CBE 548: Advanced Transport Phenomena II
Spring, 2010
Final Exam

Problem 1. Arbitrary Formulation of the Description of Mass Transfer

The multicomponent Fick diffusivities, $D_{\alpha\beta}^{\otimes}$, are defined with the following equations and constraints (BSL2, p. 767)

$$D_{\alpha\beta}^{\otimes} = -\frac{cRTa_{\alpha\beta}}{\rho_\alpha \rho_\beta} \tag{1.1}$$

$$D_{\beta\alpha}^{\otimes} = D_{\alpha\beta}^{\otimes} \tag{1.2}$$

$$\sum_{\alpha=1}^{N_c} w_\alpha D_{\alpha\beta}^{\otimes} = 0 \tag{1.3}$$

to be used in the generalized Fick equations, constitutive equations for the mass diffusive flux of component α relative to the center of mass velocity, of the form (BSL2 eq (24.2-3), p. 767)

$$\mathbf{j}_\alpha = -D_\alpha^T \nabla \ln(T) + \rho_\alpha \sum_{\beta=1}^{N_c} D_{\alpha\beta}^{\otimes} \mathbf{d}_\beta \tag{1.4}$$

where the diffusional driving forces are given by (BSL2 eq (24.1-8), p. 766)

$$cRT\mathbf{d}_\alpha = c_\alpha RT \nabla \ln(a_\alpha) + (\phi_\alpha - w_\alpha)\nabla p - \rho_\alpha \mathbf{g}_\alpha + w_\alpha \sum_{\beta=1}^{N_c} \rho_\beta \mathbf{g}_\beta \tag{1.5}$$

For binary, isothermal diffusion, we frequently write Fick's law as

$$\mathbf{j}_\alpha = -\rho D \nabla w_\alpha \tag{1.6}$$

where $\mathbf{j}_\alpha = \rho w_\alpha (\mathbf{v}_\alpha - \mathbf{v})$ and $\mathbf{v} = w_\alpha \mathbf{v}_\alpha + w_\beta \mathbf{v}_\beta$.

Rigorously derive the relationship between D and $D_{\alpha\beta}^{\otimes}$. State all assumptions made. The relationship should be expressed <u>exclusively</u> in terms of mole fractions, mass fractions and $\frac{\partial \ln(a_\alpha)}{\partial \ln(x_\alpha)}$.

Some of the following relations may be useful to you.

$$x_1\left(\frac{\partial \overline{G}_1}{\partial x_1}\right)_{T,p} + x_2\left(\frac{\partial \overline{G}_2}{\partial x_2}\right)_{T,p} = 0 \quad \text{(Gibbs-Duhem equation, binary, isothermal, isobaric)}$$

$$\ln(a_1) = \frac{\overline{G}_1 - \underline{G}_1}{RT} \quad \text{(relation between partial molar Gibbs free energy and activity)}$$

$$\frac{\partial x_\alpha}{\partial w_\alpha} = \frac{x_\alpha x_\beta}{w_\alpha w_\beta} \quad \text{(for binary systems only)}$$

Solution:
For isothermal binary diffusion in the absence of external forces and pressure diffusion, the generalized Fick equations, eq. (1.4), become

$$\mathbf{j}_\alpha = \rho_\alpha \left(D_{\alpha\alpha}^{\otimes} \mathbf{d}_\alpha + D_{\alpha\beta}^{\otimes} \mathbf{d}_\beta \right) \tag{1.7}$$

Equation (1.3) becomes for a binary system

$$w_\alpha D_{\alpha\alpha}^{\otimes} + w_\beta D_{\beta\alpha}^{\otimes} = 0 \tag{1.8}$$

which can be rearranged as

$$D_{\alpha\alpha}^{\otimes} = -\frac{w_\beta}{w_\alpha} D_{\beta\alpha}^{\otimes} = -\frac{w_\beta}{w_\alpha} D_{\alpha\beta}^{\otimes} \tag{1.9}$$

