

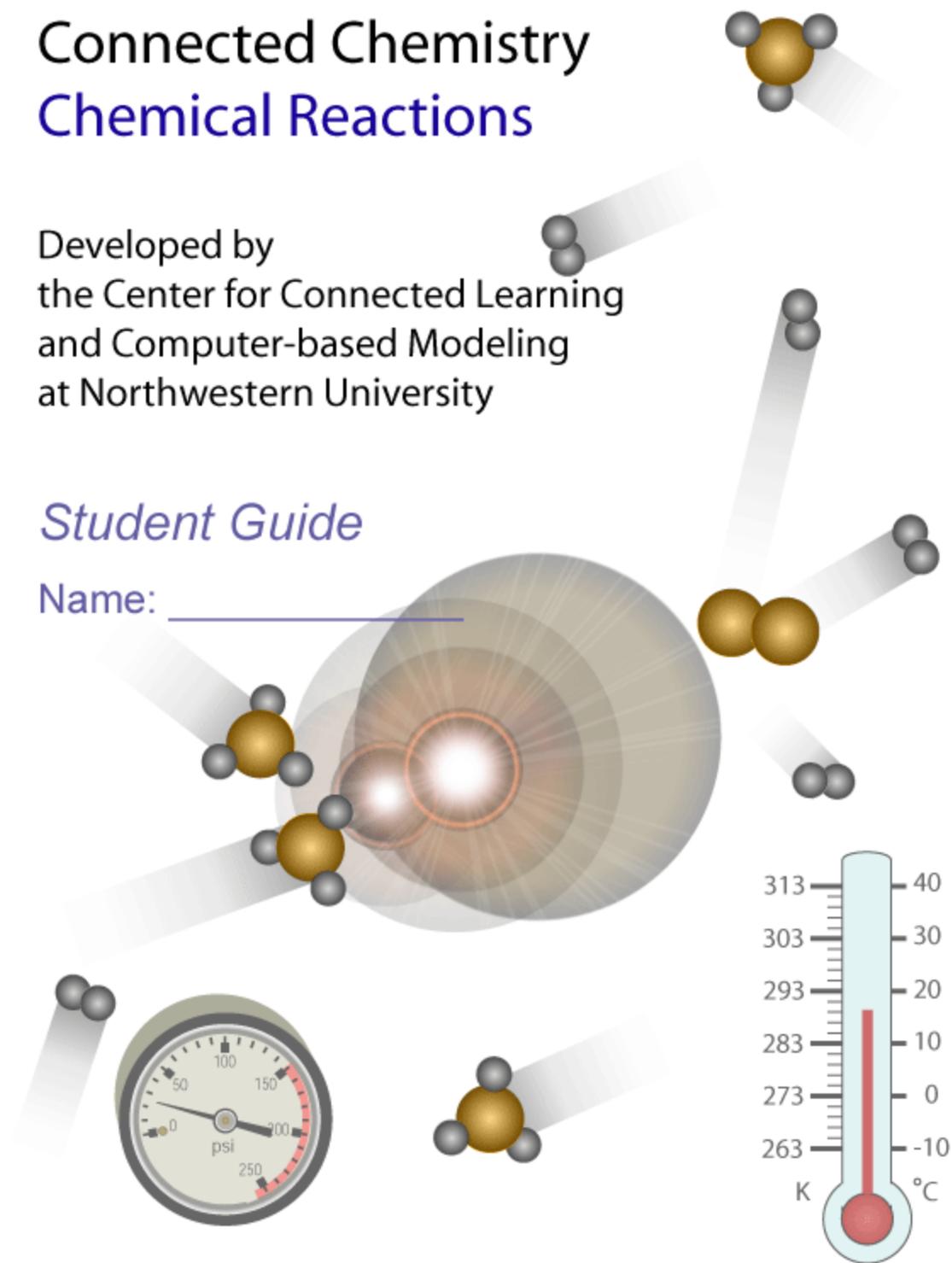
Connected Chemistry

Chemical Reactions

Developed by
the Center for Connected Learning
and Computer-based Modeling
at Northwestern University

Student Guide

Name: _____



Activity 1 – Charcoal Combustion

Have you ever seen a barbecue that used charcoal?

The grill on the right is a grill that uses charcoal as fuel. Charcoal is sold in many local stores in small bags.

Charcoal looks very similar to coal. Charcoal is composed of nearly pure carbon. In this manner it is similar to coal, which is also mostly carbon, but contains additional impurities.



Charcoal is the blackish residue that results from removing water and other volatile compounds from animal and vegetable substances. The blackish surface of wood that has been partially burned in a fireplace is typically charcoal.



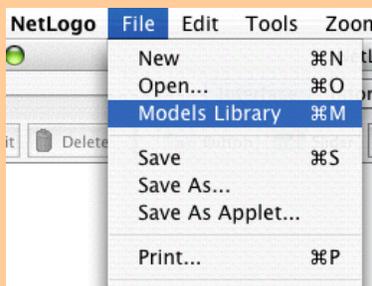
Charcoal is used in art for drawing and was also used historically as an important ingredient in gunpowder.

When charcoal burns, it undergoes a chemical reaction. The chemical reaction also releases energy in the form of heat and light.

