ChE 548
Homework Assignment V
Spring, 2010

1. Adsorption Phenomena

In the hand-out titled, "Mass Transfer Issues with Adsorption on a Surface", (contained in the file adsorption_surface_v3.pdf), we discussed equilibrium adsorption thermodynamics and looked at material and energy balances for an adsorptive system.

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

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

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

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

For component A, $k_{o,A} = 1.0 \frac{m^3}{mole}$, $\frac{\Delta S_A}{R} = -1.0$, $\frac{\Delta H_A}{R} = -300.0\,K$

For component B, $k_{o,B} = 1.0 \frac{m^3}{mole}$, $\frac{\Delta S_B}{R} = -1.0$, $\frac{\Delta H_B}{R} = -600.0\,K$

(a) Generate a plot containing
(i) the adsorption isotherm for pure A at T = 300 K for p = 10^{-4} to 10 atm.
(ii) the adsorption isotherm for pure B at T = 300 K for p = 10^{-4} to 10 atm.
(iii) the adsorption isotherms for A and B in a 50 mol % mixture at T = 300 K for p = 10^{-4} to 10 atm
Show the fractional occupancy vs pressure and vs ln(pressure). (Two plots)
(b) Explain the limits of the isotherms in these plots.
(c) Compare the amount of pure A and pure B adsorbed. Which adsorbs more? Why?
(d) Compare the mixture isotherms with the pure component isotherms. Explain the behavior of the mixture isotherms in terms of the pure component isotherms.

(e) Generate a plot containing
(i) the adsorption isotherm for pure A at T = 300 K for p = 10^{-4} to 10 atm.
(ii) the adsorption isotherm for pure B at T = 300 K for p = 10^{-4} to 10 atm.
(iii) the adsorption isotherm for pure A at T = 600 K for p = 10^{-4} to 10 atm.

(iv) the adsorption isotherm for pure B at T = 600 K for p = 10^{-4} to 10 atm.
(f) Explain the temperature dependence of the isotherms.

(g) For the adsorption of binary mixtures, selectivity is defined as

$$s = \frac{x_{ads,B} / x_{bulk,B}}{x_{ads,A} / x_{bulk,A}}$$

Calculate the selectivity for a 50/50 mol% mixture of A and B at a pressure of 1.0 atm and at T = 300 K and at T = 600 K. At which temperature is the adsorbent more selective for component B? Explain.

2. Non-Isothermal Plug-Flow Reactor Transient & Steady-State Behavior

Consider the single irreversible reaction in a Plug Flow Reactor

$$A \rightarrow 2B$$

with elementary mechanism such that the rate of the forward reaction is

$$r = kC_A$$

where the rate constant is given by

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

The activation energy for the forward reaction is 4000 J/mol. The rate constant prefactor for the forward reaction is 0.1 l/s. The heat capacities of A, B and the solvent are respectively 80.0, 140.0, and 60.0 J/mol/K. The heats of formation of A and B at a reference temperature of 298.15 K are respectively -1000.0 and -10000.0 J/mol. The inlet flowrate is 10 liters/s. The inlet temperature is 500 K. The inlet concentrations of A, B and S are 10.0, 0.0, and 30.0 mol/liter respectively. The volume of the reactor is 1000 liters. The reactor is well insulated. The initial temperature and concentrations in the reactor are the same as the inlet temperature and concentrations.

(a) Provide a plot of the steady state concentrations of A, B and S and the temperature. Explain the features.
(b) What are the steady-state temperature and conversion of A at the outlet for a reactor of length 10 m?
(c) What are the temperature and conversion of A at the outlet for a reactor of length 10 m after 100 sec?