Substitution of equation (1.9) into equation (1.7) yields

$$\mathbf{j}_\alpha = \rho_\alpha \left(-\frac{w_\beta}{w_\alpha} D_{\alpha\beta}^{\otimes} \mathbf{d}_\alpha + D_{\alpha\beta}^{\otimes} \mathbf{d}_\beta \right) = \rho \left(-w_\beta \mathbf{d}_\alpha + w_\alpha \mathbf{d}_\beta \right) D_{\alpha\beta}^{\otimes} \tag{1.10}$$

The diffusional driving forces for this system

$$cRT\mathbf{d}_\alpha = c_\alpha RT \nabla \ln(a_\alpha) \tag{1.11}$$

Substitution of equation (1.11) into equation (1.10) yields

$$\mathbf{j}_\alpha = \rho\left(-w_\beta x_\alpha \nabla \ln(a_\alpha) + w_\alpha x_\beta \nabla \ln(a_\beta) \right) D_{\alpha\beta}^{\otimes} \tag{1.12}$$

We can equate eq. (1.12) and (1.6) to yield

$$-\rho D \nabla w_\alpha = \rho\left(-w_\beta x_\alpha \nabla \ln(a_\alpha) + w_\alpha x_\beta \nabla \ln(a_\beta) \right) D_{\alpha\beta}^{\otimes} \tag{1.13}$$

Simplification yields

$$D = \left(w_\beta x_\alpha \frac{\partial \ln(a_\alpha)}{\partial w_\alpha} - w_\alpha x_\beta \frac{\partial \ln(a_\beta)}{\partial w_\alpha} \right) D_{\alpha\beta}^{\otimes} \tag{1.14}$$

Further simplification yields

$$D = \left(w_\beta x_\alpha \frac{\partial x_\alpha}{\partial w_\alpha} \frac{\partial \ln(a_\alpha)}{\partial x_\alpha} + w_\alpha x_\beta \frac{\partial x_\beta}{\partial w_\beta} \frac{\partial \ln(a_\beta)}{\partial x_\beta} \right) D_{\alpha\beta}^{\otimes} \tag{1.15}$$

Remember that for a binary system,

$$\frac{\partial x_\alpha}{\partial w_\alpha} = \frac{x_\alpha x_\beta}{w_\alpha w_\beta} \tag{1.16}$$

So that equation (1.15) becomes

$$D = \frac{x_\alpha x_\beta}{w_\alpha w_\beta}\left(w_\beta \frac{\partial \ln(a_\alpha)}{\partial \ln(x_\alpha)} + w_\alpha \frac{\partial \ln(a_\beta)}{\partial \ln(x_\beta)} \right) D_{\alpha\beta}^{\otimes} \tag{1.17}$$

From equilibrium thermodynamics, under constant temperature and pressure conditions, the Gibbs Duhem equation states

$$x_1\left(\frac{\partial \overline{G}_1}{\partial x_1}\right)_{T,p} + x_2\left(\frac{\partial \overline{G}_2}{\partial x_2}\right)_{T,p} = 0 \tag{1.18}$$

The partial molar Gibbs free energy can be related to the activity via

$$\ln(a_1) = \frac{\overline{G}_1 - \underline{G}_1}{RT} \tag{1.19}$$

$$\overline{G}_1 = RT\ln(a_1) + \underline{G}_1 \tag{1.20}$$

where $\underline{G}_1$ is the molar enthalpy of component 1 in the pure state. The derivative of the partial molar Gibbs free energy with respect to composition is

$$\left(\frac{\partial \overline{G}_1}{\partial x_1}\right)_{T,p} = \left(\frac{\partial\left(RT\ln(a_1) + \underline{G}_1\right)}{\partial x_1}\right)_{T,p} = RT\left(\frac{\partial \ln(a_1)}{\partial x_1}\right)_{T,p} \tag{1.21}$$

Substitution of (1.21) into (1.18) yields,

$$\left(\frac{\partial \ln(a_1)}{\partial \ln(x_1)}\right)_{T,p} = -\left(\frac{\partial \ln(a_2)}{\partial \ln(x_2)}\right)_{T,p} \tag{1.22}$$

Substitution equation (1.22) into (1.17) is

$$D = \frac{x_\alpha x_\beta}{w_\alpha w_\beta}\left(w_\beta - w_\alpha\right)\frac{\partial \ln(a_\alpha)}{\partial \ln(x_\alpha)} D_{\alpha\beta}^{\otimes} \tag{1.23}$$

You can see that equation (1.23) is symmetric with respect to interchange of α and β subscripts, as it must be.

