



Kinetics Student Guide Section I

Comparing Orders of Reaction for One Reactant

In this activity, you will discover how the order of the reaction affects the reactant and the reaction rate. You will build a computer model of a three reactions: zero-order, first-order and second-order. In each case, you will observe 60 seconds of a reaction which starts with a 10 mole per liter concentration of a reactant. By varying the reaction rates, you will be able to generate graphs of the reaction rates and the concentrations of the reactants.

Building the Model:


1. **Double-click** on the STELLA icon.


2. **Click once** on the icon of the world . It should change to .

3. The tool bar looks like this:



This is the source of the icons you will use to build your model.

4. **Click once** on the stock icon . Slide your pointer out into the open field and click again. A large stock should appear with the word **Noname 1** highlighted. Before doing anything else, **type** the words **Concentration A**.

5. **Click once** on the flow icon . Position your pointer *inside* the stock, then **click and drag** to a point a couple of inches to the right of the stock. Let go of the mouse button. Type the word **Rate A Disappears**.

6. **Double-click** on the **Concentration A** stock and enter the value **10 {moles per liter}**, then click **OK**. Note that units must be enclosed in { } in STELLA.

7. **Double-click** on the **Rate A Disappears** flow and enter the value **0.1 {moles per liter per second}**, then click **OK**.

Setting Time Specs:

8. Go to the **Run** menu and drag down to select **Time Specs...**

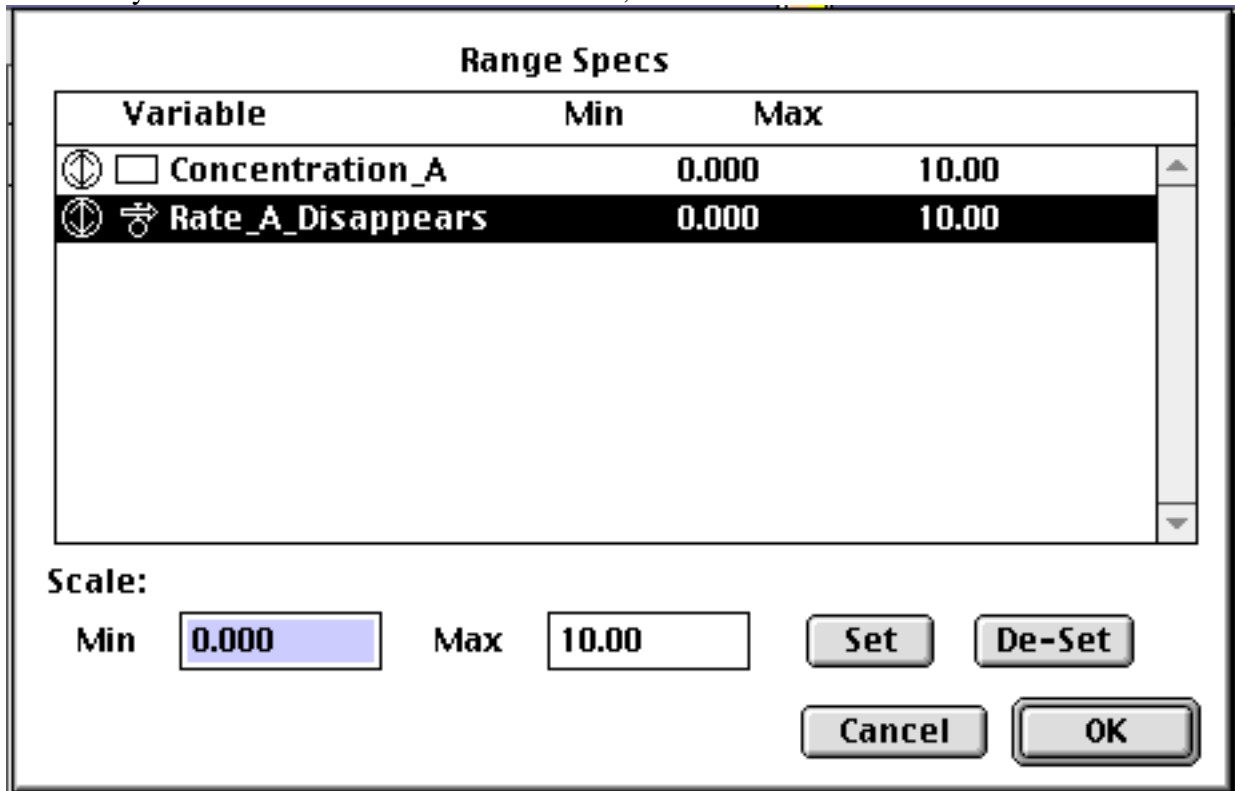
9. In the box labeled **To:**, change the 12 to **60** and in the box under **Other:**, change Time to **Seconds**. **Click OK**. Your model is now set to run a 60 second simulation of a reaction.

