

Activity 4
Type: **Modeling**
Title: **Modeling the Fuel Cell Reaction**
Time: **1–2 class sessions**

Overview

In order to understand the chemistry of fuel cells, students are introduced to oxidation-reduction (redox) reactions and half-reactions as a means of creating electric current. They then work with a computer simulation of a proton exchange membrane (PEM) fuel cell to investigate the chemical reactions that occur within a fuel cell. To deepen their understanding, they also manipulate models of oxygen and hydrogen molecules on a schematic diagram of a PEM fuel cell.

Concepts, Processes, and Issues

(with NSES 9–12 Content Standards Correlation)

1. Chemical reactions occur all around us, for instance in automobiles. *(PhysSci: 3)*
2. Chemical reactions may release or consume energy. *(PhysSci: 3)*
3. A large number of important reactions involve the transfer of electrons (oxidation/reduction reactions). *(PhysSci: 3)*

TEACHING SUMMARY

Step 1.

Introduce redox reactions.

Step 2.

Explore a computer simulation of a fuel cell.

Step 3.

Model the redox half-reactions in a fuel cell.

Step 4.

Evaluate the possibility of using fuel cells to replace internal combustion engines on buses.

Materials

For each group of two students

Fuel cell molecular modeling set (11 pieces)

PEM fuel cell diagram

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Computer with access to HyTEC Fuel Cell Simulation*

*Not supplied in kit

Advance Preparation

You can use either the DVD supplied to transfer the Fuel Cell Simulation to each computer; or if you want your students to have the opportunity to compare this computer simulation with others, arrange for them to have computers with Internet access and direct them to the simulation on the HyTEC student page of the SEPUP website at sepuplhs.org/hytec.

Background Information

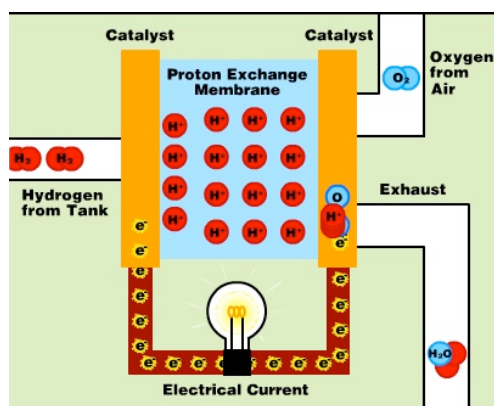
A chemical reaction that involves the transfer of electrons is called an oxidation-reduction, or redox reaction. Redox reactions are responsible for the production of electrical current in fuel cells and batteries.

Like a battery, a fuel cell is an electrochemical device that converts chemical energy into electricity. Unlike a battery, the anode and cathode reactant chemicals in a fuel cell can be replenished without interrupting the production of electricity.

In a fuel cell, the anode and cathode are made of a carbon-supported platinum catalyst fixed to a porous conductive material, such as a carbon cloth or paper. This catalyst facilitates a redox reaction without being altered or used up. Therefore, as long as the fuel cell is continuously supplied with reactant chemicals—hydrogen and oxygen, in the case of a PEM fuel cell—the fuel cell will produce electricity. This reaction typically produces electrical energy at a higher efficiency than burning the hydrogen in a heat engine to drive a generator. The only by-product is pure water.

In a PEM fuel cell, hydrogen gas is fed into the anode and oxygen gas (or air) is fed into the cathode. The platinum catalyst at the anode facilitates the splitting of the hydrogen atoms into protons (H^+) and electrons (e^-).

