ChE 263

Assignment #5

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

1. Work this problem on a worksheet titled Euler. 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 chemical timescale. The initial concentration is C_{A0} = 5 kmol/m^3, and k = 1 s^{-1}.

   a. Solve for $C_A(t)$ three ways: (1) analytically by separating variables and integrating; (2) using the Explicit Euler method; and (3) using an Implicit version of the Euler method (described below). Plot the three 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 timestep size of Δt = 0.5 s and plot to t_{end} = 7 s (14 steps).
   b. Compare the curves. Why do they have the shape they do (that is, why do they curve the way they do, and why is one curve above or below another?) Hint, think in terms of marching along a slope and where you are taking the slope when you march.
   c. Copy the figure and then "Paste Special --> as PDF" in the same document. Then change Δt from 0.5 to 1.5. Copy the figure and "Paste Special --> as PDF in the same document. Then change Δt to 2.1. That is, we want to see three plots that correspond to three different values of Δt. The Explicit Euler plots should be surprising. (What happens if you further increase Δt?)

Note: Recall, for Explicit Euler, we evaluate the rate (RHS function) at time n, then solve the whole equation for values at time n+1. That is, for dy/dt = f(y,t) we have $y_{n+1} = y_n+f(y_n,t_n)$. For Implicit Euler, we evaluate the rate (RHS function) at time n+1, and solve the whole equation for values at time n+1. That is, $y_{n+1} = y_n+f(y_{n+1},t_{n+1})$. Here, you have to write the equation out for your specific problem, then solve for y_n+1 (by hand), in terms of quantities you know (values at time n). You then have the formula to enter in Excel. Both methods give an equation for $C_{A,n+1}$ in terms of parameters or values of C_A at previous times.

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 timestep 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?