Setting Range Specs:

10. Go to the **Run** menu and drag down to select **Range Specs...**

11. **Click once** on **Concentration_A** and type 10 in the box labeled **Max** at the bottom of the window. **Click Set**. Do the same for **Rate_A_Disappears**.

12. When your window looks like the one below, **click OK**.



Setting up a Graph:

13. Go to the tool bar and **click once** on the graph icon . Slide your mouse pointer to a clear spot in the window and **click once** again.

14. **Double-click** anywhere in this graph and a new window will open.

15. **Double-click** on **Concentration_A** and **Rate_A_Disappears** in the **Allowable** box to move them to the **Selected** box.

16. **Click** on **OK**.

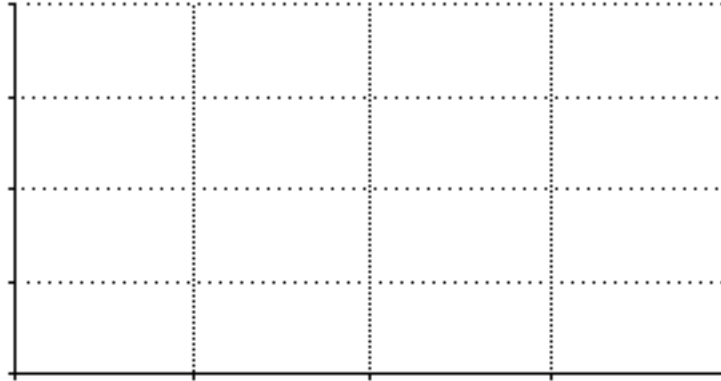
17. To prevent the graph box from disappearing every time you run the model, you should pin down the graph window.

- **Move your pointer to the horizontal bar at the top of the graph window.**
- **Drag the graph so it fits on the white space below the model.**
- **Click once on the black circle (looks like a push pin) in the upper corner of the graph.**

Using the Model:

18. To run the model, **click and hold** the **Run** option on the menu bar and **drag down to Run**.

Q1. Sketch the graph on the axes provided, labeling all parts.




Q2. Describe in full each curve on the graph.

Q3. What is the order of this reaction with respect to A? What is your evidence?

Changing the Model:

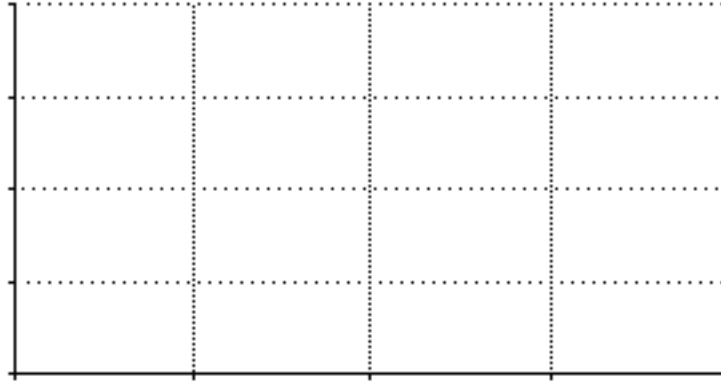
In some reactions, the rate of the reaction depends on the concentration of the reactant.

