

# Titration Curves: An Application of the Logistic Function

Think about how cold germs spread through a school. One person comes to class with a cold and infects other students. At first, the disease spreads slowly, but as more students catch cold and spread it to other classmates, the disease spreads more rapidly. The rate of infection slows down again when most students are infected and there is no one left at school to infect. The maximum number of students in the school who can contract the disease is the number of students in the school.

A logistic function is often used to model this type of situation. The logistic function is an exponential function, but it contains a ratio and offset which make its behavior interesting. The formula for a logistic function is:

$$y = \frac{A}{1 + B^{x-c}} + D$$

You can use this logistic function to model an acid-base titration activity. Chemists combine acid and base solutions while monitoring the pH of the mixture to determine the concentrations of one of the reactants in a process called *titration*. Concentrations are usually made in very small numbers such as 0.000001 or  $1 \times 10^{-6}$ . Instead of working with these small numbers, chemists use a logarithmic scale. pH is the  $-\log[\text{H}^+]$  where  $[\text{H}^+]$  is the positive hydrogen ion concentration of a solution. For example, the pH of a solution with a hydrogen ion concentration of  $1 \times 10^{-6}$  is 6. The pH scale runs from 0 to 14. Solutions with a pH of less than 7 are called acids, and solutions with a pH greater than 7 are called bases. Solutions with a pH of 7 are considered neutral.

The change of pH during the titration of an acid with a base produces a titration curve. This curve is not quite a true logistic, but it does have some of the same features as a logistic function. During the first part of the titration, the pH does not change very much because there is enough acid to react with the added base. At the equivalence point, the acid has completely reacted with the base solution. As more base solution is added to the mixture, the pH increases rapidly. Once the solution becomes basic, the pH levels off and approaches the pH of the base being added.

The point at which the most rapid change occurs is called the *equivalence point*. At this point, knowing the volume and concentration of the acid and the volume of the base added allows the chemist to calculate the concentration of the base using a simple proportion.

In this activity, you will add base to an acid and use a logistic function to model the data and locate the equivalence point.

## OBJECTIVES

- Record pH versus base volume data for an acid-base titration.
- Manually model the titration curve using a logistic function.
- Describe the role of each parameter in the logistic function.

## MATERIALS

TI-83 Plus or TI-84 Plus graphing calculator  
EasyData application  
data-collection interface  
pH Sensor  
safety goggles

distilled water in wash bottle  
25 mL household vinegar  
50 mL household ammonia  
50 mL or 100 mL graduated cylinder,  
cup, or beaker

## PROCEDURE

1. Obtain and wear goggles.
2. Prepare the pH Sensor for data collection.
  - a. Turn on your calculator. Connect the pH Sensor, data-collection interface, and calculator.
  - b. Loosen the top of the pH storage bottle, and carefully remove the bottle. Slide the top of the bottle up the shaft of the sensor so that the bottle top is out of the way. Do not remove the top from the sensor shaft.
  - c. Rinse the tip of the pH sensor with distilled water.
  - d. Place the pH sensor in a clean beaker or cup, and support it so that the beaker or cup does not fall.
  - e. Add 25 mL of vinegar to the beaker or cup. The vinegar should cover the tip of the sensor.
3. Set up EasyData for data collection.
  - a. Start the EasyData application, if it is not already running.
  - b. Select **[File]** from the Main screen, and then select **New** to reset the application.
  - c. Select **[Setup]** from the Main screen, and then select **Events with Entry**.
4. You are now ready to collect data. The data points you will collect are the pH of the mixture and the volume of base added to the mixture. In this experiment, the acid used is vinegar and the base is ammonia. It is best if one person adds ammonia while a second person operates the calculator.
  - a. Select **[Start]** to begin data collection.
  - b. Select **[Keep]** to record the pH of the vinegar before any ammonia is added.
  - c. The calculator will prompt for a value. Since you have added no ammonia, enter **0** and select **[OK]**.
  - d. Add 5 mL ammonia to the beaker or cup, and gently stir.
  - e. Select **[Keep]** to record the new pH.
  - f. Enter **5** for the total amount of ammonia you have added and select **[OK]**.
  - g. Repeat Steps d-f until you have added a total of 40 mL of ammonia. Remember that the volume of ammonia in the mixture is cumulative, so the volume data point entered increases each time you record the pH and volume. For example, the second ammonia volume data point is 10, the third is 15, and so forth until you reach 40 mL.
  - h. Select **[Stop]** to end data collection.
  - i. The graph of pH versus volume of ammonia will be displayed.
5. Examine the data pairs on the displayed graph. As you move the cursor right or left, the volume ( $x$ ) and pH ( $y$ ) values of each data point are displayed on the graph. If you want to collect more data using a fresh sample of vinegar, select **[Main]**, and repeat Step 4.

