Solution Manual to Mass Transfer Processes

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Contents

0.1   Introduction

This solution manual contains answers to review questions for all chapters and solutions to most problems in the book.

If any clarification is needed, please feel free to e-mail me. The feedback from instructions is most appreciated together with pointing out any errors which will go into updating this solution book. I will be very happy to supply additional details on any of these problems if needed.

Please note that I have taken care in the preparation of this manual, but I make no expressed or implied warranty of any kind and assume no responsibility for errors or omissions. No liability is assumed for incidental or consequential damages in connection with or arising out of the use of the information contained herein.

1   Chapter 1

1.1   Answers to Review Questions

1. *What is meant by concentration jump?*
   The concentration becomes discontinuous as we cross from one phase to another and this known as the concentration jump.

2. *What is meant by the continuum assumption and what are its implications in model development?*
   Continuum assumption assumes that the matter is continuously distributed in space and ignores the atomic/molecular nature of matter. This permits us to assign a point value to the variables such as concentration and so on. The information on the interaction of molecules is however lost and has to be supplemented by suitable constitutive model.

3. *Indicate some situations where the continuum models are unlikely to apply.*
   Continuum models are unlikely to apply if there are not sufficient number of molecules in the volume of interest. The number should be large so that the statistical average can be assigned to the ensemble of molecules. For example in high vacuum system or a plasma reactor the number of molecules are small and continuum description may not be adequate.

4. *Give an example of a system where the total concentration is (nearly) constant.*
   Gas mixture at constant total pressure and temperature.

5. *Give an example of a system where the mixture density is nearly constant.*
   Liquid mixtures of compounds with similar chemical nature.

6. *Can average molecular weight be a function of position?*
   Yes. Since in a diffusing binary system, the mole fraction of A varies along the position and correspondingly the molecular weight will vary as a function of position.

7. *What information is missing in the differential models based on the continuum assumption?*
   Information on the transport rate caused by molecular motion is missing in the context of continuum models.

8. *Why are constitutive models needed in the context of differential models?*
   Molecular level transport occurs due molecular motion and is not modeled in the continuum level of modeling. In order to incorporate these effects, a constitutive model is needed to quantify the diffusion flux.

9. *Does the Fick's law apply universally to all systems?*
   No. It is specific since it is the result of the of molecular level interactions. These are system specific. It is an accurate model for binary gas mixture at low or moderate pressures. However it is commonly used as a first level model for a large class of problems.

10. *Write a form of Fick's law using partial pressure gradient as the driving force.*
    Using $C_A = p_A/R_gT$ we can write Fick's law using partial pressure gradient as:

    $$J_{Ax} = -\frac{D_A}{R_gT}\frac{dp_A}{dx}$$

11. *What is meant by the invariant property of the flux vector?*
    A vector remains same if the coordinates are rotated or if different coordinate system (e.g., cylindrical) is used and this is known as the invariance property of the flux vector.

12. *The combined flux is partitioned into the sum of the convection and diffusion flux. Is this partitioning unique?*
    No; It is not unique. It will depends on how the mixture velocity is defined and thereby what part of the combined flux is allocated to the convection flux.

13. *State the units of the gas constant if the pressure is expressed in bar instead of Pa, (ii) if expressed in atm.* Gas constant will have a value of 8.205×10^{-5}m^3 atm/mol K if pressure is expressed atm.
    It will have a value of 8.314×10^{-5} if pressure is in bars.

14. *Express the dissolved oxygen concentration in Example in p.p.m.*
    The concentration of dissolved oxygen was calculated as 0.2739 mol/m^3. This can be converted to gm/gm using the molecular weight (32 g/g) and also using the liquid density of water. The result is 8.467×10^{-6}. This corresponds to 8.467 p.p.m.

15. *What is a macroscopic level model? What information needs to be added here in addition to the conservation principle?*
    A larger control volume or the whole reactor or separator is taken as the control volume in a macroscoipc model. The control volume does not tend to zero. Hence the local information is lost and needs to be added as additional closure information in addition to the conservation law.

16. *How is mass transfer coefficient defined? Why is it needed?* The flux across a surface is not available in the meso- or macro-models since it depends on the local concentration gradient in accordance to Fick's law. Hence the flux is represented as a product of a mass transfer coefficient and a suitably defined driving force. It it therefore needed in the meso- and macro- scale model.

