CoreModels

Enzyme Model—Catalase

A CORE LEARNING GOALS ACTIVITY FOR SCIENCE AND MATHEMATICS

Summary

Students use a computer and a preconstructed STELLA® model of enzyme activity to study the reaction rate of the enzyme catalase. They simulate the effects of variables on the enzyme catalysis rate, substrate amount and reaction product amounts. The variables are temperature, pH, amount of enzyme, and amount of substrate.

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Enzyme Model—Catalase

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OVERLOOK

Students work with a preconstructed STELLA® model (Appendixes A, B, and C) to simulate changes in the catalytic reaction rate of the enzyme catalase. They change the value of the experimental variables, one variable at a time. The variables are temperature, pH, amount of enzyme, and amount of substrate. With each run of the model, STELLA® generates graphs showing effects of that variable on the enzyme catalysis rate, amount of substrate, and amounts of reaction products.

Interpreting the graphs and the model is the essence of the activity. You may use Generic Graph Questions (Appendix D) and CoreModels Graph Interpretation Guidelines (Appendix E) for students who need help. Appendix C has the STELLA® equations, for students who are interested in how the model works.

The model is based on the action of catalase, which converts hydrogen peroxide to water and oxygen.The original model from the Creative Learning Exchange has been modified for this activity. The Maryland Virtual High School model version can be found at the MVHS web site.

ACTIVITY PARTS AT A GLANCE

Part	Title	Estimated Minutes
A	Graphing the reaction	15
B	Changing the temperature	15
C	Changing the pH	10
D	Changing the enzyme concentration	10
E	Changing the substrate concentration	10
F	Interpreting the graphs	15

PRIOR KNOWLEDGE

Computer knowledge: Students with no computer skills can do this activity, but may require an explanation of the STELLA® application before they start.

Variables: Students should know the difference between control variables and experimental variables. They should have some experience using the scientific method of investigation, testing variables one at a time.

Enzymes: Students should be familiar with enzymes and their action and should understand catalysis. This activity works best when used just after a lab session on enzymes, especially one featuring catalase, where students have measured enzyme catalysis rates.

Graphs: Students should be able to read and interpret graphs. You might do Part A as a demonstration with class discussion if your students need graph-reading instruction.

pH: Students should know what pH represents.

Times 10: Students may need a review of scientific notation and the meaning of "factor of 10."

TEACHING TIPS

Review: A quick review of enzymes and catalysis at the start of the activity could reinforce what students have learned in lab sessions and what they will learn in the computer activity.

Color: Because students will be sketching many curves on the blank graphs, they may want to use colored pencils to make each curve a different color, just as the curves are in the model.

Choosing values: In Part B, Changing the temperature, students should choose eight to ten new values, some higher and others lower than the initial temperature. Students may need guidance in selecting temperatures. They could start at 10, for example, and generate curves for 15, 20 (the initial value), 25, 30, 35, 40, and so on.

Values, again: In Part C, Changing the pH, students should choose several new values , some higher and others lower than the initial pH. Students may use a specific interval for changing the pH, like 0.2 or 0.3.

Enlarging the graph: In Part D, Changing the enzyme concentration, students may need to enlarge the H2O2 to Water graph to see that the rate doubles when the enzyme amount doubles. Students may want to enlarge graphs for many of the variable changes.

Longer simulation: In Part E, Changing the substrate concentration, you may want to have students extend the length of model simulation for increased substrate from 10 minutes to 50 minutes to see that the reaction finally stops as the substrate is exhausted.

Trouble spots: Possible problems as students work with the model:

- They forget to copy the curves STELLA® generates.
- They forget to label each curve.
- They "mess up" their graphs and need new blank graph pages.
- They fail to change the variables systematically.
- They decide to investigate the model layer and inadvertently change the model.

EXTENSIONS

Other enzymes, such as pepsin, can be investigated with the STELLA® model.

Human health requires properly functioning enzymes. Students could report on diseases such as PKU and Tay-Sachs, which are caused by enzyme malfunction.

A safe food supply depends, in part, on control of enzymes in fruits and vegetables. Students could explain how food storage conditions delay ripening of apples, pears, potatoes and other common edibles.

Extreme environments contain creatures that tolerate very high or low temperatures, very acidic or alkaline surroundings, very wet or dry conditions. How do their enzymes do it?

Acid rain changes the environment. How do organisms react to declining pH?