6. If you are satisfied with this data, select  $\overline{\text{Main}}$  to return to the Main screen. Exit EasyData by selecting  $\overline{\text{Quit}}$  from the Main screen and then selecting  $\overline{\text{OK}}$ .
7. When data collection is completed, use additional distilled water to rinse the pH sensor. Replace the storage bottle on the pH sensor.

## ANALYSIS

1. Redisplay the graph outside EasyData, and prepare to read values off of the graphs using the TRACE function.
  - a. Press  $\overline{\text{2nd}}$  [STAT PLOT].
  - b. Press  $\overline{\text{ENTER}}$  to select Plot1 and press  $\overline{\text{ENTER}}$  again to select On.
  - c. Press  $\overline{\text{ZOOM}}$ .
  - d. Press  $\overline{\text{▼}}$  until ZoomStat is highlighted. Press  $\overline{\text{ENTER}}$  to display a graph with the  $x$  and  $y$  ranges set to fill the screen with data.
  - e. Press  $\overline{\text{TRACE}}$  to determine the coordinates of a point on the graph using the cursor keys.
2. Before analyzing the collected data and the behavior of the logistic function, you need a better understanding of how the parameters ( $A$ ,  $B$ ,  $C$ , and  $D$ ) relate to one another.

$$y = \frac{A}{1 + B^{x-C}} + D$$

In this activity, the value of the parameter  $B$  is between zero and one, and the other parameters have values between 4 and 10. If  $x$  is very small so that the exponential  $B^{x-C}$  is large (remember that  $B$  is less than one), then the first term is very small. The value of  $y$  is then approximately equal to  $D$ .

On the calculator, trace to the extreme left side of the pH versus volume graph, and find the pH at the smallest  $x$  value. Record this value as  $D$  in the Data Table on the *Data Collection and Analysis* sheet. Record all values to two significant figures.

3. For a large  $x$ , or more added ammonia, then the exponential  $B^{x-C}$  becomes small, and the first term is approximately  $A$ . Then  $y$  is approximately  $A + D$ . Trace over to the extreme right side of the graph, and note the pH value at this point. This is the sum  $A + D$ . Use this pH value to calculate the value for  $A$ , and record it in the Data Table.
4. A special situation exists when  $x = C$ . This makes  $B^0 = 1$ , and the first term is  $\frac{1}{2}A$ . You can use this special situation to determine a value for  $C$  by finding the  $x$ , or the volume of added ammonia, that gives a pH with an approximate value of  $D + \frac{1}{2}A$ .

Trace across the graph to determine this value, and record it as  $C$  in the Data Table on the *Data Collection and Analysis* sheet.

5. Enter the logistic equation for the model plotted against the data.
  - a. Press  $\overline{\text{Y=}}$ .
  - b. Press  $\overline{\text{CLEAR}}$  to remove any existing equation.
  - c. Enter the logistic equation  $A/(1+B^{(X-C)}) + D$  in the  $Y_1$  field.
  - d. Press  $\overline{\text{2nd}}$  [QUIT] to return to the home screen.

### Activity 31

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- Enter values for the three parameters for which you have values:  $A$ ,  $C$ , and  $D$ . For example, to store the value for  $A$ , enter a value for the parameter  $A$ . Press  $\text{STO} \rightarrow A \text{ ENTER}$  to store the value in the variable  $A$ . Repeat for the other parameters.
- The Data Table has one parameter,  $B$ , with no value. You need to set a value for this parameter. To obtain a good fit (this is called optimizing the value), you will need to try several values for  $B$ . Start with  $B = 0.5$ , and experiment with different values until you find one that provides a good fit for the data.

To store a value for  $B$  in the calculator:

- Enter a value for the parameter  $B$ . Press  $\text{STO} \rightarrow B \text{ ENTER}$  to store the value in the variable  $B$ .
- Press  $\text{GRAPH}$  to see the data with the model graph superimposed.
- Press  $\text{STO} \rightarrow [\text{QUIT}]$  to return to the home screen.

