

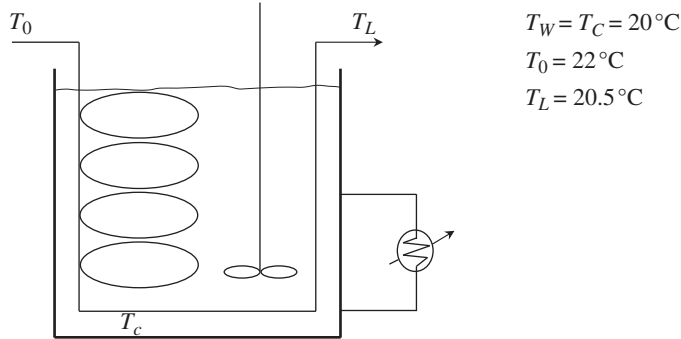
CHAPTER 1

Formulation of Physicochemical Problems

Problem 1.1

Length Required for Cooling Coil

Model 1 – Plug Flow, in section 1.2 applies:



The heat transfer coefficient is obtained from the correlation:

$$\text{Nu} = 0.026\text{Re}^{0.8} \text{Pr}^{1/3} \quad (1.1.1)$$

where

$$\text{Nu} = \frac{hD}{k}, \quad \text{Pr} = \frac{C_p\mu}{k}, \quad \text{Re} = \frac{Dv_0\rho}{\mu}$$

$$h = 0.981 \text{ kcal/m}^2\cdot\text{s}\cdot\text{K} \quad (1.1.2)$$

Substitution in Eq. 1.17 (in the text), with $T(z) = T_L$, gives:

$$\frac{20.5 - 20}{22 - 20} = \exp\left(-\frac{2 \times \pi \times 0.01 \times 0.981 \times L}{1 \times \pi \times 0.01^2 \times 10^3 \times 1}\right) \quad (1.1.3)$$

Solving the above equation for L , we get

$$\boxed{L = 7.07 \text{ m}} \quad (1.1.4)$$

Problem 1.2

Cooling of Fluids in Tube Flow: Locally Varying h

Model 1 (Section 1.2) applies up to equation 1.8:

$$v_0 A \rho C_p \frac{dT}{dz} + 2\pi R h [T(z) - T_w] = 0 \quad (1.2.1)$$

Substitution of h for $\gamma/\sqrt{z}$ gives:

$$\frac{dT}{dz} + \frac{2\pi R \gamma}{v_0 A \rho C_p} \frac{1}{\sqrt{z}} [T(z) - T_w] = 0 \quad (1.2.2)$$

Lumping parameters and changing the dependent variable, we get:

$$\frac{d\theta}{dz} + \frac{\beta}{\sqrt{z}} \theta = 0 \quad (1.2.3)$$

where:

$$\beta = (2\pi R \gamma)/(v_0 A \rho C_p) \text{ and } \theta(z) = T(z) - T_w \quad (1.2.4)$$

Separation of variables and integration using the boundary condition at $z = 0$

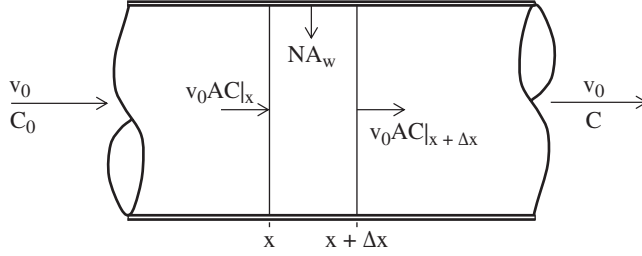
$$T(0) = T_0 \text{ or } \theta(0) = T_0 - T_w, \quad (1.2.5)$$

yields:

$$\boxed{\frac{T(z) - T_w}{T_0 - T_w} = \exp(-2\beta\sqrt{z})} \quad (1.2.6)$$

Problem 1.3

Dissolution of Benzoic Acid



Part (a):

Carrying out material balance around the shell at x with a thickness of Δx gives:

$$C|_x A v_0 - C|_{x+\Delta x} A v_0 + N A_W = 0 \quad (1.3.1)$$

where

$$N = k_C(C^* - C); \quad A = \pi D^2/4; \quad A_W = \pi D \Delta x \quad (1.3.2)$$