Genetic engineering techniques use high-temperature enzymes. Why?

Animal metabolism slows at low temperatures. What happens to enzymes in such conditions?

The model's **mathematics** and **enzyme kinematics** may interest advanced students.

Enzyme Model—Catalase

Teacher Guide—Answers

Catalysts accelerate chemical reactions that otherwise proceed slowly. The enzyme called catalase is a catalyst. It exists in plant and animal cells and breaks down hydrogen peroxide, H2O2, which is a byproduct of metabolism. Hydrogen peroxide is toxic if it accumulates in a cell.

The chemical reaction accelerated by catalase is written

$$2(H_2O_2) \xrightarrow[\text{catalase}]{} 2H_2O + O_2$$

Under favorable conditions, the reaction occurs very fast. The maximum catalytic rate for one catalase molecule is 6 million molecules of hydrogen peroxide converted to water and oxygen per minute. The reaction product is 6 million molecules of water and 3 million molecules of oxygen. (Because the oxygen molecule consists of two oxygen atoms, the number of oxygen molecules made in the reaction is half the number of water molecules.)

Part A. Graphing the reaction

Catalase, like most enzymes, is sensitive to the conditions in which it operates. The main factors that influence enzyme-catalyzed reactions are temperature, pH, enzyme concentration, and substrate concentration. In this activity, you will simulate how the enzyme catalysis rate (the rate of hydrogen peroxide conversion) changes as these factors change. The changes are shown in graphs generated by a preconstructed model **(see Appendix A)** made with the STELLA® application and adapted from a model on the Creative Learning Exchange web site.

- Open the file called Enzyme.stm to launch the STELLA® application. You will see four blank graphs and four sliders.

When you run the model, each graph will show a dependent variable plotted as a function of time. Time is the independent variable in this activity and is set in minutes. The model has been arranged so the graphs will show:

Hydrogen peroxide (expressed as number of molecules) versus time

Water (number of molecules) vs. time

Oxygen (number of molecules) vs. time

H2O2 to water rate (number of hydrogen peroxide molecules converted per minute, which is equal to the number of water molecules produced per minute) vs. time

1. Record the initial amount of each dependent variable, shown above each graph. Be sure to record the units of measure.

Amount of hydrogen peroxide **100,000,000 molecules**

Amount of water **0 molecule** s

Amount of oxygen **0 molecules**

H2O2 to water rate **27,000,000 water molecules per minute**

The sliders represent factors that can influence the enzyme catalysis rate.

2. Record the initial value on each factor's slider and indicate what it measures.

Hydrogen peroxide exponent (amount of substrate) **8 (for 10^8 molecules)**

pH **7.0 (neutral)**

Temperature **20 degrees Celsius**

Available Enzyme **5 molecules**

In laboratory work, you may have measured enzyme catalysis rates in different ways. In this computer activity, you will use the STELLA® model to change factors individually, simulating their effect on the enzyme catalysis rate.

Run the model at its initial settings.

On the four temperature-effect graphs, sketch the curves that STELLA® generates. Label each curve with the initial temperature setting. **See Appendix B.**

3. What does the shape of each curve indicate about the change in that variable over the simulated 10 minutes of enzyme activity?

3a. Hydrogen Peroxide

The hydrogen peroxide curve decreases rapidly, then levels off, indicating that most of the hydrogen peroxide molecules have been broken down when the simulation is halfway through.

3b. Water

The water curve increases rapidly, then levels off, indicating that most of the water molecules have been created by about halfway through the simulation.

3c. Oxygen

The oxygen curve increases half as rapidly as the water curve (or, to only half the height of the water curve). Then it levels off, indicating that most of the oxygen molecules are created by about halfway through the simulation.

3d. H2O2 to Water Rate

The curve starts high and stays level (steady) for a quarter of the simulation. It decreases steeply for the next quarter, then levels out. The shape indicates that the reaction is steady for the first quarter of the model run, then slows to a near stop by the end of the simulation.

4. Why do you think the curves show no change after about 5 minutes?

The curves show no change because the model reaction runs out of substrate.

Part B. Changing the temperature

Temperature affects nearly all chemical reaction rates. Rising temperature increases enzyme reactions rates until, at high temperatures, enzymes fail to work. Some of the chemical bonds of the enzyme give way and the enzyme's three-dimensional structure begins to come apart, that is, the enzyme denatures.