17. *What is meant by a cross-sectional average concentration? What is a cup mixing or the bulk concentration?*

In the cross-section average the local concentration is weighted by the local area and integrated over the cross-section. One then divides this by the total area to get the cross-sectional average.

In the cup mixing average, the local concentration is weighted by the local volumetric flow rate and integrated over the cross-section. One the divides this by the total volumetric flow rate to get the cup mixing concentration.

18. *What assumptions are involved in plug flow model?*
    The cup mixing concentration is assumed to be the same as the cross-sectional average concentration for a plug flow idealization.

19. *What assumptions are involved in a completely backmixed model?*
    The average concentration in the reactor and the exit concentration are assumed to be the same in a completely backmixed reactor.

20. *What additional closure is needed for mass transport in turbulent flow? Why?*
    The contribution of the turbulent diffusivity (eddy diffusivity) should be added in addition to molecular diffusivity to calculate the flux across a control surface. This extra term arises due to the fluctuations in velocity causing additional transport.

21. *What is an ideal stage contactor? How do you correct if the stage is not ideal?* The exit streams leaving a two phase contactor are assumed to be in equilibrium in an ideal stage contactor. If the stage is not ideal, it is corrected by using a stage efficiency factor.

22. *What is the dispersion coefficient and where is it needed?*
    Dispersion coefficient connects the cup mixing and cross-sectional averages by using a Fick's type of relation. It is needed to close the mesoscopic models in systems where a chemical reaction is taking place, e. g., tubular flow reactors.

1.2   Solutions to Problems

1. **Mass fraction to mole fractions:** Show that mass fractions can be converted to mole fractions by the use of the following equation:

$$y_i = \frac{\omega_i}{M_i}\bar{M} \qquad (1.1)$$

Derive an expression for dy_i as a function of $d\omega_i$ values. Do this for a binary mixture. Expression for multicomponent mixture becomes rather unwieldy!
Solution:
The mass fraction has the units of kg i / kg total.
The molecular weight of gas i has the unit of kg i / mol i
Dividing these we get $\frac{\omega_i}{M_i}$ which has the units of mol i/ kg total. Then dividing by the average molecular weight $\bar{M}$ which has the unit of kg total/ mol total, we get mol i/ mol total which is the mole fraction. Hence the relation is verified.
To get dy_i one should note that $\bar{M}$ is a function of ω_i.

$$\bar{M} = \left(\frac{1}{\omega_A/M_A + \omega_B/M_B} \right)$$

Hence

$$y_A = \frac{\omega_A}{M_A}\left(\frac{1}{\omega_A/M_A + \omega_B/M_B} \right)$$

and $\omega_B = 1 - \omega_A$.
Differentiating and after some algebraic manipulations we get the following relation for dy_i as a function of $d\omega_i$ values.

$$dy_A = \frac{\bar{M}^2}{M_A M_B}d\omega_A$$

2. **Mole fraction to mass fractions:** Show that mole fractions can be converted to mass fractions by the use of the following equation:

$$\omega_i = \frac{y_i M_i}{\bar{M}} \qquad (1.2)$$

Derive an expression for $d\omega_i$ as a function of dy_i values for a binary mixture.
Solution:
The mole fraction has the units of mol i / mol total.
The molecular weight gas i has the unit of kg i / mol i
Multiplying these we get kg i/ mol total and then dividing by the average molecular weight which has the unit of kg total/ mol total, we get kg i/ kg total which is the mass fraction. Hence the relation is verified.
To get $d\omega_A$ one should note that $\bar{M}$ is a function of y_i. We have for a binary :

$$\bar{M} = y_A M_A + (1 - y_A)M_B$$

Using this in the expression for ω_A and differentiating it and simplifying the algebra, we get

$$\frac{M_A M_B}{\bar{M}^2} dy_A$$

which is the required relation connecting the mass fraction gradient and the mole fraction gradient.

3. **Average molecular weight:** At a point in a methane reforming furnace we have a gas of the composition: $CH_4 = 10\%$; $H_2 = 15\%$; $CO = 15\%$ and $H_2O = 10\%$ by moles.

Find the mass fractions and the average molecular weight of the mixture. Find the density of the gas.

