Chemical reaction engineering tutorial Chapter 5 2013

1. Suppose you encounter a reaction with some stoichiometry, say: A --> 2B + C
and you are asked to determine the order of the reaction from data obtained for [A] as a function of time.

|  |  |
| --- | --- |
| time | CA |
| 0.000 min | 1.000 M |
| 10.00 mins | 0.8000 M |
| 20.00 mins | 0.6667 M |
| 40.00 mins | 0.5000 M |

Find the rate law of this reaction .

1. Consider a reaction **A + B + C-> Products** (not an elementary reaction). Several initial conditions of this reaction are investigated and the following data are obtained:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Run  | CA0 | CB0 | CC0 | r0 (initial rate) |
| 1 | 0.151 M | 0.213 M | 0.398 M | 0.480 M/s |
| 2 | 0.251 M | 0.105 M | 0.325 M | 0.356 M/s |
| 3 | 0.151 M | 0.213 M | 0.525 M | 1.102 M/s |
| 4 | 0.151 M | 0.250 M | 0.480 M | 0.988 M/s |

What is the initial rate of the reaction when all the reactants are at 0.100 M concentrations?

1. The following data were collected for a hypothetical reaction whose rate is known to only depend on the concentration of a single reactant, A. The order of the rate law with respect to A is unknown.

|  |  |
| --- | --- |
| Time (s)  | CA (M) |
| 0 | 1.00 |
| 5 | 0.82 |
| 10 | 0.67 |
| 15 | 0.55 |
| 20 | 0.45 |
| 40 | 0.20 |
| 60 | 0.09 |

Use this data to determine the order of the reaction. We assume that the reactions is either zeroth, first or second order.

4. When the concentration of A in the reaction A  B was changed from 1.20 M to 0.60 M, the half-life increased from 2.0 min to 4.0 min at 25°C. Calculate the order of the reaction and the rate constant.

|  |  |
| --- | --- |
| 5. | The progress of a reaction in the aqueous phase was monitored by following the absorbance of a reactant at various times: |

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|   | Time/s | 0 | 54 | 171 | 390 | 720 | 1010 | 1190 |
|   | Absorbance | 1.67 | 1.51 | 1.24 | 0.847 | 0.478 | 0.301 | 0.216 |

|  |  |
| --- | --- |
|   | Make appropriate plots of these data to test them for fitting zero-, first-, and second-order rate laws. Test all three even if you happen to guess the correct rate law on the first trial.  |
| 6. | For the reaction A  products, the following data were obtained. |
|   | **Time** (hrs) | CA, M | **Time** (hrs) | CA, M |
|   | 0 | 1.24 | 6 | 0.442 |
|   | 1 | 0.960 | 7 | 0.402 |
|   | 2 | 0.775 | 8 | 0.365 |
|   | 3 | 0.655 | 9 | 0.335 |
|   | 4 | 0.560 | 10 | 0.310 |
|   | 5 | 0.502 |   |   |
|   | (a) | Determine the order of the reaction and the rate constant. |
|   | (b) | Determine the rate constant for the reaction. |
|   | (c) | Using the rate law that you have determined, calculate the half-life for the reaction. |
|   | (d) | At what time will the concentration of A be 0.380 M**?** 2.  |

7. Determine the order of reaction and specific reaction rate frombatch data for reaction A→B : Graphical and numerical fit

t (min) 0 3 5 8 10 12 15 17.5

CA(mol/dm3) 4.0 2.89 2.25 1.45 1.0 0.65 0.25 0.07