CBE 450 Chemical Reactor Fundamentals
Fall, 2009
Homework Assignment #3

1. Numerical Solution of a Single Nonlinear Algebraic Equation

Consider a continuous stirred-tank reactor (CSTR) in which the following dimerization reaction goes from 2A → B with the following mass balance on A at steady state

accumulation = in – out + generation

$$0 = F_{in} C_{A,in} - F_{out} C_A - V k_{\dim er} C_A^2$$

The inlet flow rate is 1 liter/sec, as is the outlet flow rate. The inlet concentration is 10 mole/liter. The rate constant is 0.5 liter/mol/sec. The volume of the reactor is 1 liter.

(a) Solve this nonlinear equation analytically.
(b) How many roots are there?
(c) Which root is the physically meaningful root? Why?
(d) Solve this nonlinear equation using Goalseek in Excel. Provide a print-out of the spreadsheet.
(e) Solve this nonlinear equation using the Newton-Raphson method with numerical derivatives in Matlab. Note the initial guess you used to converge ot the physically meaningful root.

2. Numerical Solution of a System of Nonlinear Algebraic Equations

Consider a continuous stirred-tank reactor (CSTR) in which the following isomerization reaction goes from A → B with the following mass balance on A at steady state

accumulation = in – out + generation

$$0 = F_{in} C_{A,in} - F_{out} C_A - V k_{iso} C_A$$

The inlet flow rate is 1 liter/sec, as is the outlet flow rate. The inlet concentration is 10 mole/liter. The rate constant is

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

where k_o = 1.0 sec^{-1} and E_a = 2500 J/mol/K. The volume of the reactor is 1 liter.

The steady state energy balance is

accumulation = in – out + generation

$$0 = F_{in}H_{in} - F_{out}H - \Delta H_R V k_{iso} C_A$$

where the inlet enthalpy, $H_{in} = C_p T_{in}$, where the heat capacity is 4.0 kJ/liter/K and the inlet temperature is 300 K, where the enthalpy of the reactor is $H = C_p T$, and where the heat of reaction, ΔH_R , is -30 kJ/mol.

Find the steady state concentration of A and temperature. Provide Matlab equation input file and screen output. (You do not have to provide the entire Newton-Raphson code provided in class.)

3. Numerical Solution of a System of Nonlinear Ordinary Differential Equations

Consider a continuous stirred-tank reactor (CSTR) in which the following isomerization reaction goes from A → B with the following mass balance on A

accumulation = in – out + generation

$$V\frac{dC_A}{dt} = F_{in}C_{A,in} - F_{out}C_A - V k_{iso} C_A$$

The inlet flow rate is 1 liter/sec, as is the outlet flow rate. The inlet concentration is 10 mole/liter. The rate constant is

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

where k_o = 1.0 sec^{-1} and E_a = 2500 J/mol/K. The volume of the reactor is 1 liter.

The energy balance is

accumulation = in – out + generation

$$VC_p\frac{dT}{dt} = F_{in}H_{in} - F_{out}H - \Delta H_R V k_{iso} C_A$$

where the inlet enthalpy, $H_{in} = C_p T_{in}$, where the heat capacity is 4.0 kJ/liter/K and the inlet temperature is 300 K, where the enthalpy of the reactor is $H = C_p T$, and where the heat of reaction, ΔH_R , is -30 kJ/mol.

The initial conditions within the reactor are T(t=0) = 300 K and C_A(t=0) = 0.0 mol/liter.

(a) Find the transient behavior of the concentration and temperature. Provide the Matlab equation input file and graphical output. (You do not have to provide the entire Runge-Kutta code provided in class.)

(b) What are the long-time (steady state values) of the concentration of A and the temperature?

(c) How do the values in (b) compare with the steady state solutions obtained in problem 2?