Problem 2. Chemical Potential Gradient Driven Diffusion
Consider the steady state behavior of a three component fluid located in an isothermal and isobaric system between two boundaries. The thermodynamic state of the boundary at z = 0 is defined by the mole fraction of 1, $x_1 = 0.15$, mole fraction of 2, $x_2 = 0.84$, temperature T = 300 K, and pressure p = 1 bar. The thermodynamic state of the boundary at z = 1 m is defined by the mole fraction of 1, $x_1 = 0.10$, mole fraction of 3, $w_3 = 0.89$, temperature T = 300 K, and pressure p = 1 bar.

The chemical potential of component i in a multicomponent van der Waals gas is given by

$$\mu_i = -RT \ln\left(\frac{V_m - b_{mix}}{x_i \Lambda_i^3}\right) + \frac{RTb_i}{V_m - b_{mix}} - \frac{2}{V_m}\sum_{j=1}^{N_c} x_j a_{ij} \qquad (1)$$

where R is the gas constant, V_m is the molar volume, Λ_i is the thermal de Broglie wavelength. For this example, we will set all of the van der Waal b parameters (all b_i and b_{mix}) to zero. The values of a are as follows: $a_{11} = a_{22} = a_{33} = a_{13} = a_{23} = a_{31} = a_{32} = 0$, $a_{12} = a_{21} = 20$ Joules-m^3/mole. Consider the molar volume to be constant at $V_m = 2.35\text{x}10^{-2}$ m^3/mole.

Tasks.
(a) Using a finite difference formula, determine the average mole fraction gradients for each component, based on the boundary values.
(b) Based on the sign of the mole fraction gradients, in which direction would you expect the diffusive flux of each species to be?
(c) Using a finite difference formula, determine the average chemical potential gradients for each component, based on the boundary values.
(d) Based on the sign of the chemical potential gradients, in which direction would you expect the diffusive flux of each species to be?
(e) Based on your conclusions in parts (b) and (d), which fluxes will one actually observe, those given in part (b) or part (d)? Why?
(f) What is the common term given to the transport phenomena exhibited by one of the components?
(g) Name a chemical engineering unit operation in which this transport phenomena is frequently exploited.

Solution:
Consider the steady state behavior of a three component fluid located in an isothermal and isobaric system between two boundaries. The thermodynamic state of the boundary at z = 0 is defined by the mole fraction of 1, $x_1 = 0.15$, mole fraction of 2, $x_2 = 0.84$, temperature T = 300 K, and pressure p = 1 bar. The thermodynamic state of the boundary at z = 1 m is defined by the mole fraction of 1, $x_1 = 0.10$, mole fraction of 3, $w_3 = 0.89$, temperature T = 300 K, and pressure p = 1 bar.

The chemical potential of component i in a multicomponent van der Waals gas is given by

$$\mu_i = -RT\ln\left(\frac{V_m - b_{mix}}{x_i\Lambda_i^3}\right) + \frac{RTb_i}{V_m - b_{mix}} - \frac{2}{V_m}\sum_{j=1}^{N_c} x_j a_{ij} \tag{1}$$

where R is the gas constant, V_m is the molar volume, L_i is the thermal de Broglie wavelength. For this example, we will set all of the van der Waal b parameters (all b_i and b_{mix}) to zero. The values of a are as follows: $a_{11} = a_{22} = a_{33} = a_{13} = a_{23} = a_{31} = a_{32} = 0$, $a_{12} = a_{21} = 20$ Joules-m^3/mole. Consider the molar volume to be constant at $V_m = 2.35\text{x}10^{-2}$ m^3/mole.