In this part of the activity, you will choose different temperatures for the reaction so you can simulate how the enzyme catalysis rate, amount of substrate, and amounts of reaction products change. You will also find the optimum temperature range for catalase to operate.

- Use the Temperature slider to select temperature, or click the number box and type your values.
- Run the model after each change.
- As STELLA® generates each set of curves for each temperature, sketch the curves on the temperature-effect graphs at the end of the activity. Note that STELLA® uses a different color for each model run.
- Label each curve with the temperature you selected for that model run.

5. According to the graphs of temperature effect, how do the variables change as temperature changes?

At temperatures between about 15 °C and 45 °C, the amount of hydrogen peroxide decreases rapidly, then levels off, and the most water and oxygen molecules are produced.

6. What is the optimum temperature range for catalase to break down hydrogen peroxide?

The exact optimum temperature range is 20 to 35 °C, inclusive. Students should see a difference in the curves below 20 degrees and above 40 degrees.

7. What relationship between temperature and enzyme catalysis rate does the H2O2 to Water graph show?

At temperatures above or below the optimum range, the enzyme catalysis rate is lower.

Part C. Changing the pH

Acidity and alkalinity are measured as pH. The pH of the cellular environment greatly affects the ability of catalase to break down hydrogen peroxide. In this part of the activity, you will run the model through a range of pH settings to simulate how changes in pH affect the enzyme catalysis rate, amount of substrate, and amounts of reaction products. You will also find the optimum pH range for catalase to operate.

- Pull down the Map menu and choose Restore, then choose All Devices. The graphs will become blank and the sliders will return to their initial value.
- Run the model with the initial settings to generate curves for comparison.
- Use the pH slider to change the pH value, or click the number box and type your values.
- Choose several new values.
- Run the model after each change.
- As STELLA® generates each set of curves for each pH, sketch the curves on the pH-effect graphs at the end of the activity. Label each curve with the pH you selected for that model run.

8. What is the optimum pH range for catalase to break down hydrogen peroxide?

The optimum pH range is 6.5 to 7.5, inclusive.

9. What relationship between pH and enzyme catalysis rate does the H2O2 to Water graph show?

At pH values above or below the optimum range, the enzyme catalysis rate is lower. At very high or very low pH values, the reaction does not proceed.

Part D. Changing the enzyme concentration

The amount of enzyme available to process the substrate can control an enzyme catalytic reaction. In this part of the activity, you will use the Available Enzyme slider to simulate how doubling the amount of enzyme affects the enzyme catalysis rate, amount of substrate, and amounts of reaction products.

Use Restore All Devices.

Run the model with the initial settings.

10. What effect do you think doubling the amount of catalase will have on the enzyme catalysis rate?

Doubling the amount of catalase should double the rate.

- Use the slider to double the available enzyme value, or click the number box and type your values. Double the value once, then increase the value by a small number, like 4 or 5, so you can see changes in the graphs.
- Run the model after each change.
- As STELLA® generates curves for each value increase, sketch the curves on the available-enzyme graphs at the end of the activity. Label each curve with the available enzyme value you selected for that model run.

11. What relationship between the amount of catalase and the enzyme catalysis rate does the H2O2 to Water graph show?

    The more catalase available, the higher the enzyme catalysis rate, up to a certain amount of enzyme. (Students will probably need to enlarge the H2O2 to Water graph to see the rate change.) Between 15 and 20 molecules of catalase, all the available hydrogen peroxide designated by the model is instantly converted, so the enzyme catalysis rate decreases immediately.

12. Why do you think the enzyme catalysis rate declines rapidly?

    The rate declines rapidly because there are not enough substrate molecules in the model for more than about 15 enzyme molecules. When catalase runs out of hydrogen peroxide to convert (that is, when the 100 million molecules supplied by the model are gone), the reaction stops.

Part E. Changing the substrate concentration

The amount of substrate can control an enzyme catalytic reaction. In the model the amount of substrate is set by the hydrogen peroxide exponent. A change of 1 in the hydrogen peroxide exponent value changes the amount of substrate by a factor of 10.

In this part of the activity, you will change the value of the hydrogen peroxide exponent to simulate how changing the amount of substrate affects the enzyme catalysis rate, amount of enzyme, and amounts of reaction products.

- Use Restore All Devices.
- Run the model with the initial settings.