Dividing Eq. (1.3.1) by $\pi D \Delta x$ gives:

$$-\frac{v_0 D}{4} \left(\frac{C|_{x+\Delta x} - C|_x}{\Delta x} \right) + k_C(C^* - C) = 0 \quad (1.3.3)$$

Taking the limit as $\Delta x \rightarrow 0$, we get:

$$\boxed{-v_0 \frac{dC}{dx} + k_C \left(\frac{4}{D} \right) (C^* - C) = 0} \quad (1.3.4)$$

Part (b):

Defining $\theta = C - C^*$ and substituting into Eq. (1.3.4), we obtain:

$$-v_0 \frac{d\theta}{dx} - k_C \left(\frac{4}{D} \right) \theta = 0 \quad (1.3.5)$$

Separating the variables and integrating gives:

$$\boxed{\theta = K \exp \left(-\frac{4}{D} \frac{k_C}{v_0} x \right)} \quad (1.3.6)$$

Part (c):

Using the boundary condition at $x = 0$, $\theta = -C^*$, gives

$$K = -C^*$$

Thus, the final solution for $C(x)$ is:

$$\boxed{\frac{C(x)}{C^*} = 1 - \exp\left(-\frac{4k_C}{Dv_0}x\right)} \quad (1.3.7)$$

Part (d):

The concentration of benzoic acid leaving the tube at $x = L$ is:

$$C(L) = C^* \left[1 - \exp\left(-\frac{4k_C}{Dv_0}L\right) \right] \quad (1.3.8)$$

The total flow rate through the tube is:

$$Q_T = \pi D^2 v_0 / 4 \quad (1.3.9a)$$

The rate of benzoic acid leaving the tube is:

$$Q_B = Q_T C(L) M_B \quad (1.3.9b)$$

The weight change of the tube is:

$$\Delta W = Q_B \Delta t \quad (1.3.9c)$$

Substituting Q_T , Q_B and $C(L)$ in the expression for ΔW , we get:

$$\boxed{\Delta W = M_B C^* \Delta t v_0 \left(\frac{\pi D^2}{4} \right) \left[1 - \exp\left(-\frac{4k_C}{D} \frac{L}{v_0}\right) \right]} \quad (1.3.10)$$

Part (e):

Rearranging Eq. (1.3.10), we get:

$$\frac{\Delta W}{M_B \left(\frac{\pi D^2}{4} \right) v_0 C^* \Delta t} = 1 - \exp\left(-\frac{4k_C}{Dv_0}L\right) \quad (1.3.11)$$

Approximation of the exponential term:

$$\exp(u) = 1 + u + \dots \rightarrow 1 - \exp\left(-\frac{4k_C}{Dv_0}L\right) \approx \frac{4k_C}{Dv_0}L \quad (1.3.12)$$

Substitution the above equation into Eq. (1.3.11), rearrangement and simplification gives:

$$k_C = \Delta W / (\pi D L M_B C^* \Delta t) \quad (1.3.13)$$

Part (f):

Assumptions of the model are:

1. plug flow,
2. only resistance to dissolution of benzoic acid is due to liquid phase film resistance,
3. no axial or radial diffusion,
4. perfect radial mixing, and
5. constant wall diameter.

The maximum error can be estimated by the following equation (absolute value assures that all errors are additives, hence maximum errors):

$$\epsilon_{k_C} = \left| \frac{\partial k_C}{\partial \Delta W} \right| \epsilon_{\Delta W} + \left| \frac{\partial k_C}{\partial \Delta t} \right| \epsilon_{\Delta t} + \left| \frac{\partial k_C}{\partial D} \right| \epsilon_D \quad (1.3.14)$$

where:

$$\frac{\partial k_C}{\partial \Delta W} = \frac{1}{\pi D L M_B C^* \Delta t}, \quad (1.3.15a)$$

$$\frac{\partial k_C}{\partial \Delta t} = -\frac{\Delta W}{\pi D L M_B C^* \Delta t^2}, \quad (1.3.15b)$$