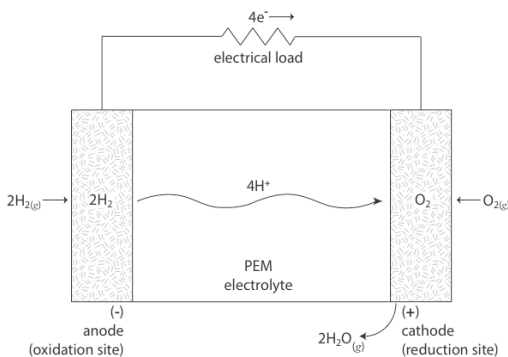
Between the anode and the cathode is an electrolyte. In PEM fuel cells (the type used in this curriculum unit, and one which is in use in various prototype cars and buses), the electrolyte is a solid



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polymer membrane that allows only protons to pass through. Because the membrane bars the passage of electrons, the electrons generated from the hydrogen at the anode are carried through an electric circuit, through a load where they can perform useful work, and then to the cathode.

At the cathode, another platinum catalyst facilitates the combining of oxygen gas with the incoming electrons (coming through the load-bearing circuit) and protons (coming through the membrane) to form water molecules. The water can be formed as either a liquid or a gas. Here, we assume it will be formed as a gas.



[insert illustration of fuel cell, different from above, that shows details of fuel cell]

The two half-reactions in a hydrogen fuel cell are shown in the table below, along with their cell potentials.

	Reaction	Cell Potential
Anode (H_2 is oxidized, loses electrons)	$2\text{H}_2(\text{g}) \rightarrow 4\text{H}^+ + 4\text{e}^-$	$E_{\text{oxid}} = 0.0 \text{ V}$
Cathode (O_2 is reduced, gains electrons)	$\text{O}_2(\text{g}) + 4\text{H}^+ + 4\text{e}^- \rightarrow 2\text{H}_2\text{O}(\text{g})$	$E_{\text{red}} = 1.18 \text{ V}$
Overall	$2\text{H}_2(\text{g}) + \text{O}_2 \rightarrow 2\text{H}_2\text{O}(\text{g})$	$E_{\text{cell}} = 1.18 \text{ V}$

Note that the electrode potentials given are based on a standard reduction potential for a 1 M aqueous solution at 25°C. These are approximate for the PEM fuel cell since it uses a solid polymer electrolyte rather than a 1 M aqueous solution. Also note that the standard cell potential increases to 1.23 V if water is formed as a liquid because additional energy is available from the heat of vaporization.

The same PEM technology can be used in a PEM electrolyzer, which operates in the nonspontaneous, reverse direction. A PEM electrolyzer requires an input of electrical energy to split water into hydrogen and oxygen gas. In the electrolytic cell the reactions are identical, but they are forced in the opposite direction.

Batteries

In a battery, redox reactions also result in the generation of electricity. In a battery, the two half-reactions of a spontaneous redox reaction are separated, and electrons are passed through an electric circuit. The reactant chemicals at the **anode**, where oxidation occurs, become depleted while delivering electrons to the circuit. The reactant chemicals at the **cathode**, where reduction occurs, also become depleted as they accept the electrons. When the concentration of reactant chemicals becomes too low, the battery stops producing enough electrical energy and needs to be replaced or recharged.

The voltage produced by the redox reaction in an electrochemical cell is determined, in part, by the chemicals used at the anode and cathode. Each chemical has a redox potential, or electromotive force (EMF), that is defined as the voltage generated when that chemical, and its associated 1 M electrolyte solution, is connected to a platinum electrode surrounded by a 1 M concentration of hydrogen gas. All other things being equal, the greater the difference in EMF between the two chemicals used in an electrochemical cell, the greater the voltage generated by that cell.

Fuel Cell Parts: Form and Function

Polymer Electrolyte

The schematic of a PEM fuel cell shown above is a simple conceptual model. This section describes the form and function of typical fuel-cell parts. A single-cell PEM fuel cell is made up of a PEM electrolyte sandwiched between two electrodes. The PEM electrolyte is a solid polymer membrane (see Figure 1 for the chemical structure). The polymer starts as a polyethylene hydrocarbon chain equivalent to a no. 2 or 4 recyclable plastic. Substituting fluorine atoms for hydrogen atoms in a process called perfluorination modifies the polyethylene and creates a modified polymer known as polytetrafluoroethylene, or PTFE. PTFE is sold under a registered trademark as Teflon[®]. The strong bonds between the fluorine and carbon atoms make PTFE durable and resistant to chemical attack. It is also strongly hydrophobic (repels water); when it is used in fuel cell electrodes it drives the water out of the electrode and prevents flooding. This same property makes it useful in outdoor clothing and footwear.