13. What effect do you think changing the amount of hydrogen peroxide by a factor of 10 will have on the enzyme catalysis rate?

Decreasing the amount of hydrogen peroxide should decrease the rate. Increasing the amount should increase the rate.

- Use the slider to decrease the hydrogen peroxide exponent value to 7, or click the number box and type your value.
- Run the model.
- As STELLA® generates curves for the new exponent value, sketch them on the substrate-amount graphs at the end of the activity. Label each curve Hydrogen Peroxide Exponent 7.
- Change the exponent value to 9, run the model, and sketch and label the curves that STELLA® generates.

14. What relationship between the amount of hydrogen peroxide and the enzyme catalysis rate does the H2O2 to Water graph show?

The graph shows that, under initial conditions (10^8 molecules), the rate is steady for about 2.5 minutes before it starts to decline. When the substrate amount decreases by a factor of 10 (to 10^7 molecules), the rate starts lower and declines very quickly. When the amount of substrate increases by a factor of 10 (to 10^9 molecules), the reaction rate remains steady for at least 10 minutes (length of model simulation).

15. Why do you think the enzyme catalysis rate curves have the shape you see in the H2O2 to Water graph?

When the number of hydrogen peroxide molecules in the model is decreased from 100 million to 10 million and the number of enzyme molecules remains at 5, the reaction starts at a lower rate and soon stops (approaches zero) because the enzyme very quickly converts all available substrate. When the number of hydrogen peroxide molecules is increased from 100 million to 1 billion, the enzyme catalysis rate starts at its maximum and stays there because the substrate is in oversupply with respect to the enzyme.

Part F. Interpreting the graphs

Simulating an enzyme catalytic reaction with a computer model allows you to change one variable while holding the others constant.

Look at the sets of graphs you have sketched for all the changes of the four variables. Questions 16 through 20 ask you to interpret the graphs.

16. How can you tell from the graphs what the optimum conditions are for each variable in this simulation?

At optimum conditions, the hydrogen peroxide amount decreases rapidly to almost zero. Water and oxygen molecules are produced most rapidly. Enzyme catalysis rate is at its highest value.

17. What are the most favorable conditions for catalase to break down hydrogen peroxide?

Catalase works best between 22 and 35 °C, with pH 6.5 to 7.5 (around neutral), and just enough catalase molecules to break down the supply of hydrogen peroxide molecules.

18. How do the curves for hydrogen peroxide and water compare?

The curves are mirror images. For every molecule of hydrogen peroxide that disappears, a molecule of water appears.

19. How do the graphs for water and oxygen compare?

The curves are the same shape, but oxygen's are half the height of water's. Half as many oxygen molecules form in the reaction as water molecules.

20. How do you think the catalase reaction simulated by the STELLA® model compares with the reaction in living organisms?

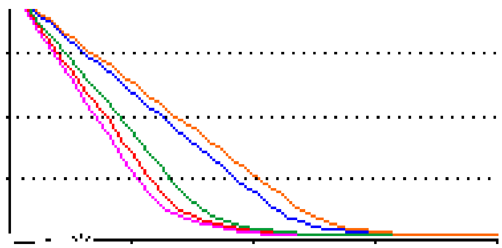
In the model, for most of the variables' values, nearly all the hydrogen peroxide molecules are used up, so the reaction stops. In living organisms, the cells are always making hydrogen peroxide, so the reaction keeps going.

Graphs of Values for Parts B, C, D and E

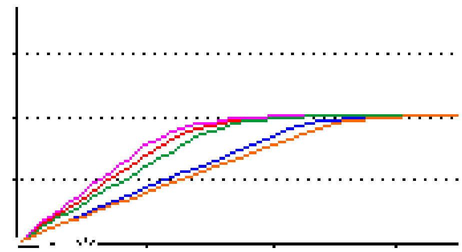
Effects of Temperature, pH, Available Enzyme and Substrate Concentration