Tasks.
(a) Using a finite difference formula, determine the average mole fraction gradients for each component, based on the boundary values.

$$\overline{\left(\frac{\partial x_1}{\partial z}\right)} = \frac{x_1(z=1) - x_1(z=0)}{1} = 0.1 - 0.15 = -0.05\,m^{-1} \tag{2.1}$$

$$\overline{\left(\frac{\partial x_2}{\partial z}\right)} = \frac{x_2(z=1) - x_2(z=0)}{1} = 0.01 - 0.84 = -0.83\,m^{-1} \tag{2.2}$$

$$\overline{\left(\frac{\partial x_3}{\partial z}\right)} = \frac{x_3(z=1) - x_3(z=0)}{1} = 0.89 - 0.01 = 0.88\,m^{-1} \tag{2.3}$$

(b) Based on the sign of the mole fraction gradients, in which direction would you expect the diffusive flux of each species to be?

One would expect that species diffuse from high mole fraction to low mole fraction.
Component 1 would move to the boundary at z = 1.
Component 2 would move to the boundary at z = 1.
Component 3 would move to the boundary at z = 0.

(c) Using a finite difference formula, determine the average chemical potential gradients for each component, based on the boundary values.

The chemical potential expressions are

$$\mu_1 = -k_B T \ln\left(\frac{V_m}{x_1 \Lambda_1{}^3}\right) - \frac{2}{V_m} x_2 a_{12} \tag{3.1}$$

$$\mu_2 = -k_B T \ln\left(\frac{V_m}{x_2 \Lambda_2{}^3}\right) - \frac{2}{V_m} x_1 a_{21} \tag{3.2}$$

$$\mu_3 = -k_B T \ln\left(\frac{V_m}{x_3 \Lambda_3{}^3}\right) \tag{3.3}$$

The average chemical potential gradients are

$$\begin{aligned}\overline{\left(\frac{\partial \mu_1}{\partial z}\right)} &= \frac{\mu_1(z=1) - \mu_1(z=0)}{1} = \\ &= -RT \ln\left(\frac{V_m}{x_1(z=1)\Lambda_1{}^3}\right) - \frac{2}{V_m} x_2(z=1) a_{12} + RT \ln\left(\frac{V_m}{x_1(z=0)\Lambda_1{}^3}\right) + \frac{2}{V_m} x_2(z=0) a_{12} \\ &= RT \ln\left(\frac{x_1(z=1)}{x_1(z=0)}\right) + \frac{2}{V_m} a_{12} \left[\left(x_2(z=0) - x_2(z=1)\right)\right]\end{aligned} \tag{4.1}$$

$$\overline{\left(\frac{\partial \mu_2}{\partial z}\right)} = RT \ln\left(\frac{x_2(z=1)}{x_2(z=0)}\right) + \frac{2}{V_m} a_{21} \left[\left(x_1(z=0) - x_1(z=1)\right)\right] \tag{4.2}$$

$$\overline{\left(\frac{\partial \mu_3}{\partial z}\right)} = RT \ln\left(\frac{x_3(z=1)}{x_3(z=0)}\right) \tag{4.3}$$

Numerical evaluation yields

$$\overline{\left(\frac{\partial \mu_1}{\partial z}\right)} = 401.6 \quad \text{kJ/mol/m} \tag{5.1}$$

$$\overline{\left(\frac{\partial \mu_2}{\partial z}\right)} = \text{-}10966 \quad \text{kJ/mol/m} \tag{5.2}$$

$$\overline{\left(\frac{\partial \mu_3}{\partial z}\right)} = 11196 \quad \text{kJ/mol/m} \tag{5.3}$$

(d) Based on the sign of the chemical potential gradients, in which direction would you expect the diffusive flux of each species to be?

One would expect that species diffuse from high chemical potential to low chemical potential.

Component 1 would move to the boundary at z = 0.
Component 2 would move to the boundary at z = 1.
Component 3 would move to the boundary at z = 0.