19. **Click once** on the connector icon . Position your pointer *inside* the stock, then **click and drag** the connector to the bubble of the flow. Once the bubble is highlighted, release the mouse button.

20. **Double-click** on the **Rate A Disappears** flow and enter the expression **0.1*Concentration_A** by typing the number and clicking on **Concentration_A** in the **Required Inputs** box.

21. Then click **OK** and **run** the model.

Q4. Sketch the graph on the axes provided, labeling all parts.



Q5. Describe in full each curve on the graph.

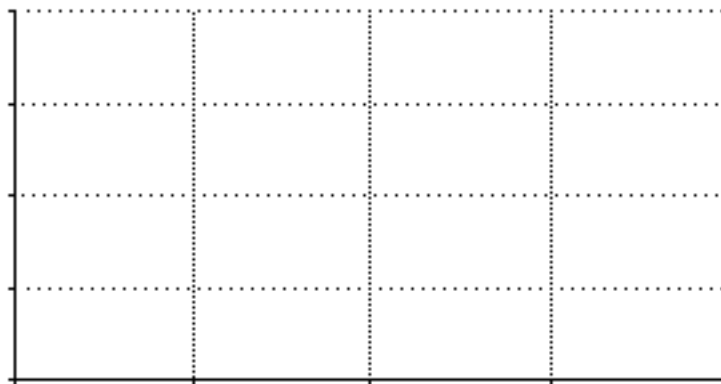
Q6. What is the order of this reaction with respect to A? What is your evidence?

Changing the Model Again:

22. Change the model so that it is second order in A and **run** the model. Note: In STELLA, x^2 means x-squared.

Q7. Describe the change you made to the model.

Q8. Sketch the graph on the axes provided, labeling all parts.



Q9. Describe in full each curve on the graph.

Q10. Referring to the graphs in Questions 1, 4 and 8, which Concentration_A curve is showing the steepest slope during the first 10 seconds? Explain what that means in the context of the problem.


Save your model as directed by your teacher.

Kinetics Student Guide Section II

Initial Concentrations of Reactants and the Initial Rate of Reaction

In this activity, you will discover how the initial concentration of a reactant affects the initial rate of reaction under different orders of reactions. To see the actual reaction rates, you will need to use a table.

1. Open the Kinetics model saved from Section I. **Un-pin** the graph by clicking on the push pin. **Close** the graph by clicking in the close box in the upper corner of the graph window.