Solution:

Assume the rest is nitrogen which was not specified as part of the problem. Calculations of this type are best done in EXCEL spreadsheet or using a simple MATLAB snippet.

```
% mass fraction calculations
 y = [0.1  0.15  0.15 0.1  0.5]
 M = [ 18 2 28 18 28 ] % note  g/mol unit
 Mbar = sum (y .*M)
 omega = y.*M/Mbar

 %% The results are
Mbar =  22.100 g/mol
omega = [   0.081448   0.013575   0.190045   0.081448   0.633484 ]
```

4. **Average molecular weight variations:** Two bulbs are separated by a long capillary tube which is 20cm long. On one bulb we have pure hydrogen while at the other bulb we have nitrogen. The mole fraction profile varies in a linear manner along the length of the capillary. Calculate the mass fraction profile and show that the variation is not linear. Also calculate the average molecular weight as a function of the length along the capillary.

Solution:

Mole fraction profile is given as linear. Hence at any location the mole fraction can be calculated as a linear interpolation between the two end point values. For example at distance X = 4cm, the mole fraction of hydrogen is $(1 - 4/20)$ = 0.8.

Correspondingly the average molecular weight at this point is $0.8 \times 2 \times 10^{-3} + 0.2 \times 28 \times 10^{-3} = 7.2$ g/mol.

The mass fraction at this point is $2 \times 0.8 / \bar{M} = 0.22$.

Similar calculations can be done at other points. For example at distance $x = 16cm$, we get the mass fraction as 0.0175.

The mass fraction profile is seen to be not linear while the mole fraction is. Similarly the average molecular weight is a function of position.

5. **Mass fraction gradient:** For a diffusion process across a stagnant film, the mole fraction gradient of the diffusing species was found to be constant. What is the mass fraction gradient? Is this also linear? The mixture is benzene-air.

   Solution:

   The mole fraction gradient is constant. Hence the mole fraction profile is linear. The average molecular weight at any location is given as the weighted average of the two species:

   $$\bar{M} = 78X + 29(1 - X)$$

   where X is a scaled distance at the two ends. (Here we assume $X = 0$ is air while $X = 1$ is benzene.)

   The mass fraction profile is related to the mole fraction profile as:

   $$\omega_A = \frac{M_A x_A}{M_A x_A + (1 - x_A)M_B}$$

   This is found to be nonlinear (due to the terms in the denominator). Correspondingly the mass fraction gradient is also nonlinear.

6. **Total concentration in a liquid mixture:** Find the total molar concentration and species concentrations of 10% ethyl alcohol by mass in water at room temperature.

   Solution:

   The total molar concentration is equal to density of the mixture divided by the average molecular weight of the mixture.

   Density of alcohol is 0.7935 g/cm^3. The average density at a mass fraction of 0.1 is calculated by interpolation using the following relation:

   $$\frac{1}{\rho} = \frac{\omega_A}{\rho_A^0} + \frac{\omega_B}{\rho_B^0}$$

   The superscripts indicate pure component values.

   The calculated value is 0.9746 g/cm^3.

   It may be noted that the solution is not ideal and hence the density is to be found from partial molar volume considerations for a more accurate result. The density from internet data base is $0.98187 g/cm^3$ which is the more accurate value.

   The average molecular weight is calculated from the following equation:

   $$\frac{1}{\bar{M}} = \sum \frac{\omega_A}{M_A}$$

   The value is found as 19.16 g/mol.

   Hence the total molar concentration, C of the mixture is $\rho/\bar{M} = (0.9784 g/cm^3)/(19.16 g/mol) = 0.0509 mol/cm^3 = 50866 mol/m^3$.

7. **Effect of coordinate rotation on flux components:** In Figure 1.1, the flux vector is $2e_x + e_y$. Now consider a coordinate system which is rotated by an angle θ. Find this angle such that the flux component N_{Ay} is zero. What is the value of N_{Ax} in this coordinate system?

Solution: The original unit vectors in the two coordinates are related to the unit vectors in the new coordinates as follows:

$$\mathbf{e_x} = \mathbf{e_x; new} \cos\theta - \mathbf{e_y; new} \sin\theta$$

$$\mathbf{e_y} = \mathbf{e_x; new} \sin\theta + \mathbf{e_y; new} \cos\theta$$

The original vector is $2\mathbf{e_x} + \mathbf{e_y}$ and this gets is transformed to:

$$\mathbf{e_x; new}[2\cos\theta\sin\theta] + \mathbf{e_y; new}[-2\sin\theta + \cos\theta]$$

New components are therefore $[2\cos\theta\sin\theta]$ and $[-2\sin\theta + \cos\theta]$.
If the flux component N_{Ay} in the new coordinates has to be zero, then

$$-2\sin\theta + \cos\theta = 0$$

The angle of rotation must then be such that $\tan\theta = 1/2$. Hence $\theta = \pi/4$.
The value of N_{Ax} is then $2\cos\theta\sin\theta$.

