = 8.314 J/mol K or 0.08205 (m^3 atm) / (kmol K)

ENCH501 SOLUTION – FINAL Dec. 12, 2003

Problem #1

(a) Dimensional Analysis

$$h = f(d, g, \rho, \sigma, \theta) \quad , \; n = 6 \text{ variables}$$

Dimensions: h: L; d: L; g: $\frac{L}{t^2}$; ρ: $\frac{M}{L^3}$; σ: $\frac{M}{t^2}$; θ: none

Number of fundamental dimensions $j = 3$ (M, L, t)

$\therefore$ Number of dimensionless quantities $n - j = 3$

By inspection, there are 2 dimensionless gps

$$\Pi_2 = h/d \quad , \quad \Pi_3 = \theta$$

Hence we need to find only Π_1 from

$$h = \phi(g, \rho, \sigma)$$

or $\Pi_1 = g^a \rho^b \sigma^c h$

$$[M]^0 [L]^0 [t]^0 = \left[\frac{L}{t^2}\right]^a \left[\frac{M}{L^3}\right]^b \left[\frac{M}{t^2}\right]^c [L]$$

Match coefficients

Length	$0 = a - 3b + 1$	$-c + 3c + 1 = 0$
mass	$0 = b + c$	$b = -c$
time	$0 = -2a - 2c$	$a = -c$

$\therefore$ $c = -\frac{1}{2}$, $a = b = \frac{1}{2}$

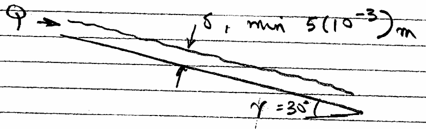
$$\therefore \quad \Pi_1 = \left(\frac{g\rho}{\sigma}\right)^{\frac{1}{2}} h \quad \text{or} \quad \frac{\rho g h^2}{\sigma}$$

Hence

$$\left[\frac{\rho g h^2}{\sigma}\right] = \psi\left[\frac{h}{d}, \theta\right]$$

→

(b)



Assume flow is laminar, no waves or ripples and steady.

from Notes, p 132 - 4, $\beta = 90 - \gamma = 60°$

The volume rate of water supply

$$Q = \frac{\rho g \delta^3 \cos\beta}{3\mu} \cdot W \qquad \text{eq. 6.7 (Notes)}$$

$$Q = \frac{(998)(9.81)(5)^3(10^{-9})}{3(1.1)(10^{-3})} \cos 60 \cdot 1.4$$

Volume rate

$Q = 0.25959$ or approx $0.26 \ m^3/s$ ⟶

Surface velocity = max. vel

from eq. 6.5 (Notes)

$$V_{max} = \frac{\rho g \delta^2 \cos\beta}{2\mu} = \frac{998(9.81)(5)^2(10^{-6})}{2(1.1)(10^{-3})}\cos 60$$

$$= 55.627 \ m/s \quad (\text{High!})$$

⟶

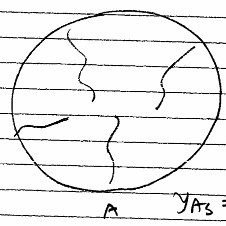
Calc. Reynolds number, $Re = \frac{\Gamma \bar{u} \rho}{\mu}$

$\bar{u} = \frac{2}{3} V_{max}$, $\Gamma = 4\delta$ (hydraulic diameter)

$$Re = \frac{4(5)(10^{-3})\,\frac{2}{3}(55.627)(998)}{1.1(10^{-3})} = 673,254$$

The flow is turbulent! Hence the calculations are invalid, or at least suspect. ⟶

Problem #2

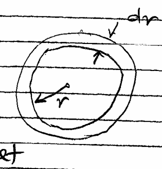


The inert gas (C) does not participate in the diffusion but it limits the sum of

$$y_A + y_B = 0.3$$

within the pellet.