In order to make an electrolyte out of the solid polymer, the PTFE is sulphonated by adding a molecular side chain that ends in a sulphonic acid group ($-\text{SO}_3\text{H}$). The sulphonic acid group is highly hydrophilic (attracts water). When water is absorbed, the sulphonic acid group ionizes, releasing a H^+ ion, or proton. The H^+ ions tend to interact with water to form hydronium ions (H_3O^+). The H^+ ions are then transported through the membrane via bulk movement of the hydronium ions as well as via transfer from one water molecule to the next. This is what allows for proton conductivity through the solid polymer proton exchange membrane.

Electrodes and Electrode Structure

The electrodes for a PEM fuel cell are typically composed of a carbon supported platinum catalyst. The catalyst is needed to lower the activation energy of the fuel cell redox reaction, thereby allowing for the practical application of this electrical power-producing device. Note that in the early days of PEM fuel cell development significant quantities of platinum were needed. This led to a large cost associated with the platinum. Today platinum loadings have been reduced to levels where they now make up only a small portion of the total cost of PEM fuel cells. The platinum catalyst is typically formed into very small particles on the surface of somewhat larger, carbon-based powders. The carbon-supported catalyst is then fixed to each side of the polymer electrolyte membrane and creates the two electrodes (anode and cathode). This electrolyte membrane (see Figure 2), with an electrode on either side, is referred to as the membrane-electrode assembly (MEA).

A thin, porous carbon cloth material is placed up against each side of the membrane-electrode assembly (MEA). This carbon cloth is referred to as the gas diffusion medium (GDM). The gas diffusion medium serves to distribute the gas reactants uniformly throughout the membrane electrode assembly. In addition, the gas diffusion medium is electrically conductive, so it serves to transport electrons to and from the electrodes, and it is treated with Teflon[®] to make it hydrophobic so that it will transport water away from the electrodes.

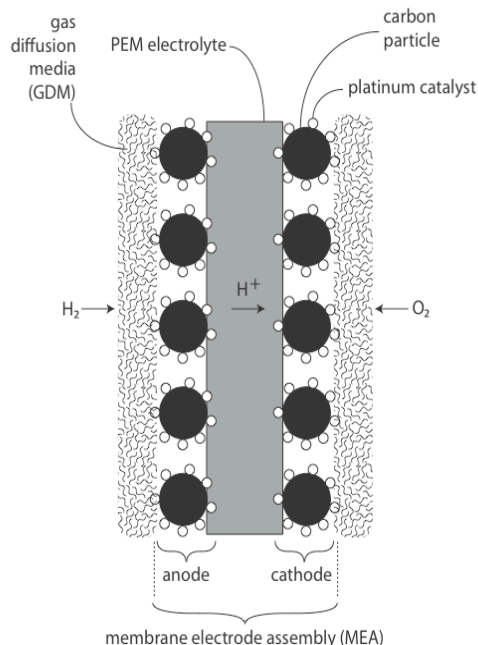


Figure 2. Simplified structure of a PEM fuel cell

In the fuel cell used in the student laboratory exercises, the MEA and GDMs described above are sandwiched between two perforated metal plates, or screens. These screens serve to distribute the reactant gases and conduct current to and from the electrodes, as well as to provide structural support and provide a uniform pressure on the MEA and

GDMs. This whole assembly is then sandwiched between two plastic endplates, which provide structural support. The overall assembly is bolted together using a gasket material to provide a gas-tight seal (see Figure 3).