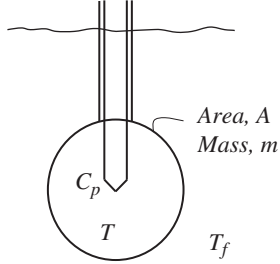
$$\frac{\partial k_C}{\partial D} = -\frac{\Delta W}{\pi D^2 L M_B C^* \Delta t} \quad (1.3.15c)$$

Substitute the values of the partial derivatives using the previous equations and the errors, $\epsilon_{\Delta W}$, $\epsilon_{\Delta t}$ and ϵ_D , from the experimental data, and simplifying:

$$\epsilon_{k_C} = \frac{\Delta W}{\pi D L M_B C^* \Delta t} \left(\frac{\epsilon_{\Delta W}}{\Delta W} + \frac{\epsilon_{\Delta t}}{\Delta t} + \frac{\epsilon_D}{D} \right) \quad (1.3.16)$$

Problem1.4

Lumped Thermal Model for Thermocouple



Heat balance equation is

$$q_C = dQ/dt \quad (1.4.1)$$

where

$$q_C = \text{heat transferred by convection} = hA(T_f - T) \quad (1.4.2a)$$

$$Q = \text{heat accumulated in the probe} = mC_P(T - T_{ref}) \quad (1.4.2b)$$

Substituting Eqs. (1.4.2) into Eq. (1.4.1), we get:

$$\boxed{mC_P \frac{dT}{dt} = hA(T_f - T)} \quad (1.4.3)$$

Part (b):

Defining $\theta = T_f - T$ and substituting into Eq. (1.4.3), we have:

$$\tau \frac{d\theta}{dt} = -\theta \quad (1.4.4)$$

where:

$$\tau = mC_P/hA \quad (1.4.5)$$

Part (c):

Separating variables and integrating Eq. (1.4.4) with the boundary condition $T(0) = T_0$, we get:

$$\frac{T - T_f}{T_0 - T_f} = \exp\left(-\frac{t}{\tau}\right) \quad (1.4.6)$$

Multiplying both sides by -1 , adding 1 to each side, and rearranging, we obtain:

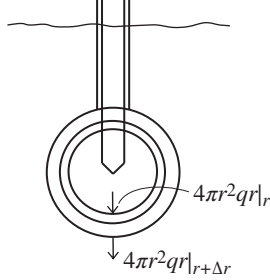
$$\boxed{\frac{T_0 - T}{T_0 - T_f} = 1 - \exp\left(-\frac{t}{\tau}\right)} \quad (1.4.7)$$

Evaluating for $t = \tau$, $(T_0 - T)(T_0 - T_f) = 0.63$, therefore:

$$\frac{T_0 - T(\tau)}{T_0 - T_f} = 0.63 \left(\frac{T_0 - T(\infty)}{T_0 - T_f} \right) \quad (1.4.8)$$

Problem 1.5

Distributed Thermal Model for Thermocouple



Heat Balance around the shell at r with a thickness of Δr is:

$$(4\pi r^2 q_r)|_r - (4\pi r^2 q_r)|_{r+\Delta r} = \partial Q / \partial t \quad (1.5.1)$$

where:

$$q_r = -k dT / dr \quad (1.5.2a)$$

$$Q = m C_P (T - T_{ref}) = 4\pi r^2 \Delta r \rho C_P (T - T_{ref}) \quad (1.5.2b)$$

Substituting Q , dividing throughout by $4\pi \Delta r$ and taking the limits as $\Delta r \rightarrow 0$, we get:

$$r^2 \rho C_P \frac{\partial T}{\partial t} = - \frac{\partial (r^2 q_r)}{\partial r} \quad (1.5.3)$$

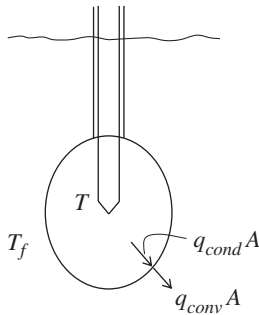
Substituting q_r from Eq. (1.5.2a) into the above equation, and rearranging, we get:

$$\rho C_P \frac{\partial T}{\partial t} = k \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial T}{\partial r} \right) \quad (1.5.4)$$

Part (b):

Heat balance at the surface of the sphere:

Heat Flux within Sphere by Conduction = Heat Flux to fluid by convection



Mathematically this continuity of heat flux is:

$$q_{cond}A = q_{conv}A \quad (1.5.5)$$

where:

$$q_{cond} = -k\partial T/\partial r|_R \quad (1.5.6a)$$

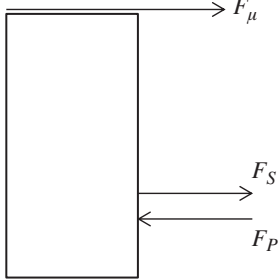
$$q_{conv} = h[T(R) - T_f] \quad (1.5.6b)$$

Substituting q_{cond} and q_{conv} into Eq. (1.5.5), we get the boundary condition at $r = R$:

$$\boxed{-k\frac{\partial T}{\partial r}\bigg|_{r=R} = h[T(R) - T_f]} \quad (1.5.7)$$

Problem 1.6

Modelling of Piston with Restraining Spring



Force Balance is:

$$\sum F_X = ma_x = m d^2x/dt^2 \quad (1.6.1)$$

Total Force (F_T) = Pressure Force (F_P) – Spring Force (F_S) – Friction Force (F_μ)
where:

$$F_P = PA, \quad F_S = Kx \quad \text{and} \quad F_\mu = \alpha \mu dx/dt \quad (1.6.2)$$

Substitution of Eq. (1.6.2) into the force balance equation (1.6.1) gives:

$$m \frac{d^2x}{dt^2} + \alpha \mu \frac{dx}{dt} + Kx = AP(t) \quad (1.6.3)$$

Part (b):

Dividing by K and defining new variables τ , ζ and $f(t)$, Eq. (1.6.3) becomes:

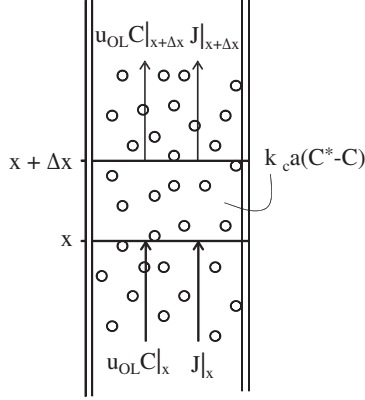
$$\tau^2 \frac{d^2x}{dt^2} + 2\zeta \tau \frac{dx}{dt} + x = f(t) \quad (1.6.4)$$

where:

Time constant:	$\tau = \sqrt{m/K}$
Damping coefficient:	$\zeta = \alpha \mu / 2\sqrt{Km}$
Effective Force:	$f(t) = AP(t)/K$

Problem 1.7

Mass Transfer in Bubble Column



Part (a):

Steady state Material Balance for Dissolved Oxygen (Liquid Phase) is:

$$A u_{OL} C|_x - A u_{OL} C|_{x+\Delta x} + A(1 - \epsilon) J|_x - A(1 - \epsilon) J|_{x+\Delta x} + k_c a (C^* - C) A \Delta x = 0 \quad (1.7.1)$$

Dividing the above equation by $A \Delta x$ and taking the limits as $\Delta x \rightarrow 0$, we get:

$$-(1 - \epsilon) \frac{dJ}{dx} - u_{OL} \frac{dC}{dx} + k_c a (C^* - C) = 0 \quad (1.7.2)$$

Substituting $J = -D_e dC/dx$ into the mass balance equation, we obtain:

$$(1 - \epsilon) D_e \frac{d^2 C}{dx^2} - u_{OL} \frac{dC}{dx} + k_c a (C^* - C) = 0 \quad (1.7.3)$$

Part (b):

Defining the following new variables:

$$z = k_c a x / u_{OL} \text{ and } y = C - C^* \quad (1.7.4)$$

the derivatives written in terms of these variables are:

$$dC/dx = (k_c a / u_{OL}) dy/dz \quad (1.7.5a)$$

$$d^2 C / dx^2 = (k_c a / u_{OL})^2 d^2 y / dz^2 \quad (1.7.5b)$$

Substituting Eqs. (1.7.5) into the dissolved oxygen equation (Eq. 1.7.3), we get:

$$(1 - \varepsilon)D_e \frac{k_C a}{u_{OL}^2} \frac{d^2 y}{dz^2} - \frac{dy}{dz} - y = 0 \quad (1.7.6)$$