(e) Based on your conclusions in parts (b) and (d), which fluxes will one actually observe, those given in part (b) or part (d)? Why?

One will observe the fluxes predicted in part (d), because part (d) is based on the thermodynamic driving force for diffusion. Following the chemical potential gradient will lead the system to a lower free energy. Here, because component 1 interacts more favorably with component 2 than it does with component 3, the advantage of the energetic driving force outweighs the disadvantage of the entropic driving force associated with going up a concentration gradient.

(f) What is the common term given to the transport phenomena exhibited by one of the components?

Component one will display “uphill diffusion”, where it diffuses up the concentration gradient.

(g) Name a chemical engineering unit operation in which this transport phenomena is frequently exploited.

In liquid-liquid extraction, a good solvent is used to extract a solute from a less good solvent. The goodness of a solvent is really an indicator of the chemical potential of the solute in that solvent. Thus, one can extract a solute to a higher concentration in the good solvent than was originally present in the less good solvent, due to the overall reduction in free energy.

A code showing the calculations is given below.

```
close all;
clear all;
format long e;
%
%  parameters
%
R = 8.314; % J/mol/K
T = 300; % K
p = 101325; % Pa
a12 = 20.0; % J-m^3/mole^2
a21 = a12;
bmix = 0;
%
% boundary one (z=0)
%
x10 = 0.15;
x20 = 0.84;
x30 = 1 - x10 - x20;
amix = x10*x20*a12 + x20*x10*a21;
Vm0 = (R*T + sqrt( (R*T)^2 - 4*p*amix) )/(2*p)
%Vm2 = (kB*T - sqrt( (kB*T)^2 - 4*p*amix) )/(2*p)
%
% boundary two (z=1)
%
x11 = 0.1;
x31 = 0.89;
x21 = 1 - x11 - x31;
amix = x11*x21*a12 + x21*x11*a21;
Vm1 = (R*T + sqrt( (R*T)^2 - 4*p*amix) )/(2*p)
%Vm2 = (kB*T - sqrt( (kB*T)^2 - 4*p*amix) )/(2*p)
%
%  assume molar volume is constant
%  (to make the problem easier for the exam)
%  This number is given.
%
Vmavg = (Vm0 + Vm1)/2
Vm0 = Vmavg;
Vm1 = Vmavg;
%
%  mole fraction gradients
%
gradx1 = x11 - x10
gradx2 = x21 - x20
gradx3 = x31 - x30
%
%  chemical potential gradients
%
gradmu1 = R*T*log( (Vm0*x11)/(Vm1*x10) ) + 2*a12*( x20/Vm0 - x21/Vm1 )
gradmu2 = R*T*log( (Vm0*x21)/(Vm1*x20) ) + 2*a21*( x10/Vm0 - x11/Vm1 )
gradmu3 = R*T*log( (Vm0*x31)/(Vm1*x30) )
```

Problem 3. Differential balances

(a) Derive the continuity equation for a conical pipe, where the cross sectional area is a function of axial position and there is only spatial variation in properties in the axial dimension.

(b) Derive the mass balance for component A for a conical pipe, where the cross-sectional area is a function of axial position and there is only spatial variation in properties in the axial dimension.

(c) What is the equation for the mass fraction of A for an isothermal, binary system in the absence of convection and the presence of a first order reaction A → B, where $A_x(z) = bz + A_o$ and Ficks law is given as $j_A = -\rho D \frac{\partial w_A}{\partial z}$ and the reaction rate is given as $r_A = -kw_A$. Assume the density, diffusivity and reaction rate constant are all constant. Put this equation in the simplest form possible.

(d) What does the steady state profile of the mass fraction of A look like in a pipe of constant cross-sectional area and the absence of reaction?

(e) Comparing the results for the constant cross-sectional area pipe and the varying cross-sectional area pipe for the case without reaction, which will yield a higher composition of A at the outlet for the same inlet conditions?