In this second investigation you will be conducting on the computer you will use **NetLogo** models to simulate and visualize the molecules involved in this chemical reaction.

Opening the first model:

1. Open NetLogo on your computer
2. In the NetLogo window, open the Model Library from the File Menu



3. Under *File > Models Library*, choose the Curricular Models/Connected Chemistry folder and open it. In the folder click on the "Connected Chemistry Charcoal Combustion" model and open it.

The Interface tab will fill up with lots of buttons, switches, sliders, and monitors:

Activity 1 – Charcoal Combustion

Exploration 1:

4. Set the INIT-GAS-TEMPERATURE to 100.
5. Press the SETUP button
6. Press the GO/STOP and observe the molecules in the model.

You should now be to recognize oxygen molecules and carbon molecules in the model.

Question #1: How are oxygen molecules represented in the model?

Question #2: How are nitrogen molecules represented in the model?

Question #3: What atoms are represented in the charcoal solid?

Exploration 2:

7. Increase the INIT-GAS-TEMPERATURE
8. Press the SETUP button
9. Press the GO/STOP and observe the molecules in the model.
10. If the gas particles do not react with the charcoal, repeat step 7.
11. Study the Gas Temperature vs. Time graph.

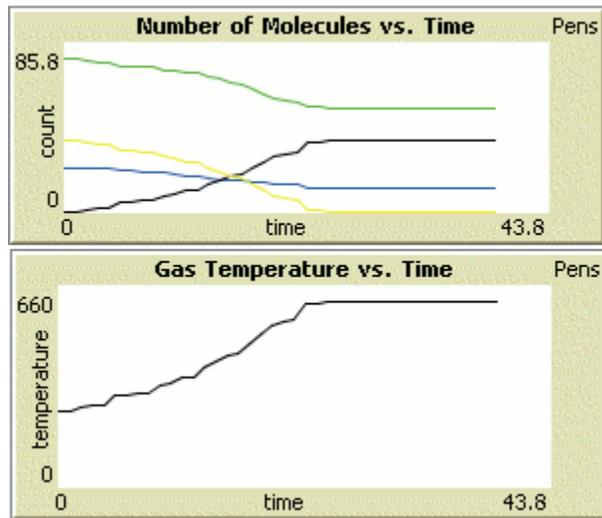
Question #4 What molecules are reacting? _____

Question #5 What molecule is produced? _____

Activity 1 – Charcoal Combustion

Question #6: On the graph of the Temperature vs. Time graph, show where:

- the reaction is starting (label as point **A**),
- where the temperature is increasing the fastest. (label as point **B**)
- where the reaction is completed (label as point **C**).



Exploration 3:

Press SETUP and study the starting layout and number of each kind of particle. Think about how you adjust the number of oxygen molecules you would start with so that ALL the oxygen molecules react with ALL the carbon atoms in the charcoal.

12. Adjust the NUMBER-OF-OXYGENS
13. Press the SETUP button
14. Press the GO/STOP and observe the reaction until it is complete
15. If any oxygen molecules or carbon atoms in charcoal remain, repeat step 12, until you find a value of NUMBER-OF-OXYGENS that react completely

Question #7 How many atoms of carbon in charcoal did you start the model with?

Question #8 How many molecules of oxygen did you start the model with?

Question #9 How many molecules of carbon dioxide did you end up with?

Question #10 What was the Gas Temperature at the end of the reaction? _____

Activity 1 – Charcoal Combustion

Exploration 4:

16. Remove the Nitrogen gas in the model, by setting the NUMBER-OF-NITROGENS slider to 0. *This will model burning charcoal in pure oxygen.*
17. Press the SETUP button
18. Press the GO/STOP and observe the reaction until it is complete
19. If any oxygen molecules or carbon atoms in charcoal remain, repeat step 12, until you find a value of NUMBER-OF-OXYGENS that react completely

Question #11 What was the Gas Temperature at the end of the reaction? _____

Question #12 Why do you think the reaction now gives a higher Gas Temperature than in question 10?

Exploration 5:

20. Change the CHARCOAL-GEOMETRY chooser setting.
21. Press the SETUP button.
22. Repeat step 20

Note that this has changed the shape of the charcoal solid, but not the number of atoms in it. Each of these shapes has a different perimeter, but the same volume. In this 2D view, changing the perimeter of a solid, causes a change in the surface area (location where an oxygen molecule can hit it).

Question #13 Which CHARCOAL-GEOMETRY setting has the largest “surface area” (number of locations where an oxygen molecule can hit it).

Question #14 What is the perimeter of the charcoal shape in this setting?

Activity 1 – Charcoal Combustion

Exploration 4:

Conduct an experiment to determine how **surface area of a solid** that reacts, affects the **rate of the reaction**. (See required questions to answer below).

Question #15 What will you use in the model to record the “rate of the reaction”?

Question #16 What are some important variables to control (or keep constant) in this experiment?

Question #17 Record your data in a table:

--

Activity 1 – Charcoal Combustion

Question #18 : What is the relationship between the surface area of a solid that reacts and the rate of the reaction?

Question #19 : If you wanted a reaction to occur as fast as possible, what could you try do to the surface area of the solid that is reacting?

