THE UNIVERSITY OF CALGARY
DEPARTMENT OF CHEMICAL & PETROLEUM ENGINEERING

ENCH 501
Mathematical Methods in Chemical Engineering

MID-TERM EXAMINATION

Tuesday, October 24, 2000 **Time : 90 minutes**

Attempt both questions
Electronic calculators are permitted
Open Notes, Open Book Examination

Problem #1 (15 points)

A flat plate, infinite in extent in the y- and z-directions, is metallic uranium. The plate is 2 cm thick. The uranium is primarily ^{238}U with 3% of the radioactive ^{235}U. The plate is bathed on both sides by deuterium oxide (heavy water) and the heat transfer coefficient h is reported to be 1256 W/m^2K. The temperature of the heavy water was maintained at 152°C under pressure. This temperature was also the temperature of the solid metal at $t = 0$.

When the boron moderators around the plate were withdrawn, the fission reaction became critical leading to the decay of ^{235}U to produce Krypton, Barium, Thorium, neutrons, other products and heat. This heat is assumed generated uniformly and at a steady rate of 5 MW/m^3 within the plate.

(a) Use the integral method to derive an expression for the temperature $T(x,t)$, within the plate.

(b) After what elapsed time does the mid-plane temperature equal 200°C? What is the temperature of the plate surface at this instant?

(c) Estimate the total amount of heat which the uranium has transferred into the D_2O by the time estimated in (b) - per m^2 of exposed surface.

Data: ***Properties of Uranium***

Density	=	18,458 kg/m^3
Heat Capacity	=	0.1167 kJ/kg K
Thermal Conductivity	=	30 W/mK

Problem #2 (10 Points)

Carbon filters are used to remove dissolved organic compounds, micro particles and minerals from water for drinking. The filter is a bed of activated charcoal particles through which tap water is passed either in batches (e.g. Brita) or continuously. Substances adsorbed and absorbed from the water ultimately saturate the filter and render it ineffective. It is desired to estimate the length of service (or life) of a filter.

It is assumed, for test purposes, that organic substance A is the primary solute in the water. This solute "permeates" the activated carbon and is uniformly distributed in each particle. That is, there are no concentration gradients inside each charcoal particle but the concentration of A in charcoal increases with contact time with the "raw" water. The filter is 15 cm long and its void volume fraction (interparticle space) is 0.4. The particles are irregular in shape, average volume per particle is 0.3 ml and surface area 3.2 cm^2. You may assume that, at each plane across the filter along the flow direction (each cross-section), each particle has water at the local concentration of A $\left(C_{A_\alpha}\right)$ fully in contact with all areas of the surface.

(a) If fresh (A free) charcoal particles are dumped into a large volume of "raw" water containing 25 mmoles/litre of A, and the charcoal absorbed 40% of the A it can ultimately absorb/adsorb in 25 minutes, what is the equilibrium (or ultimate) concentration of the solute in the charcoal? You are given $k_A = 2.6(10^{-7})\ m/s$.

(b) Set up the equations to estimate the service life for the filter? Consider that the filter is spent when 50% of substance A in the feed water exits the filter.

Hints:

(i) If the concentration of A outside a particle is C_{A_α} and inside the particle it is C_A, $k_A\,(C_{A_\alpha} - C_A)$ is mass flux equivalent to $h\left(T_\alpha - T\right)$ for heat transfer. The parameter k_A is the mass transfer coefficient.

(ii) Assume the removal of A does not change the volume flow rate for the liquid.

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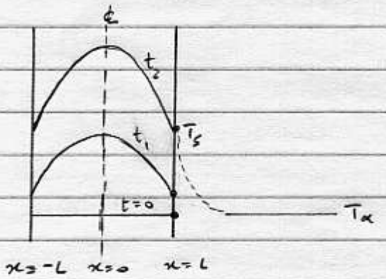
Problem #1



Because h is finite, and conditions on both sides of the plate are identical, the temperature profiles are approximately as illustrated with the surface temperature, T_s, time-dependent. In the body, $T = T(x, t)$.