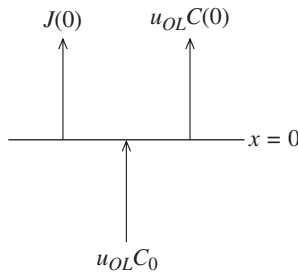
Lumping the parameters in the second order term:

$$\boxed{\alpha \frac{d^2 y}{dz^2} - \frac{dy}{dz} - y = 0} \quad (1.7.7a)$$

where

$$\alpha = \frac{(1 - \varepsilon)D_e k_C a}{u_{OL}^2} \quad (1.7.7b)$$

Part (c):



Material Balance at the Entrance of the Column gives (see the above figure):

$$Au_{OL}C_0 - Au_{OL}C|_{x=0} - A(1 - \varepsilon)J|_{x=0} = 0 \quad (1.7.8)$$

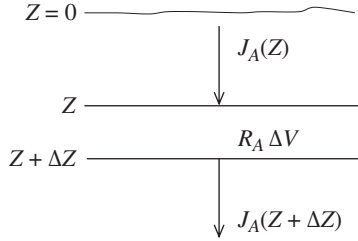
Dividing the above equation by $A\Delta x$, taking the limit as $\Delta x \rightarrow 0$ and substituting the diffusive flux $J = -D_e dC/dx$, we finally get:

$$\boxed{u_{OL}C_0 = u_{OL}C(0) - (1 - \varepsilon)D_e \left. \frac{dC}{dx} \right|_{x=0}} \quad (1.7.9)$$

The second boundary condition, $dC/dx = 0$ @ $x = L$, indicates that at the exit of the column there is no net flux of the dissolved oxygen, that is, at the end of the column the concentration of dissolved oxygen is constant with respect to axial position, because the liquid phase ends there (the top liquid interface).

Problem 1.8

Dissolution and Reaction of Gas in Liquids



The reaction rate and the diffusion flux equations are:

$$R_A = kC_A^n \quad (1.8.1)$$

$$J_A = -D_A dC_A/dz \quad (1.8.2)$$

Material Balance for Dissolved Oxygen around the shell at z with a thickness of Δz is:

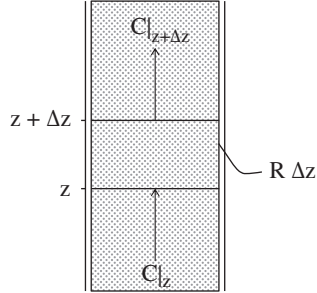
$$AJ_A|_z - AJ_A|_{z+\Delta z} - R_A A \Delta z = 0 \quad (1.8.3)$$

Dividing the above equation by $A \Delta z$, taking the limit as $\Delta z \rightarrow 0$, and substituting Fick's Law of diffusion (Eq. 1.8.2) and the rate expression (Eq. 1.8.1), we get:

$$D_A \frac{d^2 C_A}{dz^2} - kC_A^n = 0 \quad (1.8.4)$$

Problem 1.9

Modelling of a Catalytic Chemical Reactor



Part (a):

Material Balance for Toxic Gas:

$$RATE\ IN - RATE\ OUT - RATE\ REACTION = 0 \quad (1.9.1)$$

This equation is written mathematically as follows:

$$Au_0 C|_z - Au_0 C|_{z+\Delta z} - kC(z)A(1-\epsilon)\Delta z\rho_p = 0 \quad (1.9.2)$$

Dividing the above equation by $A\Delta z$ and taking the limit as $\Delta z \rightarrow 0$, we get:

$$\boxed{u_0 \frac{dC}{dz} = -(1-\epsilon)\rho_p k C} \quad (1.9.3)$$

Part (b):

Separating the variables in Eq. (1.9.3) and integrating the result with the following boundary condition:

$$@\ z = 0; \quad C(0) = C_0 \quad (1.9.4)$$

we get:

$$\ln\left(\frac{C}{C_0}\right) = -\frac{(1-\epsilon)\rho_p k}{u_0} z \quad (1.9.5)$$

Part (c):