In the computer model you should have noticed that the following conditions have to occur for a chemical reaction to happen:

1. Molecules must collide
2. Molecules have to have enough energy (moving fast enough)
3. Molecules of certain types react with each other. While other types of molecules do not react with each other. (For example: the nitrogen gas did not react with any of the other molecules)

These general conditions are true in most of the chemical reactions you will encounter. If one or more of these conditions are not met, a chemical reaction will not occur.

Question #20: In general, chemical reactions will occur more quickly if a solid is dissolved in a liquid before it is mixed with the other **reactant** (the other substance it will react with). How can this be explained in terms of what you discovered in your answers to question #15 and #16?

Activity 2 – Hydrogen Combustion

In the chemical reaction investigations you will be conducting on the computer in this chapter, you will again use **NetLogo** models to simulate and visualize the molecules involved in a chemical reaction.

This time you will study the combustion of hydrogen with oxygen.

Hydrogen and oxygen are burned by the main engines of the Space Shuttle when it is launched from the ground into space.

Recently, automotive manufacturers have increased their research into using hydrogen as an alternative to gasoline, for fueling cars and trucks.

This is due in part, to the fact that burning hydrogen does produce carbon dioxide, which is produced when burning fossil fuels (such as gasoline, coal, or charcoal). Carbon dioxide is a possible contributor to global warming and cutting down on its production, is an international goal of many governments.



The design of the car engine needs to be altered slightly to handle the burning of hydrogen fuel instead of gasoline.

Question #1 : Cars that use hydrogen as fuel only need a single tank to store the hydrogen. But the Space Shuttle needs two tanks: one for hydrogen and one for oxygen. Why does the Space Shuttle also need a storage tank for oxygen, but a car would not?

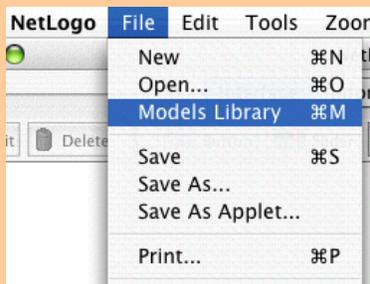
The first hydrogen refueling station was opened in Iceland in 2003 to serve a fleet of three buses that run on hydrogen fuel. Currently, there are numerous types of prototype or production cars and trucks that will/are using hydrogen fuel that are being researched for large scale production.

In the first model, you will be studying how hydrogen gas burns.

Activity 2 – Hydrogen Combustion

Opening the second model:

1. Open NetLogo on your computer
2. In the NetLogo window, open the Model Library from the File Menu



3. Under *File > Models Library*, choose the Curricular Models/Connected Chemistry folder and open it. In the folder click on the "Connected Chemistry Hydrogen Combustion" model and open it.

The Interface tab will fill up with lots of buttons, switches, sliders, and monitors:

Exploration 1:

4. Set the INIT-GAS-TEMPERATURE to 50.
5. Set the NUMBER-OXYGENS to 50.
6. Set the NUMBER-HYDROGENS to 50.
7. Press the SETUP button
8. Press the GO/STOP and observe the molecules in the model.

You should now be to recognize oxygen molecules and carbon molecules in the model.

Question #2: How are oxygen molecules represented in the model (how many atoms are in them as well)?

Question #3: How are nitrogen molecules represented in the model (how many atoms are in them as well)?

Activity 2 – Hydrogen Combustion

Exploration 2:

The hydrogen in the model does react with the oxygen at the current temperature you have set the model.

9. Set the CHANGE-IN-BOND-ENERGY to -500.
10. Set the INIT-GAS-TEMPERATURE to 100.
11. Set the HIGHLIGHT-PRODUCT? Switch to on
12. Press the SETUP button
13. Press the GO/STOP and observe the molecules in the model.

*You should now be to recognize the molecule that is produced in the chemical reaction. This **product** should be highlighted with a yellow circle around it.*

Question #4: How many atoms are in the molecule that is produced in the chemical reaction of hydrogen and oxygen?

Question #5: These atoms make up a molecule of water. How many atoms of each kind are in this molecule?

Question #6 : If this was the only product created in the chemical reaction of hydrogen and oxygen, why would the international community prefer that we use engines that burn hydrogen instead of fossil fuels (such as gasoline, coal, and charcoal).

Activity 2 – Hydrogen Combustion

Exploration 3:

Adjust the amount of oxygen and hydrogen in the model to give the highest temperature possible, and use up ALL the hydrogen molecules and ALL the oxygen molecules.

14. Set the INIT-GAS-TEMPERATURE to 100.
15. Adjust the NUMBER-OXYGEN slider.
16. Adjust the NUMBER-HYDROGEN slider.
17. Press the GO/STOP and observe the changing Gas temperature vs. time graph.

You should eventually see ALL the hydrogen molecules and ALL the oxygen molecules converted into water molecules. This may take more than 200 ticks, so you may wish to turn off the graphics to speed up the model. To turn the graphics off and on, switch the small on/off switch next to the red arrow at the top of the WORLD & VIEW:



Repeat steps 14-17 if this did not occur.