Record this optimized value for  $B$  in the Data Table.

- Display the graph with the model one more time.

⇒ Answer Question 1 on the *Data Collection and Analysis* sheet.

### EXTENSION

The calculator can perform an automatic logistic regression, although the form of the calculator's logistic expression is slightly different from the one used in the model earlier. The calculator uses the form:

$$y = \frac{c}{1 + ae^{-bx}}$$

The key difference between this and the form used earlier is that there is no additive term  $+ D$ . The other difference between this and the form used earlier is that the exponential function is based on  $e$ , rather than a direct exponential on a parameter. Because of the additive term, you will have to subtract a constant value from the data in order to use the calculator's form. Do that first. Afterward, you can perform the calculator fit and compare it to the model.

- The data in the pH column must be positive, but for this analysis, we need it to start near zero. Press  $\text{GRAPH}$  to see the collected data, and press  $\text{TRACE}$  to read values from the graph. Find the smallest pH value of the data (*not* the model) and make a note of that value.
- Press  $\text{2nd} [\text{QUIT}]$  to return to the home screen. Subtract a number just smaller than the minimum value from your pH values:
  - The pH values are stored in  $L2$ . Press  $\text{2nd} [L2]$ . Press  $\text{—}$ , and enter a value just smaller than the minimum pH.
  - Press  $\text{STO} \rightarrow \text{2nd} [L2] \text{ ENTER}$  to store the altered values back in  $L2$ .
- Have the calculator fit its logistic equation to the data.
  - Press  $\text{STAT}$  and use the cursor keys to highlight  $\text{CALC}$ .
  - Press  $\text{↓}$  until Logistic is highlighted. Press  $\text{ENTER}$  to copy the command to the home screen.
  - Press  $\text{2nd} [L1] \text{ , } \text{2nd} [L2] \text{ ,}$  to enter the lists containing the data.
  - Press  $\text{VARS}$  and use the cursor keys to highlight  $\text{Y-VARS}$ .

- e. Select Function by pressing **ENTER**.
- f. Press **ENTER** to copy  $Y_1$  to the expression.
- g. On the home screen, you'll now see the entry Logistic L1, L2,  $Y_1$ . This command will perform a logistic regression with L1 as the  $x$  and L2 as the  $y$  values. The resulting regression line will be stored in equation variable  $Y_1$ .  
Press **ENTER** to perform the linear regression. Write the values for the parameters  $a$ ,  $b$ , and  $c$  in the second column of the Extension Data Table on the *Data Collection and Analysis* sheet.

⇒ Answer Extension Question 1 on the *Data Collection and Analysis* sheet.

- h. Press **ZOOM**. Press **↓** until ZoomStat is highlighted; press **ENTER** to display a graph with the  $x$  and  $y$  ranges set to fill the screen with data.

⇒ Answer Extension Questions 2–4 on the *Data Collection and Analysis* sheet.

**DATA COLLECTION AND ANALYSIS**

Name \_\_\_\_\_

Date \_\_\_\_\_

**DATA TABLE**

<i>A</i>	<i>B</i>	<i>C</i>	<i>D</i>

**QUESTION**

1. Is the logistic equation a good model for the titration data?

**EXTENSION DATA TABLE**

	Algebraic Expression	Parameters from calculator	Parameters as calculated from model
<b>a (in terms of <i>B</i> and <i>C</i>)</b>			
<b>b (in terms of <i>B</i>)</b>			
<b>c (in terms of <i>A</i>)</b>			

**EXTENSION QUESTIONS**

1. Use the three parameters a, b and c to write down the calculator's fit equation.
2. From the graph appearance, how does the calculator's fit compare to yours?

3. How do the calculator's parameters compare to those you determined?

To answer this question you will need to determine the correlation of  $A$ ,  $B$ , and  $C$  to  $a$ ,  $b$ , and  $c$ . By comparing corresponding locations in the expressions, fill in the Extension Data Table. You will need to use properties of exponential expressions to find the correspondences. After you find these expressions, insert the values of  $A$ ,  $B$  and  $C$  from the model to calculate comparison values to those of the calculator.

4. How do the model parameters, when expressed in terms of the calculator's parameters, compare? Should they be similar?