ChE 548
Homework Assignment IV
Spring, 2010

Solving Transport Equations that are ODEs

1. Coupled Steady State Mass and Momentum Balances

The description of a flowing binary ideal gas under isothermal conditions involves a total mass balance, a balance on the mass of A and a momentum balance. These equations are provided in dimensionless form in equations 33.a to 33.d in the following paper,

Keffer, D.J., Gao, C.Y., Edwards, B.J., "On the Relationship between Fickian Diffusivities at the Continuum and Molecular Levels", *J. Phys. Chem B.* **109** 2005 pp. 5279-5288.

These equations contain three dimensionless parameters, the Peclet number, the dimensionless mass difference between components A and B, and the dimensionless temperature.

(a) Using a numerical solution technique, generate the steady state profiles using the following dimensionless initial conditions and parameters. The length of the pipe is 1. The initial density is 1. The initial velocity is 1. The initial mass fraction is 0.55. The initial gradient of the mass fraction is -0.01. The Peclet number is 5. Choose masses that correspond to neon (A) and argon (B). The dimensionless temperature is 100.
(b) What is the density, composition and velocity of the gas at the exit?
(c) Explain the physical phenomena observed in this system.
(d) How does the behavior change if you vary the Peclet number? Explain.

2. Coupled Steady State Mass and Energy Balances

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?

3. Coupled Time Dependent Mass and Energy Balances

Rework the time-dependent condensation problem described in the hand-out "Continuum Description of a Condensation Process in a System of Fixed Mass and Fixed Volume". Present the transient behavior for the first 20 seconds, where you vary the heat loss rate from 100 to 1000 J/sec. Explain the temperature, pressure and density dependence observed.