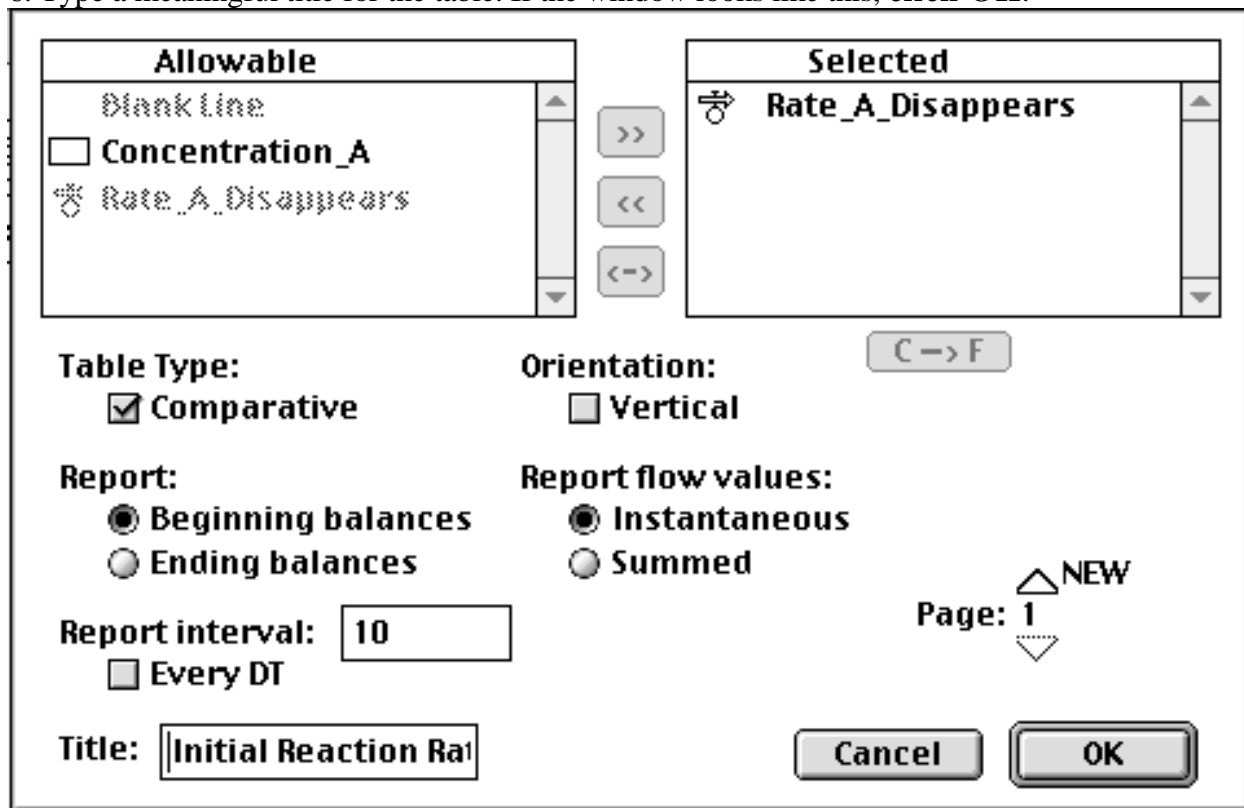
2. **Click once** on the table icon  and place it on the screen. When the table opens up, move it into the white space below the model and **pin** it down.

3. **Double-click** inside the table. Click on the **Comparative** box to check it, then double-click on **Rate_A_Disappears** to move it from the **Allowable** window to the **Selected** window.

4. Check on the **Vertical** box to un-check it.

5. **Click** on the **Every DT** box to uncheck it and type 10 in the **Report interval** box.

6. Type a meaningful title for the table. If the window looks like this, **click OK**.



Allowable	Selected
Blank Line	Rate_A_Disappears
<input type="checkbox"/> Concentration_A	
<input checked="" type="checkbox"/> Rate_A_Disappears	

Table Type: Comparative

Orientation: Vertical

Report: Beginning balances

Report flow values: Instantaneous

Report interval: 10



Every DT

Title: Initial Reaction Ra

Page: 1

Cancel OK

Problem 1 - The Zero Order Reaction Model

7. Using the dynamite icon  on the tool bar, blow up the connector  by placing the head of the dynamite on top of the small circle at the end of the connector. Take care that you do not blow up the stock accidentally! **Double-click** on the **Rate A Disappears** flow and set it to **0.01 {moles per liter per second}**. Note that the reaction rate is smaller than before.

Q1. Predict what will happen to the initial reaction rate if the initial concentration of the reactant is changed from 20 to 10 to 5 {moles per liter} and the reaction is zero order.

8. **Double-click** on the **Concentration A** stock and change it to 20. **Run** the model. Change the stock to 10 and **run** the model again. Finally, change the stock to 5 and **run** the model a third time. Your table should have four rows, one labeled **Seconds** and the other three labeled **Rate A Disappears** preceded by a 1, 2 or 3 to represent the three runs.