Part B. Effect of temperature on enzyme reactions rates

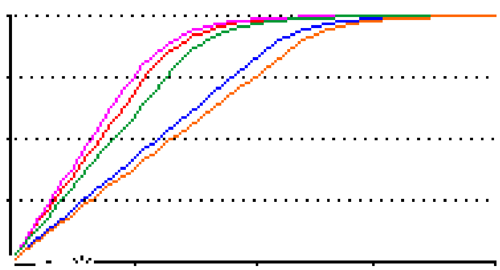
Hydrogen Peroxide



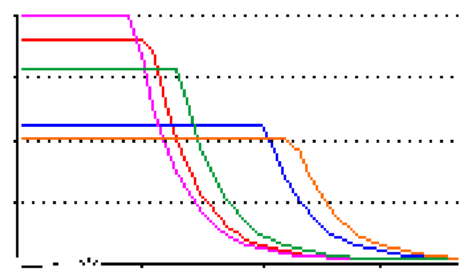
Oxygen



Water

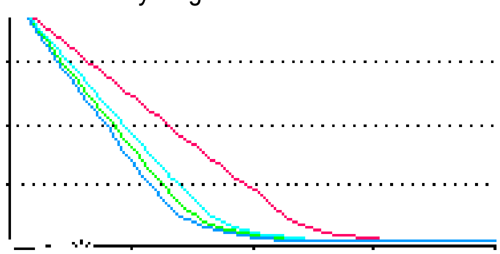


H2O2 to Water

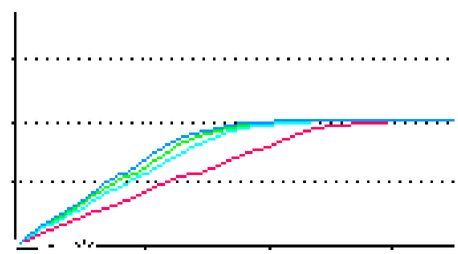


Part C. Effect of pH on enzyme reactions rates

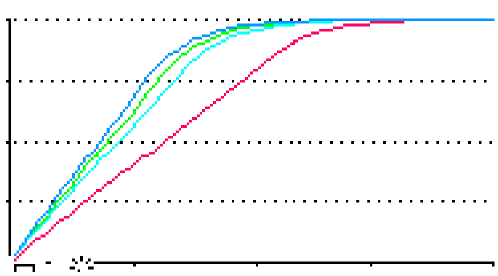
Hydrogen Peroxide



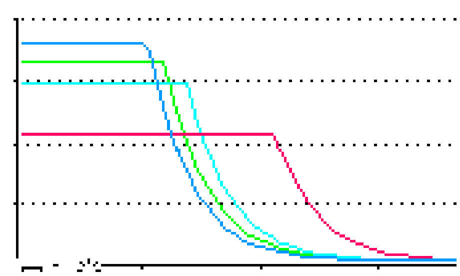
Oxygen



Water



H2O2 to Water

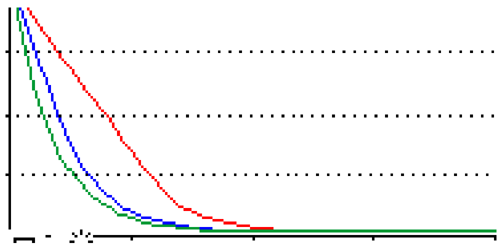


Graphs of Values for Parts B, C, D and E (cont.)

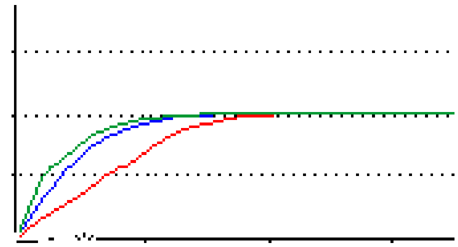
Effects of Temperature, pH, Available Enzyme and Substrate Concentration (cont.)