The maximum temperature in the model is reached when you burn as much oxygen and hydrogen as possible. This will be when there are 100 molecules of hydrogen and 50 molecules of oxygen. These will end up creating 100 molecules of water. Besides 100 molecules of hydrogen and 50 molecules of oxygen, there are other amounts of these two molecules that will always be COMPLETELY CONVERTED TO WATER. For example, 3 molecules of hydrogen and 6 molecules of oxygen will be completely converted to water.

Exploration 4:

Test other combinations of oxygen and hydrogen molecules that will convert completely to water, with no leftover amounts of pure oxygen or pure hydrogen.

18. Set the INIT-GAS-TEMPERATURE to 100.
19. Adjust the NUMBER-OXYGEN slider.
20. Adjust the NUMBER-HYDROGEN slider.
21. Press the GO/STOP and observe the reaction.
22. Record the amounts you used in the table below if successful, otherwise repeat steps 19-22.
23. Try another set of amounts that react completely

NUMBER-OXYGEN slider	NUMBER-HYDROGEN slider	Molecules of water created
100	50	100
6	3	3

Activity 2 – Hydrogen Combustion

Question #6: For every one molecule of hydrogen that reacts, how many molecules of oxygen react? _____

Question #7: For every one molecule of hydrogen that reacts, how many molecules of water are made? _____

Question #8: Account for atoms. Explain what happens to all the hydrogen atoms and oxygen atoms in questions #6 and question #7 by showing a diagram of the molecules that react, the number of atoms of each type these molecules contain, the molecules that are produced, and the number of atoms of each type these molecules contain.

Reactants			Products	
Molecules that react	the number of atoms of each type in these molecules		Molecules are produced	the number of atoms of each type in these molecules
		----React --> To make		

Hydrogen combustion reactions release large amounts of energy which speed up gas particles which increase the pressure of the gas. Strong enough gas containers (e.g. steel pistons in car engines) must be made to contain the release of energy, otherwise the container may explode. For example when you hold a match to a balloon filled with hydrogen and oxygen it will explode.

Exploration 4:

Study what happens when the gas container explodes.

24. Set the PRESSURE-LIMIT-CONTAINER to 500.
25. Set the INIT-GAS-TEMPERATURE to 50
26. Set NUMBER-OXYGEN slider to 50 and the NUMBER-HYDROGEN slider to 100.
27. Switch the SHOW-WALL-HITS switch on.
28. Press SETUP, then GO/STOP, and then press SPEED UP & TRACE ONE MOLECULE.
29. Observe the GAS PRESSURE VS. TIME graph until the container explodes. Then repeat steps 24-28 using the slow motion slider to help you answer the following questions.

Activity 2 – Hydrogen Combustion

Question #6: Explain why it took a while for the container to explode? What had to happen from the moment you first sped up a molecule to when the container exploded?

Question #7: Not all the hydrogen has reacted when the container exploded. Explain why:

Question #8: Would a smaller container speed up or slow down the reaction? _____

Question #9 : Why?

Activity 2 – Hydrogen Combustion

In reality, this combustion would occur much quicker than you observed in the model, in part, because in the model, the particles are moving much slower than in reality. But even in a 30 frame per second video clip, you can see that the process takes time.

(Optional activity for web based computer labs: Study the video clip at <http://www.chem.uiuc.edu/clcwebsite/balloon.html>, and move slowly frame by frame through the explosion to see this effect).

Hydrogen gas is much more **flammable** than charcoal. The flammability of a substance describes how easily the substance will ignite. How easy a substance will ignite is based, **in part**, on how strongly bound together the atoms are in the molecules that are trying to react. Tightly bound atoms are hard to break apart. Loosely bound atoms break apart more easily. For now, we will refer to the energy it takes to break apart the atoms to allow them to rearrange to make new molecules (products) is called the **activation energy**.

Exploration 5:

Determine what settings for ACTIVATION-ENERGY are the most flammable and least flammable.

30. Adjust the ACTIVATION-ENERGY slider.
31. Press SETUP.
32. Press the GO/STOP and then press SPEED UP & TRACE ONE MOLECULE.
33. Observe the rate of the reaction and repeat steps 30-32, until you can tell which ACTIVATION-ENERGY settings model more flammable fuels.

Question #10: What was the value for the ACTIVATION-ENERGY when the fuel was most flammable? _____

Activity 3 – Rusting

If you ride a bike, you might have noticed how important it is to not leave your bike outside, especially in the rain. If you do parts of your bike will begin to rust. When enough rust has built up on the moving parts of the bike (like the chain or wheels), it can make it very difficult to pedal.

Rust is a brownish-orange substance that you can find on certain types of metal objects. Think about what are some of the types of objects you have seen rust on.

Question #1: List some places/objects you have seen rust on?



Rust is a substance that forms from a chemical reaction with iron and oxygen. Any iron object that is exposed to oxygen might rust over time. When an iron object turns to rust, the rusted object is weaker and more brittle than the iron it used to be made of. But it is rare to find a pure iron object these days. Iron used to be used to make things like tools, cooking equipment, weapons, farming machinery, Steel, however, is still used to make lots of objects. And steel is made of mostly pure iron atoms, with a small amount (around 5% or less) of carbon atoms in it. Since steel is mostly made of iron atoms, it rusts too! Think of all the steel objects you have seen outside that you have found rust on.