Q2. Complete the table provided with the appropriate data from the model.

Run	Initial Concentration A (moles per liter)	Initial Rate A Disappears (moles per liter per second)
1	20	_____
2	10	_____
3	5	_____

Problem 2 - The First Order Reaction Model

9. Re-draw the connector from the stock to the flow so you can define **Rate A Disappears** as **0.01*Concentration_A**. Go to the **Model** menu and select **Restore ... Graphs & Tables**. The table should now be cleared of numbers.

Q3. Predict what will happen to the initial reaction rate if the initial concentration of the reactant is changed from 20 to 10 to 5 {moles per liter} and the reaction is first order.

10. **Double-click** on the **Concentration A** stock and change it to 20. **Run** the model. Change the stock to 10 and **run** the model again. Finally, change the stock to 5 and **run** the model a third time.

Q4. Complete the table provided with the appropriate data from the model.

Run	Initial Concentration A (moles per liter)	Initial Rate A Disappears (moles per liter per second)
1	_____	_____
2	_____	_____
3	_____	_____

Problem 3 - The Second Order Reaction Model

11. Define **Rate A Disappears** as $0.01 * \text{Concentration_A}^2$. Go to the **Model** menu and select **Restore ... Graphs & Tables**. The table should again be cleared of numbers.

Q5. Predict what will happen to the initial reaction rate if the initial concentration of the reactant is changed from 20 to 10 to 5 {moles per liter} and the reaction is second order.

12. **Double-click** on the **Concentration A** stock and change it to 20. **Run** the model. Change the stock to 10 and **run** the model again. Finally, change the stock to 5 and **run** the model a third time.

Q6. Complete the table provided with the appropriate data from the model.

Run	Initial Concentration A (moles per liter)	Initial Rate A Disappears (moles per liter per second)
1	_____	_____
2	_____	_____
3	_____	_____

Q7. Summarize how the initial reaction rate is affected by the initial concentration of the reactant for:

a) Zero order reactions

b) First order reactions

c) Second order reactions

Q8. What is the mathematical relationship between the order of the reaction and the reaction rate?

Save your model as directed by your teacher.

Kinetics Student Guide Section III

The Effect of Temperature on the Rate of Reaction

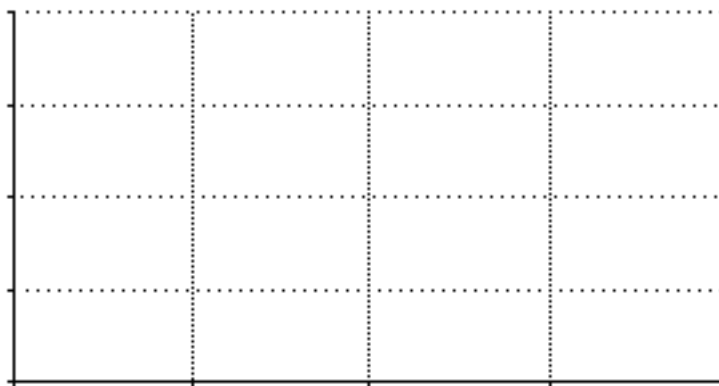
One rule of thumb (and it is a very loose rule) is that the reaction rate doubles for every 10 degree increase in temperature. In this activity, you will double the rate constant for each order of reaction to see the effect on the reaction rate. You will use the comparative graph feature so you can see the results of running the model with the two different rate constants.

1. Open the Kinetics model saved from Section II. Go to the **Model** menu and choose **Restore ...Graphs & Tables**.
2. **Un-pin** the table by clicking on the push pin. **Close** the table by clicking in the close box in the upper corner of the table window.
3. Go to the **Run** menu and drag down to select **Range Specs...** **Click once** on **Concentration_A** and **click De-Set**. Do the same for **Rate_A_Disappears**. **Click OK**.
4. **Double-click** on the icon named Graph 1. Click on the **Comparative** box to check it. **Double-click** on **Rate_A_Disappears** to move it from the **Allowable** box to the **Selected** box. **Click OK**. Pin down the graph by clicking on the push pin.