8. **Flux vector in cylindrical coordinates:** Define flux vector in terms of its components in cylindrical coordinates. Sketch the planes over which the components act. Show the relations between these components and the components in Cartesian coordinates.
   Solution:
   Flux vector is the same in cylindrical coordinates but the components are different. The flux vector is represented as:

$$N_A = \boldsymbol{e}_r N_{Ar} + \boldsymbol{e}_\theta N_{A\theta} + \boldsymbol{e}_z N_{Az}$$

The component N_{Ar} can be viewed as the mass crossing a unit area in a plane normal to the r-direction in cylindrical coordinates. The other components can be viewed in a similar manner. Thus, for example, $N_{A\theta}$ is the moles crossing a plane perpendicular to the θ direction.
The components are related to those in Cartesian by the following relations from vector transformation rules.

$$e_r = (\cos\theta)e_x + (\sin\theta)e_y$$

$$e_\theta = (-\sin\theta)e_x + (\cos\theta)e_y$$

$$e_z = e_z$$

9. **Flux vector in spherical coordinates:** Define flux vector in terms of its components in spherical coordinates. Sketch the planes over which the components act. Show the relations between these components and the components in Cartesian coordinates.
   Show the relations between these components and the components in Cartesian coordinates.
   Solution:

. The flux vector in spherical coordinates is represented as:

$$N_A = e_r N_{Ar} + e_\theta N_{A\theta} + \phi_z N_{A\phi}$$

The components are interpreted as mass crossing a unit area in a plane normal to the direction indicated in the subscript.

For example, $N_{A\theta}$ is the moles crossing a plane perpendicular to the θ direction.

The components are related to those in Cartesian by the following relations from vector transformation rules.

$$e_r = (\sin\theta\cos\phi)e_x + (\sin\theta\sin\phi)e_y + (\cos\theta)e_z$$

$$e_\theta = (\cos\theta\cos\phi)e_x + (\cos\theta\sin\phi)e_y + (-\sin\theta)e_z$$

$$e_\phi = (-\sin\phi)e_x + (-\cos\phi)e_y + (0)e_z$$

10. **Different forms of the Henry's law constant:** Express the Henry's constants reported in Table 1.4 as $H_{i,pc}$ and $H_{i,cp}$.

    Solution:

    The relation for mole fraction in the liquid is x_A equals C_A/C_{tot} Using this in the Herny law

    $$p_A = H_A x_A = (H_A/C_{tot})x_A$$

    Hence the Henry coefficient in pressure-concentration unit is given as

    $$H_{pc} = H_A/C_{tot}$$

    Henry's law in pressure-concentration form for hydrogen is therefore:

    $$H_{H,pc} = (7.099 \times 10^4; \text{atm}]/(55000; \text{mol/m}^3) = 1.2907 \text{atm m}^3/\text{mol}$$

    In the concentration-pressure unit, it is the reciprocal of this quantity, 0.7748mol/atm m^3

    Values for other gases are: Oxygen $= 0.7744$; $CO_2 = 0.0296$; ammonia $= 5.4545 \times 10^4$. in pressure-concentration unit.

11. **Henry's law constants: Unit conversions:** Henry's law constant for O_2 and CO_2 are reported as 760.2 L. atm/mol and 29.41 L. atm /mol.

    What is the form of the Henry's law used? Convert to values for the other forms shown in the text.

    Solution:

    From the units we deduce that the Henry's law is reported in pressure-concentration form.

    To get the value in pressure-mole fraction form we use $C_A = x_A C$ where C is the total concentration in the liquid. Value of 55 mol/L is used for the total concentration in water. Hence the Henry's law in pressure-mole fraction form

is:

$$H = (760.2 \text{L.atm/mol})(55 \text{mol/L}) = 4.18 \times 10^4 \text{atm}$$

Similar calculation for CO_2 shows the value of $1.617 \times 10^3 \text{atm}$

12. **Solubility of CO_2:** Henry's constant values for CO_2 is shown below as a function of temperature.