So when iron or steel chemically reacts with oxygen to make rust.

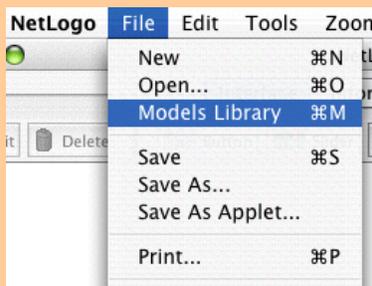
Question #2: If you tested two pieces of steel that were nearly identical, but one was left out in the air and one was put in a container of pure oxygen gas, why would both rust?

In this third investigation you will be conducting on the computer you will use **NetLogo** models to simulate and visualize the molecules involved in this chemical reaction.

Activity 3 – Rusting

Opening the second model:

1. Open NetLogo on your computer
2. In the NetLogo window, open the Model Library from the File Menu



3. Under *File > Models Library*, choose the Curricular Models/Connected Chemistry folder and open it. In the folder click on the "Connected Chemistry Rusting Reaction" model and open it.

Exploration 1:

4. Set the INIT-GAS-TEMPERATURE to 50.
5. Set the NUMBER-OXYGEN-MOLECULES to 50.
6. Set the ACTIVATION-ENERGY to 100
7. Press the SETUP button
8. Press the GO/STOP and observe the molecules in the model.

You should now be to recognize oxygen molecules and carbon molecules in the model.

Question #2: How are oxygen molecules represented in the model (how many atoms are in them as well)?

Question #3: How are iron atoms represented in the model?

Question #3: How are rust molecules represented in the model (how many atoms are in them as well)?

Activity 3 – Rusting

It can be a bit difficult to clearly see how many atoms are in each rust molecule. The molecule looks should look like it has oxygen atoms and iron atoms in it. To clearly see how many of each of these atoms are in a rust molecule, you will need to see where the boundary of one molecule ends. You can use the model to help you visualize the boundaries of the rust molecules.

Exploration 2:

9. Press the SETUP button
10. Press the GO/STOP
11. Press TOGGLE RUST MOLECULE BOUNDARIES observe the molecules in the model.

You should now be to recognize a cluster of 3 oxygen atoms and 2 iron atoms, making up each 1 rust molecule.

Now that you can see that a single molecule of oxygen is made of three oxygen atoms and two iron atoms, repeat exploration 2 to check and see if only a single molecule of rust is created when a reaction occurs between the reactants

Question #3: How many molecules of rust are created, each time a reaction occurs?

Question #4: Account for atoms. You should have seen that two molecules of rust are created each time a reaction occurs. Explain where these atoms must have come from to make these two molecules, by filling in the table from right to left (backwards) and showing a diagram of the molecules that you produced (two molecules of rust), the number of atoms of each type these molecules contain, the number of atoms of each type the reactant molecules contain, and lastly the molecules that must have reacted.

Reactants

Molecules that react	the number of atoms of each type in these molecules

----React -->
To
make

Products

Molecules are produced	the number of atoms of each type in these molecules

Activity 3 – Rusting

Exploration 3:

In Question 8, you should have determined that it takes 3 oxygen molecules and 2 iron atoms to make two rust molecules. Rerun the computer model and check this prediction.

12. Press the SETUP button
13. Press the GO/STOP
14. Adjust the slow motion slider to study this prediction.

Let the model run until most of the edges are covered in rust.

Question #5: Study the iron block with the rust on it in the model. Would this entire object weight more, less, or the same as the block of iron atoms? that you started with in the model _____

Question #6: Why? _____

Question #7: Why do you think rust is only occurring on the edges of the iron block?

In reality, iron or steel only rusts on the surface. Over time, however the rust sometimes flakes off the surface, exposing more iron or steel underneath to the air.

Activity 3 – Rusting

Exploration 4:

To mimic what happens in reality, when rust flakes off the surface of iron or steel do the following.

15. Press the SETUP button
16. Press the GO/STOP

Let the model run until most of the edges are covered in rust.

17. Press the USE MOUSE button (*it will stay black when pressed once*)
18. Set the MOUSE-INTERACTION chooser to "drag away rust"
19. Then use the computer mouse to click and hold the button down when you point at a rust molecule. With the button on the mouse pressed down, drag the rust molecule away from the iron block.

Question #8: Even if you drag all the rust away from the iron block to expose more iron to the oxygen, in theory, the block of 81 iron atoms, would never be completely converted into rust molecules. What in the model would explain why?

In reality, the rusting process does not occur very quickly. In the model, the current setting for ACTIVATION-ENERGY of 100 is too low. The low setting of this slider is helping you show how rust would react, if it required a small amount of kinetic energy to occur. In a moment, you will be asked to increase the ACTIVATION-ENERGY level to a much higher energy value. When you do so, you will find that the oxygen particles will not have enough energy to react with the iron atoms. This is a more accurate model of what happens in reality. But in reality, rusting does still occur.

Question #9: What other conditions might occur in the real world that helps things rust more quickly/easily?

You will now conduct two investigations to explore two variables that help rusting reactions occur more quickly and easily.