$(y_C = 0.7)$



A $\quad y_{As} = 0.3$

Consider a spherical shell within the pellet

at steady state

Input + Generation = Output + ~~Accum.~~ $\to 0$

$$(SN_A)\Big|_r + R_A(4\pi r^2 dr) = (SN_A)\Big|_{r+dr}$$

$$(SN_A)\Big|_r + R_A(4\pi r^2 dr) = SN_A\Big|_r + \frac{d(SN_A)}{dr}dr$$

or

$$-\frac{d(SN_A)}{dr} + R_A(4\pi r^2) = 0 \qquad (1)$$

Definition

$$N_A = -cD_{AB}\frac{dy_A}{dr} + y_A(N_A + N_B)$$

But, since $N_B = -N_A$ (from stoichiometric relation), the convective term vanishes identically and

$$N_A = -cD_{AB}\frac{dy_A}{dr} = -D_{AB}\frac{dC_A}{dr} \qquad (2)$$

since $C = P/RT$ = constant

Also the area $S = 4\pi r^2$

Hence eq. (1) becomes

$$\frac{d}{dr}\left(D_{AB}\frac{dC_A}{dr}\cdot 4\pi r^2\right) + R_A(4\pi r^2) = 0$$

Substitute for R_A

$$D_{AB}\frac{d}{dr}\left(r^2\frac{dC_A}{dr}\right) - r^2\left(k_1 C_A - k_2 C_B\right) = 0 \qquad (3)$$

write $C_A + C_B = C_{AS}$, conc. of A outside of pellet
within the pellet

or $C_B = C_{AS} - C_A$ or $y_B = y_{AS} - y_A$
constant

Equation (3) can be re-written as

$$D_{AB}\frac{d}{dr}\left(r^2\frac{dy_A}{dr}\right) - r^2\left(k_1 y_A - k_2\left(y_{AS} - y_A\right)\right) = 0 \qquad (4)$$

$$D_{AB}\frac{d}{dr}\left(r^2\frac{dy_A}{dr}\right) - r^2\left[(k_1+k_2)y_A - k_2 y_{AS}\right] = 0$$

$$\frac{d}{dr}\left(r^2\frac{dy_A}{dr}\right) - r^2\frac{(k_1+k_2)}{D_{AB}}\left[y_A - \frac{k_2 y_{AS}}{k_1+k_2}\right] = 0 \qquad (5)$$

Let $\varepsilon = \dfrac{k_2 y_{AS}}{k_1+k_2} = \dfrac{y_{AS}}{k_1/k_2 + 1} = \dfrac{0.3}{6} = 0.05$ const.

$$\beta^2 = \frac{k_1+k_2}{D_{AB}}$$

Eq. (5) becomes

$$\frac{d}{dr}\left(r^2\frac{dy_A}{dr}\right) - r^2\beta^2\left(y_A - \varepsilon\right) = 0 \qquad (6)$$

Transform equation (6) write

$$\psi(r) = r(y_A - \varepsilon)$$

$$\frac{d\psi}{dr} = (y_A - \varepsilon) + r\frac{dy_A}{dr} \quad \text{or} \quad r^2\frac{dy_A}{dr} = r\frac{d\psi}{dr} - \psi$$

Substitute into equation (6)

$$\frac{d}{dr}\left(r\frac{d\psi}{dr} - \psi\right) - r\beta^2\psi = 0$$

$$r\frac{d^2\psi}{dr^2} + \cancel{\frac{d\psi}{dr}} - \cancel{\frac{d\psi}{dr}} - r\beta^2\psi = 0$$

or $$\frac{d^2\psi}{dr^2} - \beta^2\psi = 0 \qquad (7)$$

This has a solution of the form

$$\psi = r(y_A - \varepsilon) = A_1\cosh\beta r + B_1\sinh\beta r \qquad (8)$$

The constants A_1 + B_1 are determined from the b.c.

$$r = 0, \quad \psi = r(y_A - \varepsilon) = 0$$

$$r = R, \quad \psi = R(y_{As} - \varepsilon)$$

$$A_1 = 0, \quad B_1 = \frac{R(y_{As} - \varepsilon)}{\sinh\beta R}$$

∴ The profile desired, on substitution in eq. (8), is

$$y_A = \varepsilon + \frac{R(y_{As} - \varepsilon)\sinh\beta r}{r\sinh\beta R} \qquad (9)$$

where $\beta = \left[\frac{k_1 + k_2}{D_{AB}}\right]^{1/2}$ and $\varepsilon = 0.05$

