Kinetics Worksheets

Tutorial: Ozone decomposition

Goal: In this tutorial, you will be exploring the relationship between time and concentration during a chemical reaction in order to determine reaction order, rate constants, half-lives, rate laws, and activation energies. If you have not used Excel to create graphs before, you may want to examine the <u>Making Graphs and Charts in</u> <u>Excel Guide</u>.

Instructions -

Open the kinetic data file: OZONE

The kinetic data sets are in Excel 97 format. Each set contains the reaction equation, time and concentration data, and the experimental conditions.

Question 1 (1 point)

Charting relationships: time vs. concentration: ozone

Goal: Comparing the relationship between time and reactant concentration in order to predict characteristics of the resulting graph.

Data treatment: In Excel, choose the spreadsheet for the reaction $2O_3 \rightarrow 3O_2$ at 70 'C.

Examine the time and concentration data. If time is on the X axis and concentration is on the Y axis, what do you predict would be the shape of the resulting curve?

- 1. Sloping upward as time increases
- 2. Sloping downward as time increases
- 3. Not changing as time increases
- 4. First sloping upward then leveling out
- 5. First sloping downward then sloping upward

Question 2 (1 point)

Charting relationships: time vs. inverse of concentration: ozone

Goal: Comparing the relationship between time and reactant concentration in order to predict characteristics of the resulting graph.

Data treatment:

In the Excel spreadsheet, designate a new column to the right of the concentration column as 1/concentration by labeling it 1/concentration. In the cell below the label, type in =1/B7 and press return. Click on this cell and drag the bottom right corner down to apply this formula to the data in the other cells in column B.

If time is on the X axis and 1/concentration is on the Y axis, what do you predict would be the shape of the resulting curve?

- 1. Sloping upward as time increases
- 2. Sloping downward as time increases
- 3. Not changing as time increases
- 4. First sloping upward then leveling out
- 5. First sloping downward then sloping upward

Question 3 (1 point)

Charting relationships: time vs. In concentration: ozone

Goal: Comparing the relationship between time and reactant concentration in order to predict characteristics of the resulting graph.

Data treatment:

In the Excel spreadsheet, designate a new column to the right of the concentration column as the *ln* of concentration by labeling it ln concentration. In the cell below the label, type in $=\ln(B7)$ and press return. Click on this cell and drag the bottom right corner down to take the ln of the data in the other cells in column B.

If time is on the X axis and ln concentration is on the Y axis, what do you predict would be the shape of the resulting curve?

- 1. Sloping upward as time increases
- 2. Sloping downward as time increases
- 3. Not changing as time increases
- 4. First sloping upward then leveling out
- 5. First sloping downward then sloping upward

Question 4 (2 points)

Getting a linear relationship: ozone tutorial

Goal: Now, you will graph the relationships between the time and concentration data in order to determine which of these relationships is linear.

Data treatment: In Excel, choose the spreadsheet for the reaction $2O_3$ -- $3O_2$ at 70 'C.

Plot concentration vs. time by highlighting the columns Time (hr) and [Ozone] M and then clicking the Chart

Wizard icon an the toolbar in the top part of the window (or press alt-I then alt-h). Choose an XY scatter plot and press the 'Finish' button. You can move the graph around by click and holding the mouse button on the graph and moving the mouse.

Plot *ln* concentration vs. time by first holding down the *Ctrl* key and then highlighting the columns Time (hr) and ln concentration. Then, click the Chart Wizard icon on the toolbar. Choose an XY scatter plot and press the 'Finish' button.

Plot 1/concentration vs. time by first holding down the *Ctrl* key and then highlighting the columns Time (hr) and 1/concentration. Then, click the Chart Wizard icon on the toolbar. Choose an XY scatter plot and press the 'Finish' button.

Hint: Compare your graphs to your predictions in questions 1, 2, and 3. Do your graphs look like you predicted? If not, check to make sure your graphs are really charting the data you selected!

Which graph shows a linear relationship? Hint: Make the graphs larger to help determine which is linear.