(a) The integral energy balance is as derived in the Class Notes, p. . It is, for a unit area of plate surface,

$$\frac{d}{dt}\left[\int_0^L \rho C_p (T - T_a)\, dx\right] - g^+ L + q_{x=L} = 0$$

where $q_{x=L} = -k\frac{dT}{dx}\Big|_{x=L}$ and $g^+ = \text{constant}$

The boundary + i.c. conditions for the problem are:

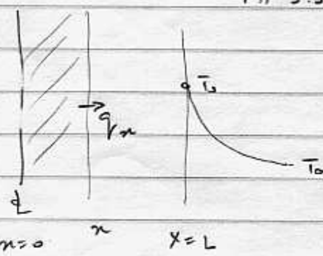
b.c. $x = 0$ $\quad dT/dx = 0$ (symmetry condition)

$\quad\quad x = L$ $\quad -k\frac{dT}{dx} = h(T - T_a)$ (convection)

i.c. $t = 0$ $\quad T = T_a$.

Assume $(T(x,t) - T_a)$ can be written as $X(x)\Gamma(t)$ – a product of two functions, $X(x)$ is the steady state solution.

At s.st.



$$g^+ x = -k\frac{dT}{dx}. \quad \text{Integrate}$$

$$\int_T^{T_s} dT = -\frac{g^+}{k}\int_x^L x\,dx \quad ; \quad T_s \text{ is surface temp. (unknown)}$$

$$T(x) - T_s = \frac{1}{2}\frac{g^+ L^2}{k}\left(1 - \frac{x^2}{L^2}\right)$$

Define $\lambda = \frac{1}{2} g^+ L^2/k$; $\frac{dT}{dx} = \lambda\left(-\frac{2x}{L^2}\right)$

But the b.c. is

$$k\lambda\left(\frac{2}{L}\right) = h(T_s - T_\infty) \quad \text{or} \quad h = \frac{2\lambda}{L}\left[\frac{1}{T_s - T_\infty}\right]$$

The steady temperature profile can be written relative to T_∞.

$$(T - T_\infty) - (T_s - T_\infty) = (T - T_\infty) - \frac{2\lambda k}{Lh} = \lambda\left(1 - \left(\frac{x}{L}\right)^2\right)$$

Simplify $\quad T - T_\infty = \lambda\left(1 - \frac{x^2}{L^2} + \frac{2}{Bi}\right)$; $Bi = \frac{Lh}{k}$

Substitute $\theta(x,t)$ into the energy equation and simplify:

i.e. $\quad \theta = \lambda\left(1 - \frac{x^2}{L^2} + \frac{2}{Bi}\right)\Gamma(t)$

$$(2\rho c_p \lambda L)\left(\frac{1}{3} + \frac{1}{Bi}\right)\frac{d\Gamma}{dt} - g^+ L + \left(\frac{2k\lambda}{L}\right)\Gamma = 0$$

I.C. $\quad t = 0 \quad \Gamma = 0$

Solve

$$\frac{T - T_\infty}{\left(\frac{g^+ L^2}{k}\right)} = \frac{1}{2}\left[1 - \left(\frac{x}{L}\right)^2 + \frac{2}{Bi}\right]\left[1 - \exp\left(-\frac{3\alpha t}{L^2}\frac{Bi}{Bi+3}\right)\right]$$

$\longrightarrow$

(b) At the mid-plane, $x = 0$, $\therefore$

$$T_{\mathcal{L}} - T_\alpha = \frac{1}{2}\left(\frac{g^+ L^2}{k}\right)\left[1 + \frac{2}{Bi}\right]\left[1 - \exp\left(-\frac{3\alpha t}{L^2}\frac{Bi}{Bi+3}\right)\right]$$

$$Bi = \frac{hL}{k} = \frac{1256(10^{-2})}{30} = 0.4187$$

$$\alpha = \frac{k}{\rho c_p} = \frac{30}{(18458)(116.7)} = 1.3927(10^{-5})$$

$$T_{\mathcal{L}} = 200\ ^\circ C, \quad T_\alpha = 152\ ^\circ C$$

$$200 - 152 = \frac{1}{2}\left(\frac{5(10^6)(10^{-4})}{30}\right)\left[1 + \frac{2}{0.4187}\right]\left[1 - \exp(-0.0512\,t)\right]$$

