<u>CHE 332 F | Applied Reaction Kinetics Tutorial 1 | September 11th, 2020</u>

Please see the document "MATLAB and Excel VBA" on Quercus for assistance accessing VBA or MATLAB. These programs will be necessary in completing future tutorials, exams and quizzes.

Learning Objective: Familiarization with numerically solving first-order linear and nonlinear ODEs for reactor balances using MATLAB and Excel. Additionally, practice uploading files on Quercus and Crowdmark.

<u>**Problem 1.1 |** Using MATLAB and/or Excel to solve First Order Linear & Nonlinear ODEs (review)</u>

It's Friday morning. You are ready to head off to your cottage for a long weekend, but a memo arrived to your mailbox from your colleague.

We have an emergency, and we need your help to figure it out… our reactor start-up is not making any sense!! I know you took CHE332, and have the skills necessary to solve this. The following is the governing design equation, but we could not solve it…

<u>Reaction:</u> $A \rightarrow 2\,B$

$$\boldsymbol{V_R \frac{dC_A}{dt} = \left(C_{A_o}\,\dot{v}_o\right) - \left(C_A\,\dot{v}\right) + V_R\, r_A} \qquad (Equation\ 1)$$

Where r_A is:

$$\boldsymbol{r_A = -k\,(C_A)^n} \qquad (Equation\ 2)$$

The following parameters are attached to the memo:

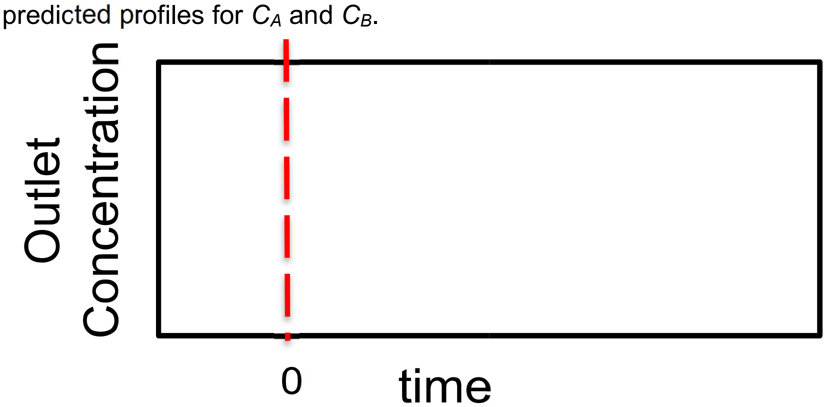
Fluid volume V_R = 1000 (L)
Inlet concentration $C_{A,o}$ = 6 (mol L^{-1})
Volumetric flowrate $\dot{v}_o = \dot{v}$ = 5 (L s^{-1})
k = 0.01

1.A. What are the units of k, in terms of n? Here, k is the reaction rate constant, and n is the reaction order in the rate law, its meaning will be discussed next week.

1.B. Combine Equations 1 and 2, then simplify them under the assumption that n=1. Then, further simplify your answer to the steady-state equation for this system.

Quercus Quiz T1.1a. Solve for C_A at steady state when n=1 (units of mol L^{-1})

1.C. For n=1, Without performing any calculations, how would you expect the concentration C_A to change upon the start of reaction? How about C_B? Assume that, at time t = 0 seconds, $C_A = C_{A,o}$ and no B has formed in the reactor. Sketch your predicted profiles for C_A and C_B.



1.D. Using either MATLAB or Excel, solve for C_A as a function of time using the initial condition in 1.C., for t between 0-1000 seconds, when n = 1. Qualitatively, does this match what you predicted?

Note: You are allowed to solve 1.D. multiple different ways; pick the one you are most familiar with. The easiest would be to use the numerical integration (RK2, RK4, Euler method) you learned in CHE222. Alternatively, in MATLAB, you could try out the built in ODE solver (ode23/ode45).

For reference, the following equations are provided (syntax here may differ from what you learned in CHE222):

$$Euler\ Method: Y_{n+1} = Y_n + \frac{d(Y_n)}{dx}(x_{n+1} - x_n)$$

$$2nd\ order\ Runge-Kutta: Y_{n+1} = Y_n + (x_{n+1} - x_n)\frac{(k_1 + k_2)}{2}, \qquad k_1 = \frac{d(Y_n)}{dx}, \quad k_2 = \frac{d(Y_n + (x_{n+1} - x_n) * k_1)}{dx}$$

1.E. Modify your code from 1.D. to show what happens when n = -1, 0, 0.5, 1, 1.5, and 2.

Crowdmark Upload T1.1. Show C_A as a function of time for each n on one plot.
For Crowdmark, you can upload either an image file, PDF, or word document. Crowdmark will be used during exams.

Quercus Quiz T1.1b. For n=1.5, at what time does C_A decrease below 2.5 (mol L^{-1})? (answer in <u>seconds</u>)

Quercus Quiz T1.1c. For n=1.5, what time does C_A decrease below 2.5 (mol L^{-1}) if $C_{A,o}$ is instead 8 (mol L^{-1})? (answer in <u>seconds</u>)

Quercus Quiz T1.1d. At what value of n is the steady-state concentration of A the highest?

<u>**Upload your Excel/Matlab file through "Upload your Tutorial 1 Code Here" under the "Assignments" tab in Quercus**</u>

<u>**Note:** Complete the Quercus quiz and Crowdmark upload by next Thursday at 4:30 PM EDT September 17th, 2020, and upload your Excel/Matlab file through the "file upload" under the "Assignments" tab. You will be required to upload your MATLAB and Excel files to receive credit on these tutorial problems.</u>