(b) The rate of conversion of A equals the rate of flux of A into the pellet.

$$-Q = 4\pi R^2 . N_{Ar}\Big|_R \qquad (10)$$

where $N_{Ar}\big|_R = -c D_{AB}\left.\frac{dy_A}{dr}\right|_R$

But $$\frac{dy_A}{dr} = \frac{r\psi' - \psi}{r^2} \quad ; \quad \psi = B_1 \sinh \beta r$$

$$= \frac{B_1}{r^2}\left[\beta r \cosh\beta r - \sinh \beta r\right]$$

$$\left.\frac{dy_A}{dr}\right|_R = \frac{R(y_{AS}-\varepsilon)}{R^2 \sinh\beta R}\left[\beta R \cosh\beta R - \sinh\beta R\right]$$

$$= \frac{(y_{AS}-\varepsilon)}{R}\left[\beta R \coth\beta R - 1\right]$$

Substitute into (10)

$$-Q = 4\pi R^2 \cdot c\, D_{AB} \frac{(y_{AS}-\varepsilon)}{R}\left[1 - \beta R \coth\beta R\right] \quad (11)$$

(c) Effectiveness factor →

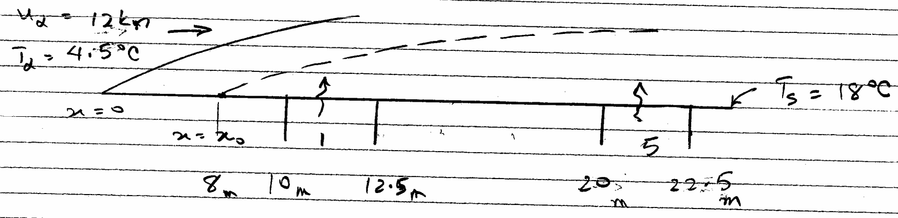
$$\eta = \frac{-Q}{\frac{4}{3}(k_1 c\, y_{AS})\pi R^3}$$

The denominator is the rate of reaction of A since any B, as formed, is carried off by the inert and ∴ reverse reaction would be negligible.

→

Problem #3

This is the problem of convective heat transfer over a flat plate, p. 113 – 117 Notes.
This problem also has an unheated leading edge.



The problem boils down to heat loss in the range 10 m → 12.5 m and 20 m → 22.5 m from the leading edge.

From Cabin 1 $$Q_1 = \int_{10}^{12.5} h_x \, dx \cdot \underbrace{(18 - 4.5)}_{°C} \cdot \underbrace{2.2 \text{ m}}_{\text{height}}$$

From Cabin 5 $$Q_5 = \int_{20}^{22.5} h_x \, dx \, (18 - 4.5) \cdot 2.2 \text{ m}$$

where $$h_x = 0.332 \, k \, Pr^{1/3} \left[\frac{u_\infty}{\nu x}\right]^{1/2} \left[1 - \left(\frac{x_0}{x}\right)^{3/4}\right]^{-1/3}$$

The integral will be evaluated approximately using the trapezoidal rule.

$$u_\infty = 12(0.51444) = 6.17328 \text{ m/s}$$

$$Pr = c_p \mu / k = 11.0582$$

$$\nu = \mu / \rho = 1.5652 (10^{-6}) \text{ m}^2/\text{s}$$

$$h_x = \lambda x^{-1/2}\left[1-\left(\frac{x_0}{x}\right)^{3/4}\right]^{-1/3} = \lambda f(x)$$

where $\lambda = 0.332\, k\, P_r^{1/3}\left[\frac{U_2}{\nu}\right]^{1/2}$

$= 837.2313468$

x, m	$f(x)$ with $x_0 = 8$ m
10	0.589797
10.5	0.5417898
11	0.5050342
11.5	0.4754223
12	0.45081467
12.5	0.42988949

$\int f(x)\,dx \doteq 6.20726$

x, m	$f(x)$
20	0.2822218
20.5	0.2770562
21	0.272164
21.5	0.2675217
22	0.2631084
22.5	0.2589057

