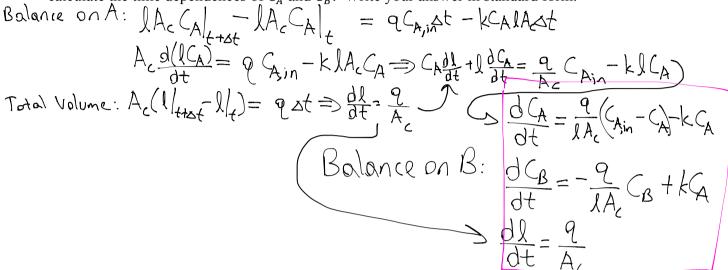ChBE 2120, Numerical Methods, Paravastu Section, Fall 2015
Quiz 2: 20 points possible

1) (10 points) Consider a semi-batch reactor, *i.e.,* a stirred tank with an input stream but no outpu. The tank is initially empty (liquid level, $l(t = 0) = 0$). The input stream is characterized by a liquid flow rate, q, and a constant concentration of compound A, $C_{A,in}$. A first order chemical reaction converts A to B with 1:1 stoichiometry: $A \xrightarrow{k} B$, where k is a first-order rate constant. Derive a system of ODE's that could be used to calculate the time dependences of C_A and C_B. Write your answer in standard form.

Balance on A: $\left. lA_c C_A \right|_{t+\Delta t} - \left. lA_c C_A \right|_t = qC_{A,in}\Delta t - kC_A l A_c \Delta t$

$$A_c \frac{d(lC_A)}{dt} = q C_{A,in} - k l A_c C_A \Rightarrow C_A \frac{dl}{dt} + l \frac{dC_A}{dt} = \frac{q}{A_c} C_{A,in} - k l C_A$$

Total Volume: $A_c(\left. l \right|_{t+\Delta t} - \left. l \right|_t) = q\Delta t \Rightarrow \frac{dl}{dt} = \frac{q}{A_c}$

$$\boxed{\frac{dC_A}{dt} = \frac{q}{lA_c}\left(C_{A,in} - C_A\right) - kC_A}$$

Balance on B: $$\boxed{\frac{dC_B}{dt} = -\frac{q}{lA_c}C_B + kC_A}$$

$$\boxed{\frac{dl}{dt} = \frac{q}{A_c}}$$

2) (10 points) The Matlab function ODEHeun correctly implements Heun's method. Write SemiBatchReactor.m, which would be passed to the variable Yprime in ODEHeun in order to solve the ODE derived in Problem 1. Use the following values for the constants: $A_c = 10$; $q = 1$; $k = 2$; $C_{Ain} = 1$

```
function [ tSolution, Ysolution ] = ODEHeun( Yprime, tRange, Y0, h )
    tSolution = tRange(1):h:tRange(2);
    [numberOfEquations, ~] = size(Y0);
    Ysolution = zeros(numberOfEquations, length(tRange));
    Ysolution(:, 1) = Y0;
    for (i = 2:length(tSolution))
        Y0 = Ysolution(:, i-1) + h * Yprime(tSolution(i-1), Ysolution(:, i-1));
        Ysolution(:, i) = Ysolution(:, i-1) + h * 1 / 2 * (Yprime(tSolution(i-1), Ysolution(:, i-1)) + Yprime(tSolution(i),
        Y0));
    end
end

function [ Yprime ] = SemiBatchReactor( t, Y )  %to be passed to ODEHeun into Yprime
```

$A_c = 10$;
$q = 1$;
$k = 2$;
$CAin = 1$;
$CA = Y(1,1)$;
$CB = Y(2,1)$;
$l = Y(3,1)$;
Yprime $= [q/l/A_c * (CAin - CA) - k*CA; -q/l/A_c*CB + k*CA; q/A_c]$;

```
end
```