Activity 3 – Rusting

Exploration 5:

20. Set the ACTIVATION-ENERGY slider to 300.
21. Press the SETUP button
22. Press the GO/STOP

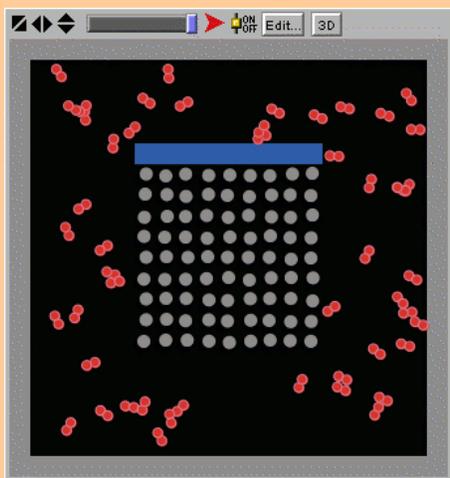
You should see that no rust is currently forming.

23. Press the USE MOUSE button (*it will stay black when pressed once*)
24. Set the MOUSE-INTERACTION button to "shine UV light"
25. Then use the computer mouse to click and hold the button down on a location where there are oxygen molecules.

You should see oxygen molecules speeding up (increasing the temperature of the gas). Keep shining UV light on gas molecules until you see rust molecules forming.

Exploration 6:

26. Set the ACTIVATION-ENERGY slider to 300.
27. Press the SETUP button
28. Press the USE MOUSE button (*it will stay black when pressed once*)
29. Set the MOUSE-INTERACTION button to "add water"
30. Then use the computer mouse to click and hold to paint water on one edge of the iron block. The picture here shows what this would look like after you painted water on the top edge of the iron block:



31. Press the GO/STOP

Watch what happens. Where does the rust form? Why might it appear to form there?

Activity 3 – Rusting

In exploration 5, you should have seen that speeding up the gas particles can help provide enough energy to the reactants, to allow the rusting reaction to occur. This is way in which you can get the rusting reaction to occur. Before you sped up the gas particles, and had a high activation energy for the reaction, there was never a time when the reactants had enough energy to react. This is similar to what happens in reality. Oxygen and rust can be made to react the reactants are bombarded with ultra-violet (UV) light.

Scientists believe that this is one reason why the surface of the planet Mars is covered in particles of rust. The visible surface of Mars that is brownish-orange is due to the vast amount of rust on the surface



Question #9: Where do you think the ultra-violet light came from to cause this rust to form on Mars?

In many types of chemical reactions, there is sometimes more than one way to get a chemical reaction to occur. Sometimes the reactants can be made to react more easily, when they are in the presence of another molecule. In the model, you saw that the water helped the rusting reaction occur. Water in reality, does actually help rusting occur. It does this by helping the reactants form products more easily by moving the atoms through a series of steps that require less energy, than going directly into making rust. These series of steps are sometimes referred to as a **chemical pathway**. The details of what happens in that pathway aren't important right now. Instead, you should recognize that water decreases the amount of energy required to turn oxygen gas and iron into rust.

Question #10: In this model spots where there was water were represented as blue squares. If you wanted to include a more accurate representation of water at the molecular what would you want the water to look like?

The water is not used up in the chemical reaction for rust. It is simply a **catalyst**. A catalyst is a chemical substance that increases the rate of reaction without being consumed. The catalyst lowers the activation energy required, allowing the reaction to proceed more quickly or at a lower temperature.

Activity 3 – Rusting

In the computer model you should see that there is a chooser called IRON-BLOCK-GEOMETRY. The chooser has options that allow you to change shape and size of the iron block. If you look at the rest of the interface, you will see there also the other widgets that let you control initial temperature, activation energy, water location, etc...

Design an experiment to test a question that you would like to investigate with this model AND that you think the model is capable of helping you investigate.

Question #11: What question would you like to investigate?

Question #12: What particular variable(s) are you interested in measuring the effect of (independent variable(s))

Exploration 7:

Question #13 : Describe a series of steps (procedure) that someone could follow to perform your investigation:

Now Conduct Your Experiment!

Activity 3 – Rusting

Question #13: What are the results of your investigation?

Question #14: Use what you have learned so far about particle behavior to explain why or how the results occurred:

Activity 4 – The Haber Process

Let's review what must happen for chemical reaction to occur:

1. Molecules must collide
2. Molecules have to have enough energy (moving fast enough)
3. Molecules of certain types react with each other types of molecules do not react with each other. (For example: the nitrogen gas did not react with any of the other molecules)

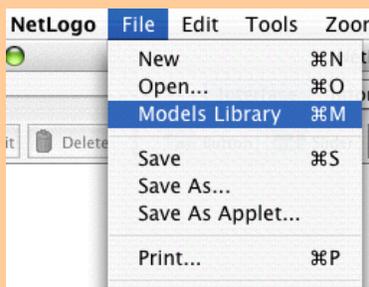
Let's think more about the last requirement. If molecules collide and have enough energy, they may break apart into atoms and those atoms may rearrange into new molecules. Think about what might happen if the new molecules were to collide together.

Question #1: Now imagine a nitrogen molecule N_2 collides with some hydrogen molecules H_2 and this creates a new product; what might also happen when the molecules of this newly created product collide together?