Solution

(a) Derive the continuity equation for a conical pipe, where the cross-sectional area is a function of axial position and there is only spatial variation in properties in the axial dimension.

accumulation = in – out + generation

$$acc = \frac{\partial(\Delta V \rho)}{\partial t} \tag{3.1}$$

where the differential volume is $\Delta V = A_x \Delta z$. The in and out terms are

$$in = A_x \rho v_z\big|_z \tag{3.2}$$

$$out = A_x \rho v_z\big|_{z+\Delta z} \tag{3.3}$$

Substitute into the balance equation

$$A_x \Delta z \frac{\partial(\rho)}{\partial t} = A_x \rho v_z\big|_z - A_x \rho v_z\big|_{z+\Delta z} \tag{3.4}$$

Divide by the volume

$$\frac{\partial(\rho)}{\partial t} = \frac{1}{A_x} \frac{A_x \rho v_z\big|_z - A_x \rho v_z\big|_{z+\Delta z}}{\Delta z} \tag{3.5}$$

Take the limit as the differential length goes to zero.

$$\frac{\partial(\rho)}{\partial t} = -\frac{1}{A_x}\left(\frac{\partial A_x \rho v_z}{\partial z}\right) \tag{3.6}$$

Use the product rule to split terms.

$$\frac{\partial \rho}{\partial t} = -\left(\frac{\partial \rho v_z}{\partial z}\right) - \rho v_z \left(\frac{\partial \ln A_x}{\partial z}\right) \tag{3.7}$$

The second term disappears if the cross-sectional area is constant.

(b) Derive the mass balance for component A for a conical pipe, where the cross-sectional area is a function of axial position and there is only spatial variation in properties in the axial dimension.

accumulation = in – out + generation

$$acc = \frac{\partial(\Delta V \rho w_A)}{\partial t} \tag{3.1}$$

where the differential volume is $\Delta V = A_x \Delta z$. The in and out terms for convection and diffusion are

$$in = A_x \rho w_A v_z\big|_z + A_x j_A\big|_z \tag{3.2}$$

$$out = A_x \rho w_A v_z\big|_{z+\Delta z} + A_x j_A\big|_{z+\Delta z} \tag{3.3}$$

The generation term is

$$gen = \Delta V r_A \tag{3.4}$$

Substitute into the balance equation

$$A_x \Delta z \frac{\partial(\rho w_A)}{\partial t} = A_x \rho w_A v_z\big|_z - A_x \rho w_A v_z\big|_{z+\Delta z} + A_x j_A\big|_z - A_x j_A\big|_{z+\Delta z} + \Delta V r_A \tag{3.5}$$

Divide by the volume

$$\frac{\partial(\rho w_A)}{\partial t} = \frac{1}{A_x}\frac{A_x \rho w_A v_z\big|_z - A_x \rho w_A v_z\big|_{z+\Delta z} + A_x j_A\big|_z - A_x j_A\big|_{z+\Delta z}}{\Delta z} + r_A \tag{3.6}$$

Take the limit as the differential length goes to zero.

$$\frac{\partial(\rho w_A)}{\partial t} = -\frac{1}{A_x}\left(\frac{\partial A_x \rho w_A v_z}{\partial z}\right) - \frac{1}{A_x}\left(\frac{\partial A_x j_A}{\partial z}\right) + r_A \tag{3.7}$$

Use the product rule to split terms.

$$\frac{\partial(\rho w_A)}{\partial t} = -\left(\frac{\partial \rho w_A v_z}{\partial z}\right) - \rho w_A v_z\left(\frac{\partial \ln A_x}{\partial z}\right) - \left(\frac{\partial j_A}{\partial z}\right) - j_A\left(\frac{\partial \ln A_x}{\partial z}\right) + r_A \tag{3.8}$$

You can simplify this by subtracting the continuity equation from this equation.

$$\rho\frac{\partial(w_A)}{\partial t} = -\rho v_z\left(\frac{\partial w_A}{\partial z}\right) - \left(\frac{\partial j_A}{\partial z}\right) - j_A\left(\frac{\partial \ln A_x}{\partial z}\right) + r_A \tag{3.9}$$