Problem 1 - The Second Order Reaction Model

5. Define **Rate A Disappears** as $0.01 * \text{Concentration_A}^2$. Define **Concentration A** as **10 {moles per liter}**.
6. **Run** the model.
7. Change the **Rate A Disappears** flow to $0.02 * \text{Concentration_A} * \text{Concentration_A}$ and **run** the model again.

Q1. Sketch the graph on the axes provided, labeling all parts.



Q2. Describe the effect that doubling the rate constant has on the lines you see on the graph.

Problem 2 - The First Order Reaction Model

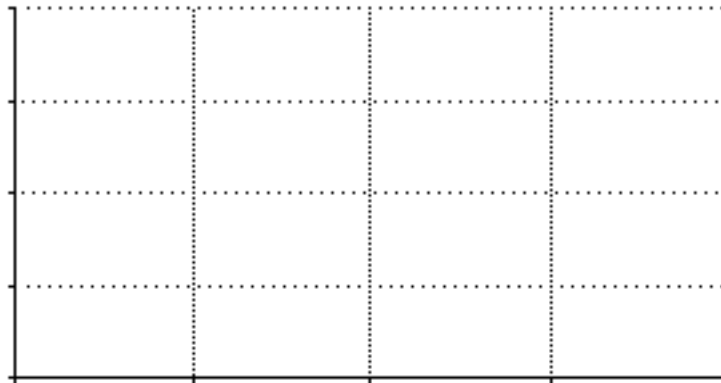
8. Define **Rate A Disappears** as $0.01 * \text{Concentration_A}$.

9. Go to the **Model** menu and select **Restore ... Graphs & Tables**.

10. **Run** the model.

11. Change the **Rate A Disappears** flow to $0.02 * \text{Concentration_A}$ and **run** the model again.

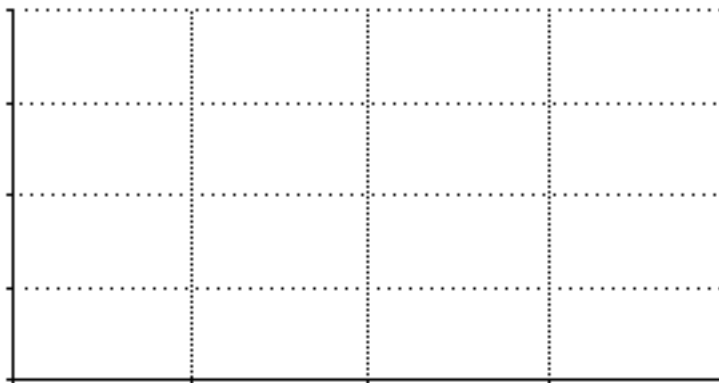
Q3. Sketch the graph on the axes provided, labeling all parts.



Q4. Describe the effect that doubling the rate constant has on the lines you see on the graph.

Problem 3 - The Zero Order Reaction Model

Q5. Without returning the model to a zero order reaction, predict what the comparative graph should look like if the first run has **Rate A Disappears** set to **0.01 {moles per liter per second}** and the second run has **Rate A Disappears** set to **0.02**. Sketch your prediction on the axes provided, labeling all parts.



Q6. Describe the effect that doubling the rate constant has on the lines you see on the graph.

Conclusions:

Q7. Summarize how the initial reaction rate is affected by doubling the rate constant for:

- a) Zero order reactions
- b) First order reactions
- c) Second order reactions

Q8. Summarize how the reaction rate graph is affected by doubling the rate constant for:

- a) Zero order reactions
- b) First order reactions
- c) Second order reactions

Save your model as directed by your teacher.