From Eq. (1.9.5), we derive the concentration at the exit of the reactor:

$$C_L = C_0 \exp \left(-\frac{(1 - \varepsilon)\rho_P k L}{u_0} \right) \quad (1.9.6)$$

Part (d):

Multiplying and dividing the argument of the exponential term by the cross-sectional area, A , we get:

$$C_L = C_0 \exp \left(-\frac{AL(1 - \varepsilon)\rho_P k}{u_0 A} \right) \quad (1.9.7)$$

However:

$$\text{Volumetric Gas Flow rate} = F = u_0 A \quad (1.9.8a)$$

$$\text{Mass of Catalyst Inside the Reactor} = W = AL(1 - \varepsilon)\rho_P \quad (1.9.8b)$$

The exit concentration (Eq. (1.9.7)) becomes:

$$C_L = C_0 \exp \left(-\frac{Wk}{F} \right) \quad (1.9.9)$$

Part (e):

For 95 % conversion:

$$\frac{C_0 - C_L}{C_0} = \frac{C_0 - C_0 \exp \left(-\frac{Wk}{F} \right)}{C_0} = 0.95 \quad (1.9.10)$$

Simplifying and rearranging the above equation, we get:

$$-\frac{Wk}{F} = -\ln(0.05) \quad (1.9.11)$$

Solving for the mass of catalyst, we finally obtain:

$$\boxed{W = \frac{3F}{k}} \quad (1.9.12)$$

Part (f):

Accounting for axial diffusion, Eq. (1.9.2) can be rewritten as follows:

$$Au_0C|_z - Au_0C|_{z+\Delta z} + A\varepsilon J|_z - A\varepsilon J|_{z+\Delta z} - kC(z)A(1-\varepsilon)\Delta z\rho_P = 0 \quad (1.9.13)$$

Dividing the above equation by $A\Delta z$ and taking the limit as $\Delta z \rightarrow 0$, we get:

$$-u_0 \frac{dC}{dz} - \varepsilon \frac{dJ}{dz} - (1-\varepsilon)\rho_P kC = 0 \quad (1.9.14)$$

Substituting the equation for the axial dispersion, $J = -DdC/dz$, the above equation becomes:

$$\boxed{\varepsilon D \frac{d^2 C}{dz^2} - u_0 \frac{dC}{dz} - (1-\varepsilon)\rho_P kC = 0} \quad (1.9.15)$$

Part (g):

Defining the following variables and parameters:

$$y = C/C_0, \quad x = z/L, \quad Pe = u_0 L/D\varepsilon; \quad N = Wk/F \quad (1.9.16)$$

The derivatives can be written in terms of the new variables as follows:

$$\frac{dC}{dz} = C_0 \frac{dy}{dz} = C_0 \frac{dy}{dx} \frac{dx}{dz} = \frac{C_0}{L} \frac{dy}{dx} \quad \frac{d^2 C}{dz^2} = \frac{C_0}{L^2} \frac{d^2 y}{dx^2} \quad (1.9.17)$$

Substituting dC/dz and $d^2 C/dz^2$ in the material balance equation (Eq. 1.9.15):

$$\varepsilon D \frac{C_0}{L^2} \frac{d^2 y}{dx^2} - \frac{u_0 C_0}{L} \frac{dy}{dx} - (1-\varepsilon)\rho_P kC_0 y = 0 \quad (1.9.18)$$

Multiplying by $L/C_0 u_0$ and using $W = (1-\varepsilon)\rho_P LA$ and $F = u_0 A$, the above equation becomes:

$$\frac{D\varepsilon}{u_0 L} \frac{d^2 y}{dx^2} - \frac{dy}{dx} - \frac{Wk}{F} y = 0 \quad (1.9.19)$$

From the definition of Pe and N , the final equation is:

$$\boxed{\frac{1}{Pe} \frac{d^2 y}{dx^2} - \frac{dy}{dx} - Ny = 0} \quad (1.9.20)$$

For the boundary conditions:

$$u_0 C_0 = -\varepsilon D \frac{C_0}{L} \frac{dy}{dx} \Big|_{x=0} + u_0 C_0 y|_{x=0} \quad \frac{C_0}{L} \frac{dy}{dx} \Big|_{x=1} = 0 \quad (1.9.21)$$

which are written in terms of new variables as:

$$1 = y|_{x=0} - \frac{1}{Pe} \frac{dy}{dx} \Big|_{x=0} \quad \frac{dy}{dx} \Big|_{x=1} = 0 \quad (1.9.22)$$

