CHE 332 F | Applied Reaction Kinetics Tutorial 2 | September 18th, 2020

Learning Objective: Be able to understand the meaning and differentiate the various rates (species dependent, species independent, extensive vs. intensive rates); understand Arrhenius rate law and its applications; stoichiometric table; be an expert in uploading files on Quercus and Crowdmark.

Problem T2.1 | Species Dependent and Species Independent Rates

The stomach of a hippopotamus digests compounds A and B and converts them into C and D in the following reaction:

$$2A + 0.5\ B \rightarrow C + D$$

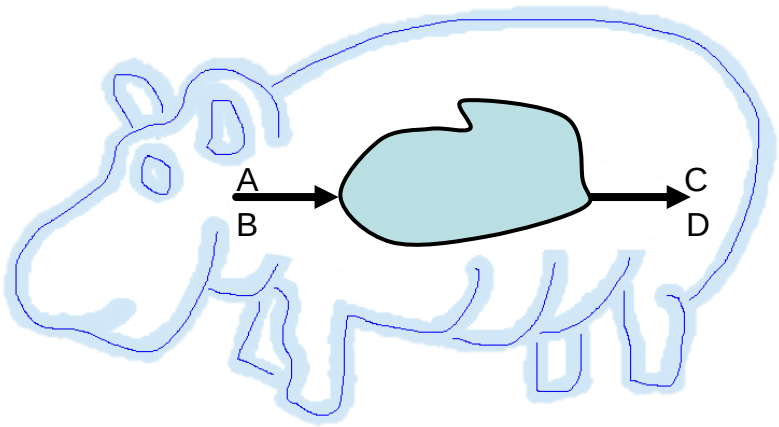
The rate of reaction is given by:

$$r = kC_A^2$$

Where k is the rate constant (L mol^{-1} s^{-1}) and C_A is the concentration of A inside the stomach. The volume of the stomach is V_R (L) and A and B are fed at rates of $F_{A_{in}}$ and $F_{B_{in}}$ (mol s^{-1}). There is no accumulation in the stomach, and it is well-mixed.

Following are the parameters for this problem:

- V_R=1000 L
- Inlet concentration $C_{A,in} = 5\ mol\ L^{-1}$
- Inlet volumetric flowrate $\dot{v}_{in} = 4\ L\ s^{-1}$
- $k = 0.01\ L\ s^{-1}\ mol^{-1}$



1.A. Write the molar balance of A. Express the equation in terms of C_A.

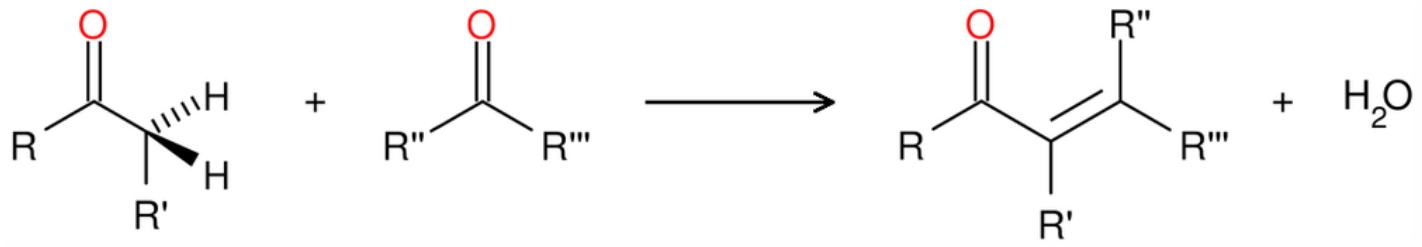
1.B. Equation in 1.A. could be solved by 1) analytically and 2) numerically. Submit the analytical form of the equation and the time dependent profile of C_A on Crowdmark. Use the initial condition of at time t = 0 seconds, $C_A = C_{A,in}$. Plot the graph for t between 0 and 1000 seconds using MATLAB.

1.C. Write the molar balance of B.

Quercus Quiz T2.1. From the time dependent profile of C_A in 1.B., what is the time needed for C_A to be reduced by 50%?

Problem T2.2| The Arrhenius Equation

You were just given the following aldol condensation reaction which follows **elementary rate law**:



(A) (B) (C)

2.A. Given the provided reaction, determine the rate constant (k) at each temperature shown in the Table below.

Temperature	Species A	Species B	Rate (mol C /(L min)$^{-1}$)
^{0}C	mol/L	mol/L	
40	2	0.2	59
65	1.5	0.6	2683
72	3	1	108947
90	1.8	3	878876
105	0.2	1	1777222

2.B. Using the Table provided, determine the reaction rate at 130°C given that A and B were supplied in equimolar amounts at 2.5 mol/L.

Quercus Quiz T2.2 What is the activation energy for the aldol condensation reaction **in kJ**?

Upload your Figure from 2.B. onto Crowdmark and the Excel file from 3.B. through "Upload your Tutorial 2 File Here" under the "Assignments" tab in Quercus

Problem (Quercus Quiz) T2.3. What is the rate constant at 250°C provided that the first order reaction is A → B has a rate constant of 0.02s^{-1} at 200°C and has an activation barrier of 80 kJ mol^{-1}?

Problem T2.4 | (Quercus Quiz)

T2.4a. Species independent vs species dependent rate.

C is produced in the reaction A+3B → 2C at a rate of 120 molC L^{-1} h^{-1}. What is the reaction rate of B?

A 120 mol L^{-1} h^{-1}

B -120 mol L^{-1} h^{-1}

C -60 mol L^{-1} h^{-1}

D -180 mol L^{-1} h^{-1}

T2.4b. Unit of intensive vs. extensive rate. Which of these describes the unit of intensive rate of reaction?

A mol h^{-1}

B mol L^{-1} h^{-1}

C h^{-1}
D mol^{-1} L h^{-1}

T2.4c. By conducting reactions in a batch reactor of volume 1 L, the reaction rate equation was found to be $r_A = -kC_A$. The rate expression for a batch reactor of volume 5 L would be:

A $r_A = -0.2kC_A$
B $r_A = -kC_A$
C $r_A = -5kC_A$

Elementary rate law.
T2.4d. Write the rate equation for the production of B in the elementary reaction of 2A → B given rate constant k and concentrations of A and B of C_A, and C_B, respectively. (2 min)

A $r_B = kC_A^2$
B $r_B = 2kC_A^2$
C $r_B = -2kC_A^2$
D $r_B = -kC_A^2$

Limiting vs. excess reactant.
T2.4e. 50 mol h^{-1} of A, 100 mol h^{-1} of B, and 10 mol h^{-1} of C enter an ideal CSTR and react according to 2A+3B → C + D. Which species is the excess reactant? (1 min)
A A
B B
C C
D D

Words mass balance.
T2. 4f. F_{j0} and F_j are the inlet and outlet molar flow rate of species j in a **well-mixed** reactor of volume V. If r_j is the rate of generation of species j, which of the following is the correct mole balance on the reactor?
A $r_jV = d(VCj)/dt$
B $F_{j0} + F_j + r_jV = d(VCj)/dt$
C $F_{j0} - F_j + r_jV = d(VCj)/dt$
D $F_{j0} - F_j - r_jV = d(VCj)/dt$

Note: Complete the Quercus quiz and Crowdmark upload by next Thursday at 4:30 PM EDT September 24th, 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.