Temperature, K	280	300	320
H, bar	960	1730	2650

Fit an equation of the type:

$$\ln H = A + B/T$$

What is the physical significance of the parameter B? Find the solubility of pure CO_2 in water at these temperature.

Solution:

The plot $\ln H$ as $1/T$ should be linear and the constants A and B can be found from this plot. However, it is best to use a linear regression model in MATLAB. The following MATLAB code is useful for the linear regression and can be used in general for other problems.

```
% Linear regression:   problem 1.12 CO2 solubility data.

% P = POLYFIT(X,Y,N) finds the coefficients of a polynomial P(X) of
  %  degree N that fits the data Y best in a least-squares sense. P is a
  %  row vector of length N+1 containing the polynomial coefficients in
  %  descending powers, P(1)*X^N + P(2)*X^(N-1) +...+ P(N)*X + P(N+1).
 x  = [ 280 300 320 ] %% temperature values
 y = [960 1730 2650 ]  %% henry values in bars
 Y = log (y)
 X = 1./x
 P = polyfit (X, Y, 1 ) % linear fit here.
 Y1 = P(2) + P(1) * X  %% fitted constants
 %%% comparison plots
 plot ( X,Y, '*' ); hold on
 plot (X, Y1)
 delh = 8.314 * P(1)  % heat of solution Answer= -19 kJ/mol
 % solutions: B = -2.2792e+003;  % A=  15.0215
```

The fitted constants are found to be $B = -2.2792e + 003$ and $A = 15.0215$
The parameter B is a measure of heat of solution in accordance with van't Hoff equation:

$$B = \frac{\Delta H_s}{R}$$

From the fitted data we find the heat of solution of CO_2 as -19 kJ/mol which is close to experimental value of -19.4kJ/mol reported in the literature.

13. **Vapor pressure calculations: the Antoine equation:** The Antoine constants for water are: $A = 8.07131$; B=1730.63; $C = 233.426$ in the units of mm Hg for pressure and deg C for temperature. Convert this to a form where pressure is in Pa and temperature is in deg K;

Also rearrange the Antoine equation to a form where temperature can be calculated explicitly. This represents the boiling point at that pressure. What is the boiling point of water at Denver, CO (mile high city)?

Solution:

$$p(\text{Pa}) = p(\text{mm})\frac{1.0135 \times 10^5 Pa/atm}{760 mm/1 atm}$$

Taking log

$$\log_{10} p(\text{mm Hg}) = \log_{10} p(\text{Pa}) - \log(0.0075) = \log_{10} p(\text{Pa}) - 2.1249$$

Using this in Antoine equation and substituting for $\log_{10} p(\text{mm Hg})$ we get

$$\log_{10} p(\text{Pa}) = 2.1229 - \frac{B}{C + T(K) - 273}$$

or

$$\log_{10} p(\text{Pa}) = 10.1962 - \frac{1730.63}{T(K) - 39.57}$$

which is the required relation with pressure in Pa and temperature in deg K. The equation can be rearranged to be explicit in temperature and the following relation is obtained:

$$T = \frac{B}{\log_{10} p - A} - C$$

The pressure at Denver at normal condition is given as:

$$p/p_0 = \exp(-\frac{M_{air}gh}{R_g T})$$

from the equation of hydrostatics. Here p_O is the pressure at sea level. $M_w = 20 \times 10^{-3} kg/mol$ and h = elevation = 1 mile = 1600 m.

Hence p = 367 mm Hg. Substituting in the Antoine equation we find the boiling point of water as 95 deg Celsuis.

14. **van't Hoff relation:** Given the Antoine constants for a species, can you calculate the heat of vaporization of that species? Find this value for water from the data given in Problem 1.12.   Solution:

One should use the van't Hoff relation as a first approximation. The relation is:

$$\frac{d \ln P; vap}{dT} = \frac{\Delta H; vap}{R_g T^2}$$

The integrated form is:

$$\ln P; vap = \frac{-\Delta H_{vap}}{R_g T} + A$$

This is similar to the Antoine equation with a minor difference on the temperature term. Overall, a plot of $\ln P; vap$ vs $1/T$ should be linear. From the slop eof this plot the heat of vaporization can be estimated.

Using the Antoine equation we find $P = 0.0419 bar$ at $T = 303K$.