Solve for t: $\quad t = 114.2\ s$ $\longrightarrow$

At the surface, $x = L$

$$T_s - T_\alpha = \frac{1}{2}\left(\frac{g^+ L^2}{k}\right)\left(\frac{2}{Bi}\right)\left(1 - \exp\left(-\frac{3\alpha t}{L^2}\frac{Bi}{Bi+3}\right)\right)$$

$$= 39.69\ ^\circ C$$

$$T_s = 39.69 + T_\alpha = 191.69\ ^\circ C \longrightarrow$$

(c) There are 2 ways one may approach the problem.

(i) $\quad Q = \int_0^t q(t)\,dt \quad ; \quad q(t) = -k\left.\frac{dT}{dx}\right|_{x=L}$

or (ii) $\quad Q = \underbrace{g^+ L t}_{\text{heat generated}} - \underbrace{\int_0^L \rho c_p (T - T_i)\,dx}_{\text{heat stored}}$

The second method may be easier. Both are obvious from the energy integral equation

$$Q = g^+ L t - (\rho C_p)\left(\frac{1}{2}\frac{g^+ L^2}{k}\right)\left(1 - exp\left(-\frac{3\alpha t}{L^2}\frac{Bi}{Bi+3}\right)\right) \cdot$$

$$\int_0^L \left(\gamma - \frac{x^2}{L^2}\right) dx \quad ; \quad \gamma = 1 + \frac{2}{Bi}$$

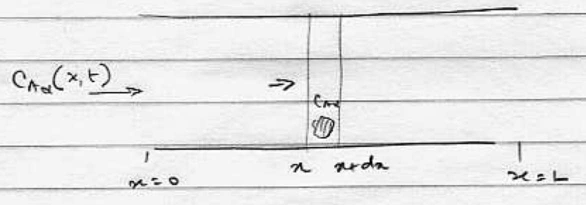
$$\int_0^L \left(\gamma - \frac{x^2}{L^2}\right) dx = \gamma x - \frac{1}{3}\frac{x^3}{L^2}\Big|_0^L = \gamma L - \frac{L}{3} = L\left(\gamma - \frac{1}{3}\right)$$

$$Q = g^+ L \left[114.2 - \frac{1}{2}\frac{(10^{-2})}{1.3927(10^{-5})} \cdot 0.9971 \cdot 10^{-2}(5.4434) \right]$$

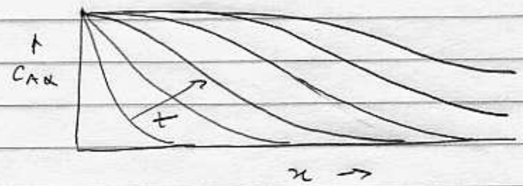
$$= 5(10^6)(10^{-2})(114.2 - 19.5)$$

$$= 4.736\,(10^6)\ J$$

Problem # 2

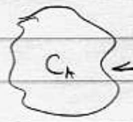


The concentration of A in the water changes with both position and time. That is, $C_{A\alpha}(x,t)$



The profile in the liquid for A may be expected to appear as in plot to the left

(c) Consider a particle in a large volume of liquid.



The problem can be handled by the lumped analysis method

Material balance on species A ⇒ particle

$$\text{Input} + \underset{0}{\cancel{\text{Gen}}} = \underset{0}{\cancel{\text{Output}}} + \text{Accum.}$$

$$k_A A (C_{A\alpha} - C_A) = \frac{d(\forall C_A)}{dt}$$

$$-\frac{k_A A}{\forall} = \frac{dC_A}{C_A - C_{A\alpha}} = d \ln (C_A - C_{A\alpha})$$

Integrate with $C_A = 0$ at $t = 0$

$$\frac{C_{A\alpha} - C_A}{C_{A\alpha}} = \exp\left[-\frac{k_A A}{\forall} t\right]$$

Given $C_{A\alpha} = 25$ mmoles/litre
$k_A = 2.6\,(10^{-7})$ m/s
$A = 3.2\ cm^2 = 3.2\,(10^{-4})\ m^2$
$V = 0.3\ cm^3 = 0.3\,(10^{-6})\ m^3$
$t = 25$ min or 1500 s