In the next model you will investigate the **Haber Process**. The **Haber Process** is a manufacturing method that uses a chemical reaction between nitrogen and hydrogen to make ammonia. Ammonia is a common household substance that is sometimes used for cleaning and disinfecting. It is also used as a fertilizer for plants. It has a very distinct smell, which is noticeable in window cleaning fluids, such as Windex[™].

Opening the second model:

32. Open NetLogo on your computer
33. In the NetLogo window, open the Model Library from the File Menu



34. Under *File > Models Library*, choose the Curricular Models/Connected Chemistry folder and open it. In the folder click on the "Connected Chemistry Haber Process" model and open it.

Activity 4 – The Haber Process

Exploration 1:

1. Set the NUMBER-H₂ slider to 50
2. Set the NUMBER-N₂ slider to 100
3. Keep the rest of the settings as they were when you opened the model.
4. Press SETUP

Notice there are two types of molecules in the model to start with

5. Press the GO/STOP and observe the molecules in the model until you see a reaction occur.

You should now be able to recognize a few new gas molecules that are made of some of the atoms that were in the molecules you started with.

Question #2: How are hydrogen (H₂) molecules represented in the model (how many atoms are in them as well)?

Question #3: How are nitrogen (N₂) molecules represented in the model?

Question #4: The new molecule that is created in the chemical reaction in the model is ammonia. How is this represented in the model?

Exploration 2:

6. Set the NUMBER-H₂ slider to 0
7. Set the NUMBER-N₂ slider to 0
8. Set the NUMBER-NH₃ slider to 50
9. Keep the rest of the settings as they were when you opened the model.
10. Press SETUP

Notice there is only one types of molecules in the model to start with

11. Press the GO/STOP and observe the molecules in the model until you see a reaction occur.

Activity 4 – The Haber Process

Question #5: What molecules are created when ammonia molecules react with each other?

Were you surprised to see that sometimes when ammonia molecules collide, they break back apart and reform nitrogen gas and hydrogen gas? This is what you should have observed in the model, and is an example of a “reverse reaction”. We will call this a “reverse reaction” since what happened was the reverse of the first reaction we saw in exploration 1.

In exploration 1, we saw a “forward reaction” that could be summarized as follows:



This representation shows that one nitrogen molecule and three hydrogen molecules react to make two ammonia molecules.

In exploration 2, you saw a “reverse reaction” that could be summarized as follows:



Notice that direction of the reaction arrow is different in this summary. The arrow is facing in the reverse direction, showing that the ammonia is reacting to make the nitrogen and hydrogen.

So in this model, two things are happening. When the right number of nitrogen and hydrogen molecules hit each other with enough energy, they react to make ammonia molecules. And when the right number of ammonia molecules hit each other with enough energy, they react to make nitrogen and hydrogen molecules. Since both the “forward reaction” and “reverse reaction” are occurring in this model, we can summarize both of these events as a **reversible reaction**. A **reversible reaction** is a reaction which can occur in either direction (forward or backward).



Activity 4 – The Haber Process

Exploration 3:

12. Set the NUMBER-H₂ slider to 0
13. Set the NUMBER-N₂ slider to 0
14. Set the NUMBER-NH₃ slider to 100
15. Keep the rest of the settings as they were when you opened the model.
16. Press SETUP
17. Press the GO/STOP and observe the temperature graph, and the number of molecules graph.

You should notice over time that both graphs eventually start to level off and appear to become stable (the value is not changing much overall, only fluctuating up and down).

Question #6: Why does the number of molecules of H₂, N₂, and NH₃ eventually become stable, showing only slight fluctuation, but little overall change?

Question #7: How many total molecules need to collide together for the forward reaction to occur? _____

Question #8: How many total molecules need to collide together for the reverse reaction to occur? _____

Question #9: Therefore, which event is more likely to occur: the forward reaction or the reverse reaction? _____

Question #10: How does your answer to question #7 provide a possible explanation, why there are less NH₃ than there are N₂ when the system becomes stable?

Activity 4 – The Haber Process

Look at the monitor that shows the % OF FORWARD REACTIONS and the % OF REVERSE REACTIONS. Both of these numbers should be showing a value less than 100%. This means that when the right numbers of each type of molecule collide, the molecules don't always react. They may lack the required amount of energy to do so.

Question #11: Which reaction is occurring more often, even when the right number of each type of molecule collide? _____

Your answer to question 8 should suggest that one of the reactions (forward or reverse), is less likely to occur, because the molecules don't have enough energy.

Question #12: Which reaction requires more energy to occur, the forward or the reverse reaction? _____

Reversible reactions can be tricky to think about since there are competing forces at work. For example, your answer to question #7 should suggest the reverse reaction is more likely to occur because of where the molecules are located, but your answer to question #8 should suggest that the forward reaction is more likely to occur because of the energy required for the reaction is less.

This sort of trade-off between competing forces is part of what accounts for the stability of the system. When this system is stable it is said to be in **equilibrium**. Equilibrium is a state of a system, when forces that are counteracting each other are balancing the effect of each other out.