Similarly $P = 1.0008 bar$ at $T = 373K$.

Taking the slope of $\ln P$ as $1/T$. the value of heat of vaporization is found as $4.1 \times 10^4 J/mol$ which is an average value over the temperature range. It may be noted that the heat of vaporization is a mild function of temperature which is ignored in these calculations.

15. **Concentration jump:** A solid rock of NaCl is in contact with water. Calculate the concentration of NaCl on the water side and salt side of the interface in mol/m^3.

    Solution: On the salt side the concentration is that corresponding to the density of solid salt which has a value of $2.16 g/cm^3$. Dividing by molecular weight, the concentration on the salt side is $37000\ mol/m^3$.

    On the water side the salt concentration corresponds to the saturation solubility of the salt. This is found from data sources as 39 g in 100 g water. Dividing by molecular weight and using the density of solution as $1 g/cm^3$ as an approximation, we find the concentration of salt on the water side as 6.495 mol/m^3.

16. **A well mixed reactor - mass balance calculation:** Consider a well stirred reactor where a reaction $A \to B$ is taking place. The volumetric flow rate is 1 m^3/s and the reactor volume is 0.3 m^3. Inlet concentration of A is 1000 mol/m^3 and the exit concentration is 200 mol/m^3. What is the rate of reaction of A in the system? If the reaction is first order and the contents are well mixed, what is the value of the rate constant?

    Solution:

    In - Out + Generation = 0

$$\text{In} = 1\text{m}^3/\text{s} \times 1000\text{mol/m}^3 = 1000\text{mol/s}$$

$$\text{Out} = 1\text{m}^3/\text{s} \times 200\text{mol/m}^3 = 200\text{mol/s}$$

Hence generation = -800 mol/s. Dividing by the volume of the reactor of 0.3 m^3 we get the rate of reaction as -2667mol/m^3; s which is to be interpreted as the average rate of reaction in the well mixed reactor. The representative concentration is the exit concentration of 200mol/m^3. Dividing the rate by this concentration and assuming a first order reaction, we get the rate constant of 13.33 s^{-1}.

17. **Mass transfer coefficient calculation:** A naphthalene ball ($M_A = 128g/mol$ and $\rho_A = 1145kg/m^3$) is suspended in a flowing stream of air at 347K and 1atm pressure.. The vapor pressure of naphthalene is 666 Pa for the given temperature. The diameter of the ball was found to change from 2.1 cm to 1.9 cm over a time interval of one hour. Estimate the mass transfer coefficient from the solid to the flowing gas.

    Solution:

    The mass balance is:

    Accumulation = -out by evaporation

    The accumulation term is calculated as $d/dt(4\pi R^3/3\ \rho_s/M_S)$ as shown in the text.

    Since the change in radius is small, the term dR/dt can be calculated from a finite difference approximation as:

    $$\frac{dR}{dt} = \frac{R(t+dt-R(t)}{dt} = 0.1cm/3600s = 2.78 \times 10^{-5}cm/s.$$

    Hence the evaporation rate is $4\pi R^2 \rho_s M_s(dR/dt)$.. Using the density and molecular weight reported, we find the evaporation area rate of $1.25E-05mol/s$.

    This is represented in terms of the mass transfer coefficient, k_m as $4\pi R^2 k_m C_{As}$. The concentration at the surface C_{aS} is calculated from thermodynamic considerations as p_{vap}/R_gT. Using the data of vapor pressure, we find $C_{As} = 666/8.314/347 = 0.2309mol/m^3$.

    Hence the mass transfer coefficient is 0.0431 m/s.

18. **A model for VOC loss from a holding tank:** Wastewater containing a VOC at a concentration of 10mol/m³ enters an open tank at a volumetric flow rate of 0.2m³/min and exits at the same rate. The tank has a diameter of 4m and the depth of liquid in the tank is 1m. Concentration of VOC in the exit stream and the rate of release of VOC is requested by the EPA.

    Use the conservation law to set a up a model. State further assumptions you may need to complete the model. List the parameters needed to solve the problem.

    Solution:

    The mass balance is:

    In - Out + Generation - transferred to gas phase = 0

    The mathematical expressions are needed for each term and these are given as follows.

    In $= QC_{A,i}$

    Out $= QC_{A,e}$

    Generation $= -VR_A$; minus since VOC is consumed. The R_A is the average rate of reaction in the tank ($\langle R_A \rangle$). The volume is the reactor is assumed to be constant since the VOC evaporation is expected to be small.