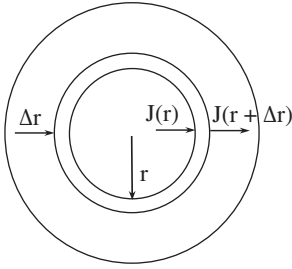
Therefore, for the two models:

$$\text{Model 1: } \boxed{\frac{dy}{dx} + Ny = 0} \quad (1.9.23)$$

$$\text{Model 2: } \boxed{-\frac{1}{Pe} \frac{d^2y}{dx^2} + \frac{dy}{dx} + Ny = 0} \quad (1.9.24)$$

It is seen that Model 2 reduces to Model 1 when $Pe \gg 1$, as the second order term becomes negligible.

Part (h):



Material Balance inside the catalyst gives the following equation:

$$(4\pi r^2)J|_r - (4\pi r^2)J|_{r+\Delta r} - kC_P(r)(4\pi r^2)\Delta r\rho_P = 0 \quad (1.9.25)$$

Dividing the above equation by $4\pi\Delta r$, we get:

$$-\frac{r^2 J|_{r+\Delta r} - r^2 J|_r}{\Delta r} - kC_P r^2 \rho_P = 0 \quad (1.9.26)$$

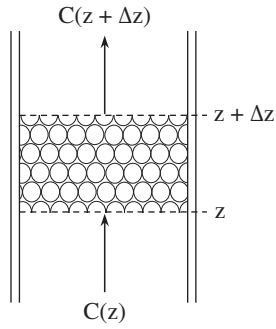
Taking the limit as $\Delta r \rightarrow 0$ and substituting Fick's Law of diffusion, $J = -D_e dC_P/dr$, we obtain:

$$\boxed{D_e \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dC_P}{dr} \right) - \rho_P k C_P = 0} \quad (1.9.27)$$

Part (i):

The boundary conditions state that at the surface of the particle, ($r = R$), the concentration of the toxic gas in the catalyst is the same as that in the flowing gas. In

the interior of the catalyst particle the concentration profile is a continuous function of r .



Material Balance Excluding Catalyst Volume gives:

$$\text{RATE IN} - \text{RATE OUT} - \text{RATE ENTERING CATALYST} = 0 \quad (1.9.28)$$

Mathematically, the above equation can be written as:

$$C(z)u_0A|_z - C(z)u_0A|_{z+\Delta z} - (1 - \epsilon)a[-J(R)]A\Delta z = 0 \quad (1.9.29)$$

where we note that $J(R)$ is a negative flux and:

$$a = \frac{\text{surface area}}{\text{volume particle}} = \frac{4\pi R^2}{4\pi R^3/3} = \frac{3}{R} \quad (1.9.30)$$

Dividing Eq. (1.9.29) by $A\Delta z$, taking the limit as $\Delta z \rightarrow 0$ and substituting the expression for a and $J(R) = -D_e dC_p/dr|_{r=R}$, we obtain:

$$\boxed{-u_0 \frac{dC}{dz} = (1 - \epsilon) \frac{3}{R} D_e \frac{dC_p}{dr} \Big|_{r=R}} \quad (1.9.31)$$

Problem 1.10

Dimensional Analysis of a Correlation

Part (a):

Solve $2 = 3x + y$

$$1 = 3x$$

$\therefore x = 1/3$ and $y = 4/3$

Given $c = 0.35$, show that

$$P_m = \text{Power/mass} = g u_{0g}.$$

Take $\epsilon = \text{void fraction}$

$$P_m = \frac{(A u_{0g})[\rho_L g h(1 - \epsilon)]}{\rho_L A h(1 - \epsilon)} = \frac{\text{vol.flow (hydro head)}}{\text{mass liquid}}$$

$$\therefore P_m = g u_{0g}$$

and given $\delta = d$ (eddy scale)

$$\boxed{D_e = 0.35(g u_{0g})^{1/3} d^{4/3}} \quad (1.10.1)$$

END OF CHAPTER 1