Question #13: Let's think about what would happen in some extreme cases. For example, if you could shrink the container very small so all the molecules were packed more closely together, then does that increase or decrease the chance of a reaction?

Exploration 4:

18. Set the NUMBER-H₂ slider to 0
19. Set the NUMBER-N₂ slider to 0
20. Set the NUMBER-NH₃ slider to 100
21. Set the INITIAL-WALL-POSITION to 5.
22. Keep the rest of the settings as they were when you opened the model.
23. Press SETUP
24. Press the GO/STOP and observe the temperature graph, and the number of molecules graph.

You should notice over time that both graphs eventually start to level off and like before, but the system is far less stable.

Activity 4 – The Haber Process

Question #14: Why does the number of each kind of molecule in the system show more fluctuations with this smaller volume?

Exploration 5:

With the model still running (GO/STOP is still pressed down)

25. Press MOVE WALL

26. Click in the black space in the WORLD & VIEW far to the right of the orange wall in the model.

You should notice the orange wall jump to the new location where you clicked.

27. Press the GO/STOP to resume the model run and observe the temperature graph, and the number of molecules graph.

You should notice that both graphs over time have less fluctuations and the system starts to adjust to new stable value.

Question #15: Why does the system now have a new set of stable values for the number of each kind of molecule?

Notice that the overall pressure in the system dropped when you increased the volume. From chapter 1 of Connected Chemistry (Ideal Gas Law), you should have expected this. But also notice that because there are now less ammonia molecules there are also more hydrogen and nitrogen molecules than before.

Question #16: How would these additional molecules affect the pressure in the system?

Activity 4 – The Haber Process

The competing effect of increased volume that should lead to a decreased pressure, but that also creates more molecules because of a new equilibrium state for the system is summarized as **Le Chatelier's Principle**, which states, that reversible reactions tend to partially “reverse” the outcome that you expect in an ideal gas situation.

For example, in an ideal gas if you quadrupled the volume, you would expect to end up with a quarter of the pressure you started. But because the equilibrium state of the chemical reaction in the system also changes, the number of particles changes (increasing). This results in the pressure of the system end up being more than the expected 25% you would get with an ideal gas.

Le Chatelier's Principle can seem kind of mysterious at first, since it often sounds as if the system is responding in an intelligent manner to the changes that are made to it to try to counteract those changes. In reality, it is only a matter of an opposing effect in the reversible chemical reaction between the molecules, working against the effects one would expect from molecules if they were an ideal gas only.

Let's look at a similar situation in the system to help us better understand the interplay of competing effects.

If you adjust the INITIAL-GAS-TEMPERATURE and run the model again, this will also affect the overall stability of the system.

Exploration 6:

28. Set the NUMBER-N₂ slider to 50
29. Set the NUMBER-H₂ slider to 150
30. Set the INITIAL-WALL-POSITION to 20
31. Adjust the INITIAL-GAS-TEMPERATURE value to 5.
32. Press SETUP
33. Press the GO/STOP and run the model until the number of molecules graph is relatively stable and the system as at equilibrium.
34. Record how many molecules of ammonia you produced in the table below.
35. Gradually increase the INITIAL-GAS-TEMPERATURE and repeat steps 32-35

INITIAL-GAS-TEMPERATURE	Number of ammonia molecules produced
5	
10	
15	
20	
25	
30	

Notice that there is an optimal value for producing the most ammonia. It is not necessarily the highest or lowest temperature possible. Again, competing forces in the reversible reaction help determine what temperature this occurs at.

Activity 4 – The Haber Process

Exploration 7:

36. Set the NUMBER-N₂ slider to 50, Set the NUMBER-H₂ slider to 150
37. Set the INITIAL-WALL-POSITION to 20
38. Adjust the INITIAL-GAS-TEMPERATURE value to 5.
39. Press SETUP
40. Press the GO/STOP and run the model until the number of molecules graph is relatively stable and the system as at equilibrium. Now STOP the model.
41. Record how much TIME it took to reach a stable value of number of molecules.
42. Gradually increase the INITIAL-GAS-TEMPERATURE and repeat steps 32-35

INITIAL-GAS-TEMPERATURE	Time it took to reach a stable value
5	
10	
15	
20	
25	
30	

Notice that the time it takes to reach an equilibrium value is different for various temperatures. And the fastest time occurs when the temperature is the highest.

In the real world the production of ammonia in a manufacturing plant is a tricky process to optimize.

The manufacturing process is called the **Haber Process**. It is a well known process, because many of the competing effects have to be weighed in deciding what temperature and pressure the ammonia should be created at.



Higher temperatures result in a faster production of ammonia, but also increasing how often the reversible reaction occurs. This increased probability of reverse reactions means that less overall ammonia is produced. A lower temperature would produce more ammonia (because the reverse reaction would rarely if ever occur), but the forward reaction also occurs less frequent (again due to not enough energy in every collision). So now the process takes very long to make the increased amount of ammonia.

The **Haber Process** tries to balance the competing forces of Le Chatelier's Principle and the competing forces on the overall outcome of the reaction (e.g. how much ammonia is made vs. how fast its made); a medium temperature is used as a compromise to maximize the combined but cancelling effects of going to too high or too low a temperature, yielding a high amount of product, but also doing so quickly.