$\int f(x)\,dx \doteq 3.376$

$\therefore Q_1 = (837.23)(6.207)(13.5)(2.2) = 154.342$ kW

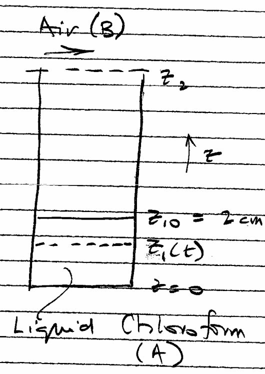
$Q_5 = (837.23)(3.376)(13.5)(2.2) = 83.947$ kW

$$\frac{Q_1}{Q_5} = 1.8386$$

Hence considerably more heat is lost from cabin #1 compared to cabin 5.

$\longrightarrow$

Problem #4



This is a problem of diffusion in a stagnant medium – air.
It is assumed that the chloroform, $CHCl_3$ is fully saturated with air.

See Notes, p 171-4

Pseudo-steady system (eq. 6.116, Notes)

$$N_A\Big|_{z=0} = -\frac{\rho_L}{M_A}\frac{dz_1}{dt} \qquad (1)$$

where

$$N_A\Big|_{z_1} = \frac{c D_{AB}}{z_2 - z_1}\ln \frac{y_{B2}}{y_{B1}} \qquad \text{(eq. 6.114)}$$

In this system, $z_1(t)$. Integrate eq. 1 subject to the condition $t=0$, $z_1 = z_{10}$

Hence $$(z_1 - z_2)^2 - (z_{10} - z_2)^2 = 2\Gamma t \qquad (2)$$

where $$\Gamma = \frac{M_A c D_{AB}}{\rho_L}\ln\frac{y_{B2}}{y_{B1}} \; ; \quad y_{B2} = 1.0, \quad y_{B1} = 1 - y_{A1}$$

Substitute for L.h.s. of eq. (2) – the conditions: $t=0$, $z_{10} = 2\,cm$; $t = 19$ hrs $\approx 68{,}400\,s$; $z_1 = 0.8\,cm$.

$$\left[(0.8 - 9)^2 - (2-9)^2\right]10^{-4} = 2\Gamma t$$

$$18.24\,(10^{-4}) = 2\Gamma\,(68400)$$

$$\therefore \quad \Gamma = 1.333\,(10^{-8}) \quad m^2/s$$

In the terms for Γ, c and y_{A1} need to be evaluated.

$$c = \frac{P}{RT} = \frac{(692/760)}{0.08205\,(303.15)} = 0.0366606 \;\frac{kmol}{m^3}$$

and from Raoult's law,

$$y_{A1} = \frac{P_{vp}^A}{P}$$

where P_{vp}^A is extrapolated from data provided.

From Clasius – Clapeyron eq. $\ln P \propto 1/T$

T °C	$1/T$, K^{-1}	$\ln P$
20	0.003411	5.065376
25	0.003354	5.288267
30	0.003299	?

The unknown $\ln P = 5.503806$, or $P^{A}_{vp} = 245.625$ mm Hg

$\therefore \; y_{A1} = \dfrac{245.625}{692} = 0.355$

(a) Solve for D_{AB} from

$$1.33\dot{3}\,(10^{-8}) = \frac{119.38\,(0.0366606)\,D_{AB}}{1470.4} \ln \frac{1}{1-0.355}$$

$$m^2/s \qquad \frac{\cancel{kg}}{\cancel{kmol}} \; \frac{\cancel{kmol}}{\cancel{m^3}} \; \frac{m^2}{s} \; \frac{\cancel{m^3}}{\cancel{kg}\,s}$$ dimensionally consistent

$\therefore \; D_{AB} = 1.023\,(10^{-5})\ m^2/s$

Diffusion coeff. of chloroform in air

(b) For all the liquid chloroform to be evaporated, use equation 6.118 (Notes)

$$z_0 z_2 - \frac{z_{10}^2}{2} = \Gamma t_0$$

Substitute numbers

$$(2\times 9 - 2)(10^{-4}) = 1.333\,(10^{-8})\,t_0$$

Time to completely evaporate the liquid $t_0 = 120{,}000$ s

or 33.33 hours.