ChE 263

Assignment #5

The assignment is due midnight **before** the beginning of the next class period. Upload completed assignment to Learning Suite.

1. A first order reaction is governed by A---> B and has rate

$$\frac{dC_A}{dt} = -kC_A$$

where C_A is the concentration (kmol/m^3), t is time, and k is a rate constant. The initial concentration is C_{A0} = 5 kmol/m^3, and k = 1 s^{-1}.

a. Solve for $C_A(t)$ two ways: (1) analytically by separating variables and integrating; (2) using the Explicit Euler method. For the Euler method, evaluate the rate (RHS function) at time n, then solve the whole equation for values at time $n+1$.

$$\frac{dC_A}{dt} \approx \frac{C_{A_{n+1}} - C_{A_n}}{t_{n+1} - t_n} = f(C_{A_n})$$

$$C_{A_{n+1}} = f\left(C_{A_n}\right)\Delta t + C_{A_n}$$

Plot the two versions of $C_A(t)$ on the same plot. Label and format the plot including axis labels, and legends, etc. so that you can clearly communicate the solution. Use a time step size of Δt = 0.5 s and plot to t_{end} = 7 s (14 steps).

b. Compare the curves. Why are they different?

c. Copy the figure and paste as an image in the same document. Change Δt from 0.5 to 1.5. Copy the figure as an image again. Change Δt to 2.1. Observe the three plots that correspond to three different values of Δt.

2. We are performing a chemical reaction as follows:

A + B --> C Reaction 1
B + C --> D Reaction 2

Product C is desired, but as soon as some C is formed, some B reacts with it to form an undesired product D.

The rate of change of the concentrations of each of the species is given by
$dA/dT = -k_1\ A\ B$
$dB/dt = -k_1\ A\ B - k_2\ B\ C$
$dC/dt = k_1\ A\ B – k_2\ B\ C$
$dD/dt = k_2\ B\ C$
(Here, symbols A, B, C, and D denote the species concentrations in mol/L). The initial concentrations are **A_0=1, B_0=1, C_0=0, D_0=0**. Also, **k_1 = 1** L/mol-s, and **k_2 = 1.5** L/mol-s

a) **Solve** for the concentrations of A, B, C, and D as functions of time. Use a time step size of **dt=0.2 s** and solve to **t=3 s**. Also solve for the selectivity defined as **S = C/(C+D)** as a function of time. (S is initially undefined, but you can set it equal to 1 at t=0.) Use Euler's equation applied to each d(Species)/dt above: dy/dt = f(y,z,w,etc.) --> $y_{n+1} = y_n + \Delta t*f(y_n,z_n,w_n, etc.)$.
b) **Plot** the concentrations of A, B, C, D, and S as functions of time on the same plot. Label the axes as "time (s)" and “concentration (mol/L)”.
c) What is the **final value of the selectivity**? (Color the cell yellow)
d) Assuming the values of C_0, D_0, k_1 and k_2 are fixed, **how can you increase the final value of the selectivity** given the above reactions?