(c) What is the equation for the mass fraction of A for an isothermal, binary system in the absence of convection and the presence of a first order reaction A → B, where $A_x(z) = bz + A_o$ and Ficks law is given as $j_A = -\rho D\frac{\partial w_A}{\partial z}$ and the reaction rate is given as $r_A = -kw_A$. Assume the density, diffusivity and reaction rate constant are all constant. Put this equation in the simplest form possible.

$$0 = -\left(\frac{\partial j_A}{\partial z}\right) - j_A\left(\frac{\partial \ln A_x}{\partial z}\right) + r_A \tag{3.10}$$

$$j_A = -\rho D\frac{\partial w_A}{\partial z} \tag{3.11}$$

$$r_A = -kw_A \tag{3.12}$$

Substitution of the diffusive flux, reaction rate and cross-sectional area into equation (3.10) yields

$$0 = \rho D\frac{\partial^2 w_A}{\partial z^2} + \rho D\frac{b}{bz + A_o}\frac{\partial w_A}{\partial z} - kw_A \tag{3.13}$$

This can be further simplified as

$$0 = \frac{\partial^2 w_A}{\partial z^2} + \frac{b}{bz + A_o}\frac{\partial w_A}{\partial z} - \frac{k}{\rho D}w_A \tag{3.14}$$

(d) What does the steady state profile of the mass fraction of A look like in a pipe of constant cross-sectional area and the absence of reaction?

$$0 = \frac{\partial^2 w_A}{\partial z^2} \tag{3.15}$$

This solution of this ODE is a straight line.

$$w_A(z) = w_{A,o} + \left.\frac{\partial w_A}{\partial z}\right|_{z_o} z \tag{3.16}$$

(e) What does the steady state profile of the mass fraction of A look like in the pipe with linearly varying cross-sectional area and the absence of reaction?

$$0 = \frac{\partial^2 w_A}{\partial z^2} + \frac{b}{bz + A_o}\frac{\partial w_A}{\partial z} \tag{3.17}$$

Let $X = \frac{\partial w_A}{\partial z}$

$$0 = \frac{\partial X}{\partial z} + \frac{b}{bz + A_o} X \tag{3.18}$$

$$\frac{\partial X}{X} = -\frac{b}{bz + A_o}\partial z \tag{3.19}$$

Integrate.

$$\ln\left(\frac{X}{X_o}\right) = -\ln\left(\frac{bz + A_o}{bz_o + A_o}\right) \tag{3.20}$$

$$X = \frac{bz_o + A_o}{bz + A_o} X_o \tag{3.21}$$

Substitute in for *X*.

$$\frac{\partial w_A}{\partial z} = \frac{bz_o + A_o}{bz + A_o}\left.\frac{\partial w_A}{\partial z}\right|_{z_o} \tag{3.22}$$

$$\partial w_A = \frac{bz_o + A_o}{bz + A_o}\left.\frac{\partial w_A}{\partial z}\right|_{z_o} \partial z \tag{3.23}$$