Estimate C_A from eq.

$$\frac{25 - C_A}{25} = \exp\left[-\frac{2.6(10^{-7})(3.2)(10^{-4})}{0.3(10^{-6})}\,1500\right]$$

$$= \exp[-0.414] = 0.6597$$

$$C_A = 25\,(1 - 0.6597) = 8.5 \text{ mmols/litre.}$$

This is 40% of $=^m$ value

$$\therefore\ C_{A\,eq} = \frac{8.5}{0.4} = 21.27 \text{ mmols/litre}$$

(b) To estimate the service life of the filter, perform a balance on a differential element of the domain. Let liquid flow rate $\frac{}{\text{unit area}} = Q$

superficial velocity

1) Balance on A in the liquid

Input $= Q \cdot C_{A\alpha}(x, t)$

Out $= Q \cdot \left(C_{A\alpha} + \frac{dC_{A\alpha}}{dx}\,dx\right)$

Accum $= \frac{d}{dt}\left(\varepsilon\,dx\,C_{A\alpha}\right)$; ε = void fraction

No reaction. Hence

$$0 = Q\frac{\partial C_{A\alpha}}{\partial x} + \varepsilon\frac{\partial C_{A\alpha}}{\partial t} \qquad (1)$$

Subject to the conditions

$x = 0$, $C_{A\alpha} = C_{A0}$ (input condition)

$t = 0$, $C_{A\alpha} = 0$ (fresh filter)

$\Rightarrow$? t at which $C_{A\alpha}(L, t) = 0.5\, C_{A0}$

In equation ① Q is a parameter. $C_{A\alpha}(z,t)$ depends on the value of Q. ε is a constant.

The accumulation or depletion of A from the liquid depends on the functioning of charcoal particles.

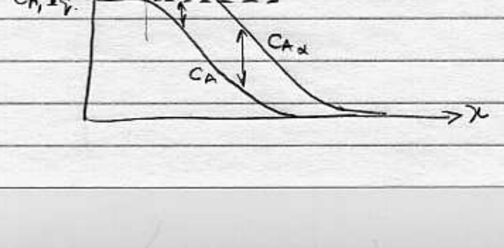
□ Transfer from liquid into solid of solute.
In same differential element / unit cross-sectional area of filter bed, the solid volume $= dx\,(1-\varepsilon)$

Mass transfer area in element $= \frac{A}{V}(1-\varepsilon)\,dx$

Rate of mass transfer into solid = Rate of A loss from liquid

$$k_A \left[\frac{A}{V}(1-\varepsilon)\,dx \right] (C_{A\alpha} - C_A) = \varepsilon\, dx \frac{\partial C_{A\alpha}}{\partial t} \qquad ②$$

* The driving force $\rightarrow (C_{A\alpha} - C_A)$ is valid as long as $C_{A\alpha} \le C_{A,eq}$.
Otherwise it is $(C_{A,eq} - C_A)$



□ Mass Transfer into each particle (local condition).

$$k_A \frac{A}{V}(C_{A\alpha} - C_A) = \frac{dC_A}{dt} \qquad (3)$$

subject to the same 'driving' force limitations as (2)
condition: $t=0$, $C_A = 0$

Make the pseudo-steady assumption - i.e. $C_{A\alpha}$ does not change rapidly at any fixed x. Then solve (3)

$$C_A = C_{A\alpha}\left[1 - \exp\left(-\frac{k_A A}{V} t\right)\right] \qquad (4)$$

Let $\gamma = k_A A/V$

substitute (4) into (2)

$$\gamma(1-\varepsilon)\exp(-\gamma t)\, C_{A\alpha} = \varepsilon \frac{\partial C_{A\alpha}}{\partial t} \qquad (5)$$

Subst. (5) into (1)

$$\int_{C_{Ao}}^{C_{Ao}/2} dC_{A\alpha} = -\frac{C_{A\alpha}\gamma}{Q}(1-\varepsilon)\exp(-\gamma t)\int_0^L dx$$

⟶