Introduction to Reactor Design, 3K4

Tutorial 6/Assignment 4

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Objectives of this short assignment:

- To calculate rate expression constants.
- Ensure you are comfortable specify the experiments and analyzing the data from them to get the rate constants in the model.

Take a look at this job posting I received in my mailbox today, from Amgen: "Looking for a Grad Co-op for our Pilot Plant Operations to develop dynamic models of biopharmaceutical manufacturing processes. Perform optimization analyses using these models. Develop effective methods for communicating the results of these analyses. Develop stand-alone simulation tools from these models that will enable Amgen staff to independently design processes and investigate operating condition and process parameter options. Candidates should have significant experience with MATLAB and Simulink."

Even though 3K4 is about reactors, the skills learned in this course are 100% what they are asking for above (except for the optimization and communication parts). This tutorial in particular is looking at "developing dynamic models (rate expressions are dynamic models) for manufacturing processes". Feel free to use MATLAB, Polymath or Python, or even Excel.

Question 1

The following data were collected in an experiment to determine the reaction order and rate constant. The species starts to decompose to products according to:

$$\mathrm{A} \longrightarrow \mathrm{B} + \mathrm{C}$$

The following concentration against time data were collected:

Time [min]	C_A[**mol.m**$^{-3}$]
0	154
50	114
100	87
150	76
200	70
250	58

Determine the reaction order and rate constant.

Question 2

Problem modified from Cutlip and Shacham

The liquid phase reaction between ethylene dibromide and potassium iodide, in methanol can be written as:

$$\text{A} + 3\text{B} \longrightarrow \text{C} + 2\text{D} + \text{E}$$

The concentration of A was measured over time in a batch reactor, and is report in terms of conversion of A in the table. The batch had $C_{A0} = 20\,\text{mol.m}^{-3}$ and $C_{B0} = 150\,\text{mol.m}^{-3}$.

1. Confirm if the reaction is zeroth order with respect to A and B, and if so, what is the reaction rate constant.
2. Confirm if the reaction is first order with respect to A and zeroth order with respect to B; if so, what is the reaction rate constant.
3. If the reaction rate is first order with respect to A and B, then:

$$\frac{1}{(\theta_B - 3)C_{A0}} \ln\left(\frac{1 - \frac{3X_A}{\theta_B}}{1 - X_A}\right) = kt$$

   Confirm if this might be the case, and what would be the value of the rate constant k, where $\theta_B = \dfrac{C_{B0}}{C_{A0}}$.

Time [s]	$X_A[-]$
0	0
30	0.29
41	0.36
48	0.41
56	0.46
62	0.49
73	0.54
84	0.58

Question 3

Problem modified from Cutlip and Shacham

The reaction of acetic acid and cyclohexanol in dioxane solution is catalyzed by sulphuric acid. It is studied in a well-mixed batch reactor at 320 K.

$$\text{A} + \text{B} \longrightarrow \text{C} + \text{D}$$

The reaction rate is thought to occur as $-r_A = k_A C_A^{\alpha} C_B^{\beta}$, so there are 3 unknown constants in the rate expression.

One way to operate the batch experiments is to place one of the species in excess, e.g. species B so that essentially C_B during the experiment is approximately equal to C_{B0}, with only C_A varying.

The following data were collected under such conditions, where $C_{B0} = 8\,\text{mol.L}^{-1}$

Time [s]	C_A[**mol.L^{-1}**]
0	1.0
30	0.96
45	0.94
75	0.90
120	0.85
150	0.82
210	0.77
255	0.73

1. Substitute in $C_B = C_{B0}$ in the rate expression above, and use that to determine the lumped rate constant $k'_A = k_A C_{B0}^{\beta}$, where $-r_A = k'_A C_A^{\alpha}$, and also determine the coefficient α.

Then the reaction is run again, this time with species A in excess, so that C_A during the experiments is approximately equal to $C_{A0} = 15\,\text{mol.L}^{-1}$.

Time [s]	C_B[**mol.L^{-1}**]
0	2.0
120	1.7
150	1.65
180	1.56
210	1.55
240	1.50
270	1.46
300	1.42

2. Use a similar idea as in the previous part to solve for the 2 constants in the expression $-r_A = k''_A C_B^{\beta}$.
3. Now use these data to determine all constants in the rate expression $-r_A = k_A C_A^{\alpha} C_B^{\beta}$.

END