    Finally the mass transfer is modeled as the driving force times a mass transfer coefficient. An overall coefficient from the bulk liquid to bulk is used here

denoted as $\bar{K}_m$. The mathematical representation for the transport rate is therefore: $A\bar{K}_m(\langle C_A \rangle - H_A C_{A;\text{gas}})$. Here A is the transfer area. This completes the equations for all the terms needed in the macroscopic balance.

The parameters and assumptions needed are the following:

– A mixing pattern in the liquid is to be assumed so that the average concentration needed in the rate equation and in the mass transfer equation can be assigned.

– The concentration in the gas phase needs to be known or has to be calculated from a separate mass transfer model for the gas phase. (or assumed as zero if evaporation is to a large body of gas).

– The partition coefficient of the VOC H_A needs to be known from thermodynamic database.

– Value of the average mass transfer coefficient $\bar{K}_m$ per unit transfer area needs to be known or estimated or measured.

19. **Averaging:** Velocity profile in laminar flow is

$$v_z(r) = v_{max}[1 - (r/R)^2]$$

What does v_{max} represent? How is it related to the pressure drop? Find the average velocity.

The concentration distribution at a given axial position for a solid dissolving from the wall is given by Equation 1.24. Find the cross-sectional average concentration. and compare the value with the cup mixing concentration calculated in Example 1.2.

Solution:

v_{max} is the velocity at $r = 0$ and hence it represents the center line velocity. The average velocity is calculated by performing the following integration:

$$< v > = \frac{1}{\pi R^2} \int_0^R 2\pi r v_{max}[1 - (r/R)^2] dr$$

Note that $2\pi r dr$ is the local area for flow at any radial location r and is used in the equation as the weighting factor for the velocity.

The result is $< v > = v_{max}/2$. An useful result worth memorizing.

The cross-sectional average is calculated by doing the following integration:

$$< c >_A = \frac{1}{\pi R^2} \int_0^R 2\pi r v_{max}[1 - (r/R)^2] c_A(r) dr$$

For the given problem c_A as a function of r is given as:

$$c_A = \frac{C_A(r)}{C_{As}} = (r/R)^2 - (r/R)^4/4 + 1/4$$

Using this and performing the integration we get the cross-sectional concentration as $2/3 = 16/24$.

The cup mixing concentration was found in the text as: $13/24$.

20. **Cup mixing vs cross-sectional average:** The variation of scaled concentration in a laminar flow tubular reactor was measured fitted to the following

equation at a specified axial position:

$$c_A = 0.5[1 - (r/R)^2 + (r/R)^4/2]$$

Calculate the center, wall, cup mixing and cross-sectional average concentrations.

Solution:

The center concentration is obtained simply by substituting $r = 0$. and equal to 0.5.

The wall concentration is obtained by substituting $r = R$ and is equal to 0.25.
The cup mixing concentration is calculated as the ratio of the the two integrals shown next:

$$C_{Ab} = \frac{\int_A vC_A dA}{\int_A v dA} = \frac{\langle vC_A \rangle}{\langle v \rangle}$$

The velocity profile in laminar flow is given in the previous problem. The concentration profile is given as a part of the problem statement. Using these in the definition of the cup mixing concentration, the integrals are evaluated using WOLFRAM integral tool.

The cross-section concentration is calculated from the following integral:

$$\langle C \rangle_A = \frac{\int_A C_A dA}{\int_A dA}$$

where $dA = 2\pi r dr$.

The integrated value is $1/3$ using symbolic integration in MATLAB and this is the cross-sectional concentration.

21. **Turbulent flow velocity profile:** Velocity profile in turbulent flow is commonly modeled by the 1/7-th law:

$$v_z(r) = v_c[1 - (r/R)]^{1/7}$$

What does v_c represent? Find the average velocity. Compare the difference between the average velocity and the center line velocity.

Solution:

The average velocity is calculated as:

$$< c >_A = \frac{1}{\pi R^2} \int_0^R 2\pi r v_{max}[1 - (r/R)]^{1/7} c_A(r) dr = \frac{49}{60} v_{max}$$

Center velocity is v_{max} and is therefore 60/49 times the average velocity. Another useful result to remember.

This may be contrasted with the laminar flow where the center velocity is twice the average velocity.