Part D. Effect of available enzyme on enzyme reactions rates

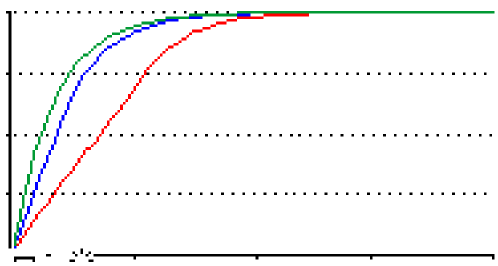
Hydrogen Peroxide



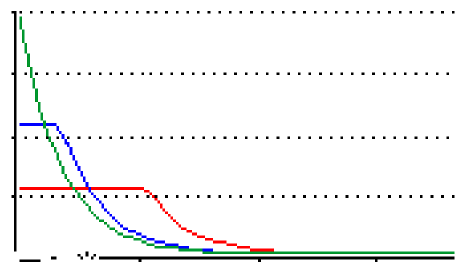
Oxygen



Water

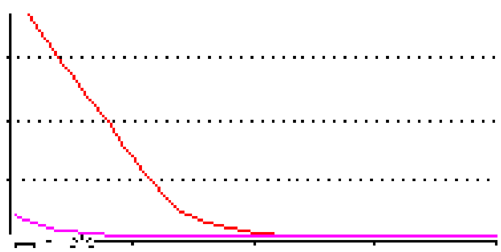


H2O2 to Water

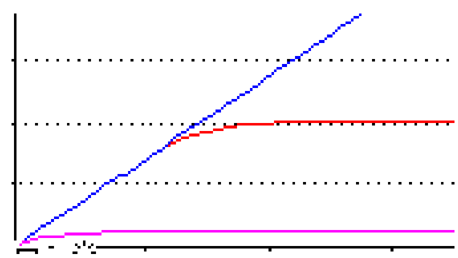


Part E. Effect of substrate amount on enzyme reactions rates

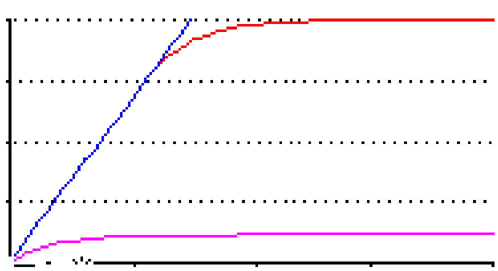
Hydrogen Peroxide



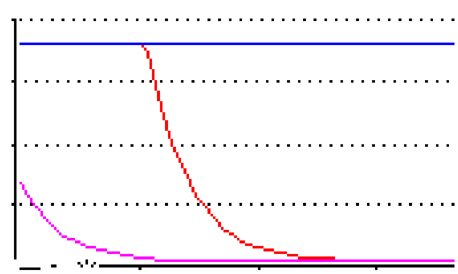
Oxygen



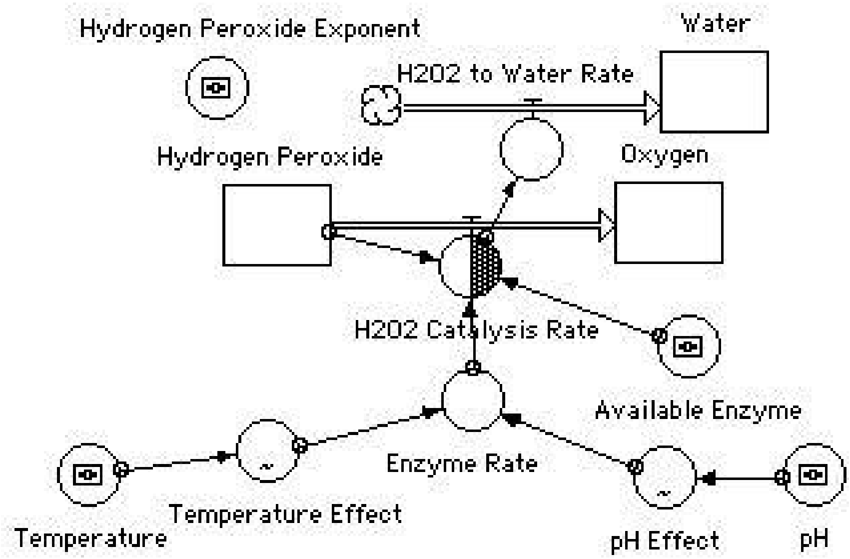
Water



H2O2 to Water



Appendix A
Enzyme Model—Catalase



The chemical reaction accelerated by catalase is written

$$2(H_2O_2) \xrightarrow[\text{catalase}]{} 2H_2O + O_2$$

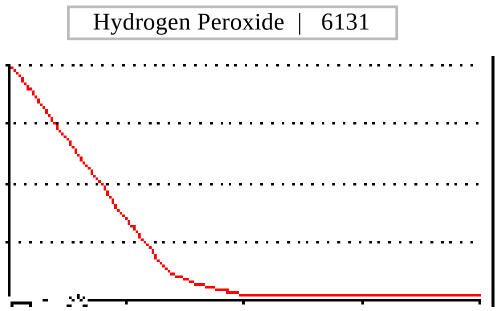
Initial values of each dependent variable:

- Amount of hydrogen peroxide **100,000,000 molecules**
- Amount of water **0 molecules**
- Amount of oxygen **0 molecules**
- H2O2 to water rate **27,000,000 water molecules per minute**

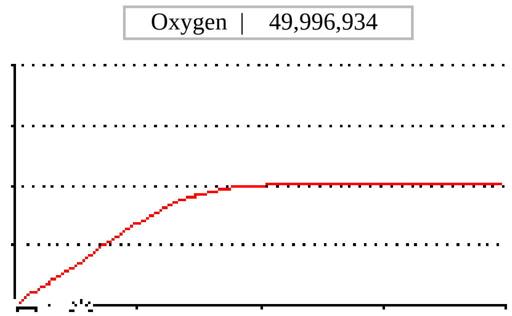
Initial values of each influencing factor's slider:

- Hydrogen peroxide exponent (amount of substrate) **8**
- pH **7.0 (neutral)**
- Temperature **20 degrees Celsius**
- Available Enzyme **5 molecules**

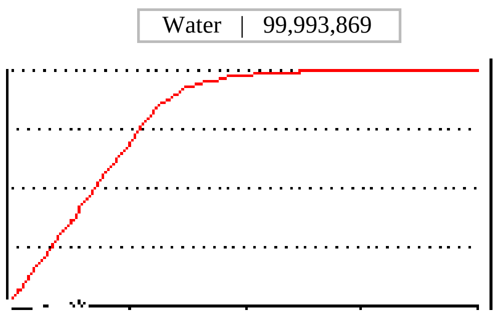
Appendix B
Enzyme Model—Initial Run



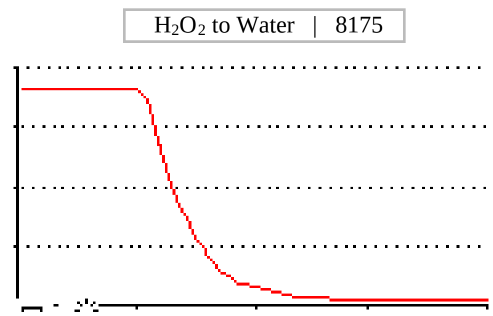
Graph: Hydrogen Peroxide



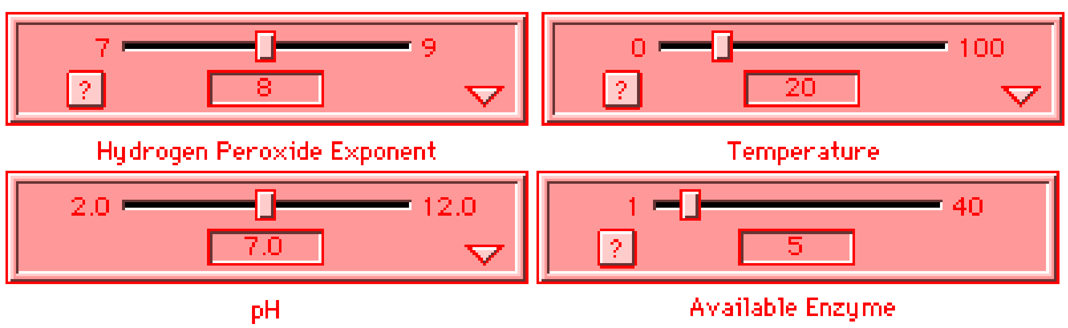
Graph: Oxygen



Graph: Water



Graph: H2O2 to Water



Each graph shows a dependent variable plotted as a function of time.

Time is the independent variable in this activity and is set in minutes.

The model has been arranged so that the graphs will show:

Hydrogen peroxide (expressed as number of molecules) versus time
Water (number of molecules) vs. time
Oxygen (number of molecules) vs. time
H2O2 to Water rate vs. time

The enzyme catalysis rate (H2O2 to Water) is the number of hydrogen peroxide molecules converted per minute, which is equal to the number of water molecules produced per minute.