Integrate

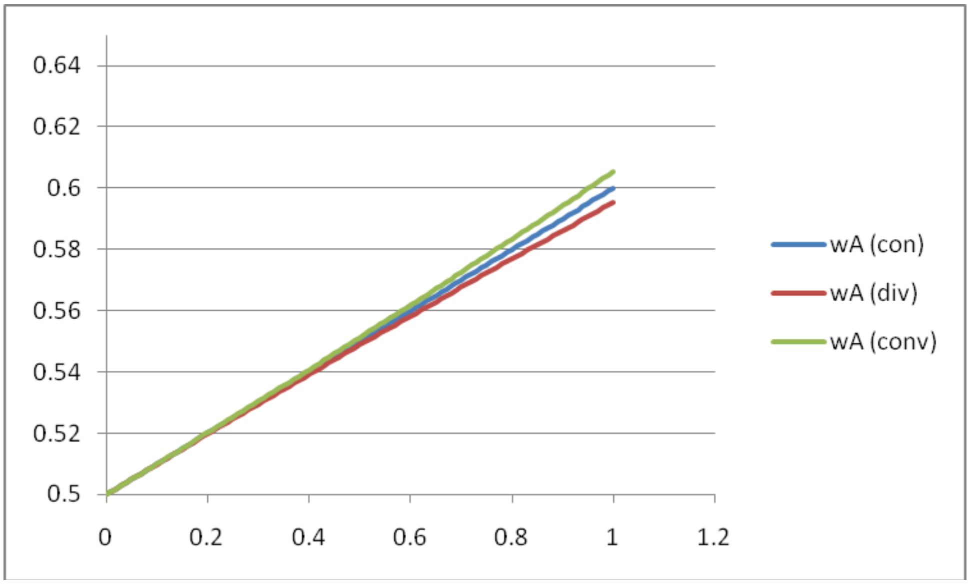
$$w_A - w_{A,o} = \frac{bz_o + A_o}{b} \left.\frac{\partial w_A}{\partial z}\right|_{z_o} \ln\left(\frac{bz + A_o}{bz_o + A_o}\right) \tag{3.24}$$

(e) Comparing the results for the constant cross-sectional area pipe and the varying cross-sectional area pipe for the case without reaction, which will yield a higher composition of A at the outlet for the same inlet conditions?

The question is whether the quantity $\frac{bz_o + A_o}{b} \ln\left(\frac{bz + A_o}{bz_o + A_o}\right)$, which is the factor in front of the initial slope in equation (3.24), is greater than or less than 1.

If b is positive and the pipe is diverging, then the composition of A at the outlet will be lower than the constant cross-sectional area pipe. If b is negative and the pipe is converging, then the composition of A at the outlet will be higher than the constant cross-sectional area pipe.

Typical Plot (not required) shown below



The following equations are provided for the exam. The continuity equation is

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{v}) \quad , \tag{A.1}$$

where ρ is the mass density, **v** is the center-of-mass velocity, and *t* is time. In BSL2, this is equation (3.1-4) on page 77 [1].

The mass balance on component A is

$$\rho \frac{\partial w_A}{\partial t} = -\rho \mathbf{v} \cdot \nabla w_A - \nabla \cdot \mathbf{j}_A + \sum_{i=1}^{N_R} r_{i,A} \quad , \tag{A.2}$$

where w_A is the mass fraction of component *A*, $\mathbf{j}_A$ is the diffusive mass flux of component *A* relative to the center-of-mass velocity, N_R is the number of independent chemical reactions in the system, and $r_{i,A}$ is the rate of production of component *A* in reaction *i*, in units of mass/volume/time. In BSL2, this is equation (19.1-14) on page 584.

The momentum balance is

$$\rho \frac{\partial \mathbf{v}}{\partial t} = -\rho \mathbf{v} \cdot \nabla (\mathbf{v}) - \nabla p - \nabla \cdot \boldsymbol{\tau} - \rho \nabla \hat{\Phi} \quad , \tag{A.3}$$

where *p* is the pressure, $\boldsymbol{\tau}$ is the extra stress tensor, and $\hat{\Phi}$ is the specific external field imposed by, for example, gravity. This equation is a the difference of equation (3.2-9) on page 80 of BSL2 and the continuity equation , equation(1).

The energy balance is

$$\frac{\partial \rho \left(\frac{1}{2} v^2 + \hat{U} + \hat{\Phi} \right)}{\partial t} = -\nabla \cdot \rho \left(\frac{1}{2} v^2 \mathbf{v} + \hat{U} \mathbf{v} + \hat{\Phi} \mathbf{v} \right) - \nabla \cdot \mathbf{q} - \nabla \cdot p \mathbf{v} - \nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{v}) \quad , \tag{A.4}$$

where $\hat{U}$ is the specific (per mass) internal energy, $\hat{\Phi}$ is the specific potential energy due to an external field, and **q** is the heat flux due to conduction. This is equation (11.1-9) on page 336 in BSL2.