

## Quiz 2: 20 points possible

- 1) (10 points) Consider a semi-batch reactor, *i.e.*, a stirred tank with an input stream but no output. 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.

- 2) (10 points) The Matlab function ODEHeun below correctly implements Heun's method. Write SemiBatchReactor, the function that would be passed to the variable Yprime in ODEHeun in order to solve the ODE derived in Problem 1. Constant values:  $A_c = 10$ ;  $q = 1$ ;  $k = 2$ ;  $C_{A,in} = 1$

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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
```

end