ChE 548
Advanced Transport Phenomena II
Final Exam
Friday, May 1, 2009
8:00-10:00 AM

Problem 1. Mass Transfer
Consider diffusion of through a reactive membrane of component A, which can react to form B via the first order, irreversible reaction, A → B. The rate constant is given by

$$k = k_o \exp\left(-\frac{E_a}{RT}\right) \tag{1.a}$$

where the rate of reaction is given by

$$rate = k\rho_A \tag{1.b}$$

The heat of reaction for this reaction is small and the system can be assumed to be isothermal. The prefactor is $k_o = 1.0x10^{-2}\frac{1}{s}$, the activation energy is $E_a = 1.0x10^{4}\frac{J}{mol}$, R is the ideal gas constant, $R = 8.314\frac{J}{mol \cdot K}$, and the temperature is $T = 300\,K$. There is no convection in the membrane. The Fickian diffusivity is $D = 1.0x10^{-5}\frac{m^2}{s}$ and can be considered independent of composition. The membrane is of thickness $L = 0.05\,m$. One of boundaries of the membrane is fixed at $\rho_A = 0.7\frac{kg}{m^3}$ and $\rho_B = 0.0\frac{kg}{m^3}$.

(a) Write the transient total mass balance and mass of A balance.
(b) Determine the mass fraction of component A at the far side of the membrane at steady state.
(c) If you want the conversion to be 90%, how thick would the membrane have to be?

Problem 2. Reference States in Energy Balances
The enthalpy of component i can be written as

$$H_i(T,p) = \int_{T_{ref}}^{T} C_{p,i}(T,p)dT + \int_{p_{ref}}^{p}\left(\frac{\partial H_i}{\partial p}\right)_{T=T_{ref}} dp + H_{f,i}(T_{ref}, p_{ref}) \tag{1}$$

where $H_{f,i}$ is the enthalpy of formation at the reference state. Typically we ignore the pressure dependence of the enthalpy. It can be ignored in this problem as well.

Consider a system with accumulation, convection and diffusion of a binary mixture, in which the mixture enthalpy is ideal

$$H_{mix}(T,p) = w_A H_A(T,p) + w_B H_B(T,p) \quad (2)$$

The total conduction in the system is due to thermal conduction and enthalpy carried by diffusion,

$$\mathbf{q} = -k_c \nabla \cdot \mathbf{T} + H_A \mathbf{j}_A + H_B \mathbf{j}_B \quad (3)$$

(a) If the system is non-reactive, show that the enthalpy of formation drops out of the energy balance.
(b) If there is a chemical reaction term, show that the enthalpy of formations terms in the energy balance become the heat of reaction term.

Problem 3. Adsorption
Consider a system where an ideal gas adsorbs onto a surface via the Langmuir adsorption isotherm.

$$\theta_i = \frac{K_i c_i}{1 + \sum_{j=1}^{N_c} K_i c_i} \quad (1)$$

where c_i is the molar concentration of component i (mole/m^3), θ_i is the fractional occupancy of the surface, and K_i is the adsorption/desorption equilibrium coefficient with units of m^3/mole. The equilibrium coefficient is given in terms of the entropy and enthalpy of adsorption as

$$K_i = k_{o,i} \exp\left(\frac{\Delta S_i}{R}\right) \exp\left(-\frac{\Delta H_i}{RT}\right) \quad (2)$$

(a) As the temperature increases, what happens to the amount of material adsorbed? Why?
(b) As the pressure increases, what happens to the amount of material adsorbed? Why?
(c) For a binary system, will the selectivity, s, (defined below), will the selectivity increase or decrease with temperature? Why?

$$s = \frac{x_{ads,B} / x_{bulk,B}}{x_{ads,A} / x_{bulk,A}} \quad (3)$$

Possibly Useful Information:

The solution to an ODE of the form, $\frac{\partial^2 y(x)}{\partial x^2} = ky(x)$, is $y(x) = c\exp\left(-\sqrt{k}\,x\right)$.

Balance Equations
total mass:

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

where ρ is the mass density, **v** is the center-of-mass velocity, and *t* is time.

mass balance on component A

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

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.

momentum balance:

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

where *p* is the pressure, **τ** is the extra stress tensor, and $\hat{\Phi}$ is the specific external field imposed by, for example, gravity. If gravity is the source of the external field then we have $\mathbf{g} = -\nabla \hat{\Phi}$

energy balance

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

where $\hat{H}$ is the specific (per mass) enthalpy, $\hat{\Phi}$ is the specific potential energy due to an external field, and **q** is the heat flux due to conduction.