Appendix C
Enzyme Model—STELLA® Equations

Hydrogen_Peroxide(t) = Hydrogen_Peroxide(t-dt)+(- H2O2_Catalysis_Rate) * dt
INIT Hydrogen_Peroxide = 1*10^(Hydrogen_Peroxide_Exponent)
DOCUMENT: The amount of hydrogen peroxide in this stock is number of molecules and not absolute concentration (M). The value is set at more than the maximum catalytic rate of catalase at its optimal temperature and pH, which is 6 million H2O2 molecules (see H2O2 Catalysis Rate and H2O2 to Water flows).
OUTFLOWS:

H2O2_Catalysis_Rate(o) = min(Enzyme_Rate*Available_Enzyme,Hydrogen_Peroxide)
DOCUMENT: The enzyme catalysis rate equals the minimum of the amount of hydrogen peroxide and the catalase catalytic rate multiplied by the amount of available enzyme. Because two molecules of hydrogen peroxide are converted into two molecules of water and one molecule of oxygen (O2), this model uses a conversion multiplier to halve the amount of oxygen accumulated per catalytic event. (See H2O2 Catalysis Rate (i).)

Oxygen(t) = Oxygen(t - dt) + (H2O2_Catalysis_Rate) * dt
INIT Oxygen = 0
DOCUMENT: The number of oxygen molecules created is one-half the number of hydrogen peroxide molecules that break down in the reaction. Therefore, the model uses a conversion multiplier to halve the amount of oxygen accumulated per catalytic event.
INFLOWS:

H2O2_Catalysis_Rate(i) = H2O2_Catalysis_Rate(o) * CONVERSION MULTIPLIER

CONVERSION MULTIPLIER = 0.5

DOCUMENT: The enzyme catalysis rate equals the minimum of the catalase catalytic rate multiplied by the amount of available enzyme and the amount of hydrogen peroxide. Because two molecules of hydrogen peroxide are converted into two molecules of water and one molecule of oxygen (O2), this model uses a conversion multiplier to halve the amount of oxygen accumulated per catalytic event. (See H2O2 Catalysis Rate (i).)

Water(t) = Water(t - dt) + (H2O2_to_Water) * dt
INIT Water = 0
DOCUMENT: The water measured here is metabolic water, water that is produced from the conversion of hydrogen peroxide by catalase.
INFLOWS:

H2O2_to_Water = H2O2_Catalysis_Rate
DOCUMENT: This model "measures" metabolic water because that number of molecules is equal to the number of H2O2 molecules converted; so H2O2 to Water is set to equal H2O2 Catalysis Rate catalysis without a conversion multiplier.

Appendix C (cont.)
Enzyme Model—STELLA® Equations

Available_Enzyme = 5
DOCUMENT: Amount is number of molecules of catalase.

Enzyme_Rate = 6e6 * pH_Effect*Temperature_Effect
DOCUMENT: The catalytic rate of catalase (the number of molecules of substrate converted per enzyme molecule per minute) is affected by both the pH and the temperature of the reaction. Each factor has an optimal value.

Hydrogen_Peroxide_Exponent = 8
DOCUMENT: This convertor sets the exponent for the number of hydrogen peroxide molecules in the stock and is used in the slider that controls initial hydrogen peroxide amount.

pH = 7.0

Temperature = 20
DOCUMENT: Temperature is in degrees Celsius.

pH_Effect = GRAPH(pH)
(0.00, 0.00), (1.08, 0.00), (2.15, 0.00), (3.23, 0.00), (4.31, 0.2), (5.38, 0.8), (6.46, 1.00), (7.54, 1.00), (8.62, 0.8), (9.69, 0.2), (10.8, 0.00), (11.8, 0.00), (12.9, 0.00), (14.0, 0.00)
DOCUMENT: This model uses a standard bell-shaped curve of the effect of pH on catalase catalysis rate. The curve has a maximum at pH 7.0 and drops to zero at pH 4.0 and near pH 11.0. This curve can be described by an algebraic equation using simple Michalis-Menton theory where Vmax (pH)= [Eo] (kcat pH). See Fersht's Enzyme Structure and Mechanism.

Temperature_Effect = GRAPH(Temperature)
(0.00, 0.01), (7.14, 0.1), (14.3, 0.5), (21.4, 1.00), (28.6, 1.00), (35.7, 1.00), (42.9, 0.9), (50.0, 0.5), (57.1, 0.005), (64.3, 0.00), (71.4, 0.00), (78.6, 0.00), (85.7, 0.00), (92.9, 0.00), (100.0, 0.00)
DOCUMENT: Using data from Lehninger's Biochemistry in the model, we assume that catalase operates at its maximum rate from 20 to 37 degrees C and is denatured at about 60 degrees.