- 1. The plot of concentration vs. time
- 2. The plot of ln concentration vs. time
- 3. The plot of 1/concentration vs. time

Question 5 (2 points)

Determining reaction order: ozone decomposition tutorial

Goal: Here, you will use the linear relationship from question #4 to determine the reaction order. Reaction order is necessary to calculate the rate law in question #6.

Equation analysis:

If concentration vs. time is linear, the data will fit to the following equation:

$$[\mathbf{c}] = -\mathbf{k}(\mathbf{t}) + [\mathbf{c}]_0$$

where k is the rate constant and c is the initial concentration. This is the equation that describes zero-order kinetics.

If *ln* concentration vs. time is linear, the data will fit to the following equation:

$$\ln \left[c \right] = -k(t) + \ln \left[c \right]_0$$

where k is the rate constant and c is the initial concentration. This is the equation that describes first-order kinetics.

If 1/concentration vs. time is linear, the data will fit to the following equation:

$$1/[c] = kt + 1/[c]_0$$

where k is the rate constant and c is the initial concentration. This is the equation that describes second-order kinetics.

Reaction order: On the basis of the equation used to obtain a linear fit of the data, what is the reaction-order for ozone decomposition?

- 1. Zero-order
- 2. First-order
- 3. Second-order

Question 6 (2 points)

Rate Law determination: Ozone Decomposition

Rate laws: It is possible to determine the rate of a given reaction:

 $A + B \rightarrow C + D$

from the reaction order and either the reduction of the reactant concentration or the increase in the product concentration.

For example, the kinetic rate law for the above reaction takes the form:

rate = $k[A]^x [B]^y$

where x is the reaction order, [A] and [B] are the concentrations of the reactants, and rate = -d[A]/dt = -d[B]/dt. Write the rate laws for the given reaction.

Your answer should be in the form: rate=k[reactant]^x

Question 7 (2 points)

Rate constant: ozone decomposition tutorial

Goal: Here, you will calculate the rate constant by examining the charts you generated for question #4. The rate constant is required to determine the reaction half-life in question #9.

Calculate the slope of the line for the graph in question #5 that has a linear relationship. To do this, first click on a data point on graph to highlight the data points. This may take a couple of tries, but continue clicking on the data points until they are all highlighted.

At the top of the Excel window, click on the Chart pull-down menu and select 'Add Trendline...' A new window will appear. In the new window, click on the 'Options' tab, check off 'Display equation on chart'. Click the 'ok' button. The equation displayed on the chart is in the form y = mx + b where m is the slope and b is the y-intercept. The value of the slope is the rate constant k for ozone decomposition at 70'C.

You may need to change the number of decimal places displayed by the equation box in Excel for the slope in order to match the number of significant figures in your initial data set. You can do this by double-clicking the equation. In the new window that appears, click on the 'Number' tab. In the 'Category' column, select 'Number'. In the 'Decimal places' box, enter the number of decimal places that you want.

Write the value of the slope in the space below. Write your answer in scientific notation. (For example, enter 2.34e-2 for 2.34×10^{-2} . Don't forget the units!) You have just calculated the rate constant for this reaction.

Question 8 (2 points) Half-life Estimation - Ozone Decomposition

Goal: Estimate the half-life of this reaction at time = 0.

The half-life is defined as the time at which the concentration of the reactant(s) is half the initial concentration. Examine the original data in the spreadsheet and estimate the time for the concentration to decrease by half.

- 1. 100 seconds
- 2. 300 seconds
- 3. 1000 seconds
- 4. 10 seconds
- 5. 600 seconds

Question 9 (2 points)

Half-life Determination: ozone decomposition tutorial

Half-life: Now, we will calculate the half-life more precisely. Look back through your work in this tutorial, and determine which equation to use in your calculations. Determine the half-life for ozone decomposition at 70 'C and enter it in the space below.

Hint 1: If c is the initial concentration, then at the half-life, the concentration is c/2.

Hint 2: Compare your answers to questions #8 and #9. Be sure they are consistent and make sense. Don't forget the units!