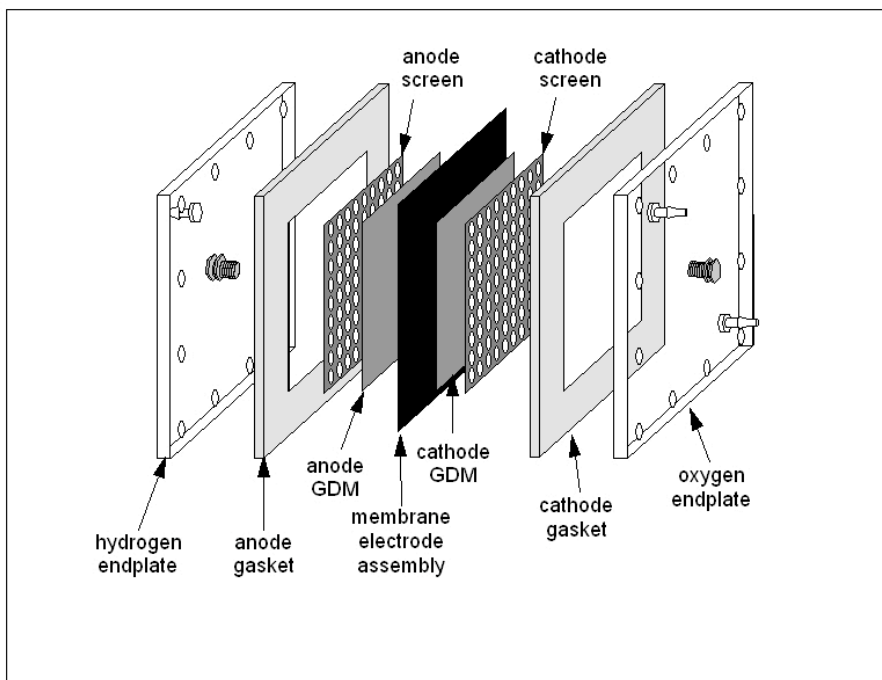


Figure 3. Overall assembly of a fuel cell

The maximum theoretical open circuit voltage of a single fuel cell, as defined by the standard reduction potential for the fuel cell redox reaction, is 1.18 V (assuming the water is formed as a gas). In practice, the open circuit voltage (the voltage when no electrical load is connected) for a well-working fuel cell is approximately 0.9 V, and a power producing cell typically operates in the range of 0.6 V to 0.7 V.

A Fuel Cell Stack

In order to build enough voltage to produce useful electrical power, fuel cells must be stacked electrically in series. This can be accomplished in the classroom by simply connecting the negative electrode of one student fuel cell to the positive electrode of another. In practice, however, a fuel cell “stack” is fabricated as a complete unit.

A fuel cell stack consists of numerous cells that are stacked physically against one another so that their electrodes are connected in series (the anode of one cell is connected to the cathode of the adjacent cell). The number of cells stacked in series determines the operating voltage range of the fuel cell stack, and the active area of the fuel cell membranes determines the current generating potential of the cells (a larger active area equals greater current generating capacity). A fuel cell engineer uses these attributes—the area of the cells and the number of cells in series—to design a fuel cell

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stack that meets specified current and voltage requirements. Since current times voltage equals power, the number of cells and the cross sectional area of the cells defines the electrical power a given fuel cell stack can deliver. Figure 4 shows the conceptual assembly of a three-cell stack (three cells stacked in series). By examining the figure you can see how the hydrogen and oxygen gases (the reactants) are fed to each of the cells. The hydrogen is fed to the anode and the oxygen is fed to the cathode of each cell. A manifold within the stack delivers the gases to each cell. In Figure 4 you can also see how the cells are stacked in series, with the anode of one cell being physically connected to the cathode of the adjacent cell. Note that you may want to compare Figure 4 with the exploded diagram of a three-cell stack depicted in Extension of Activity 3 in the Student Book.

Note that in a real fuel cell stack, gaskets and structural end plates would be added along with bolts that hold the whole unit together. The plates that channel the gases and transport the current to and from the electrodes are typically made out of graphite (note that the anode and cathode screens in the student fuel cells serve these functions and they are made of stainless steel). Graphite is used because it is highly electrically conductive, chemically resistant, and easy to machine into properly shaped pieces with grooves that channel the gases to the electrodes.

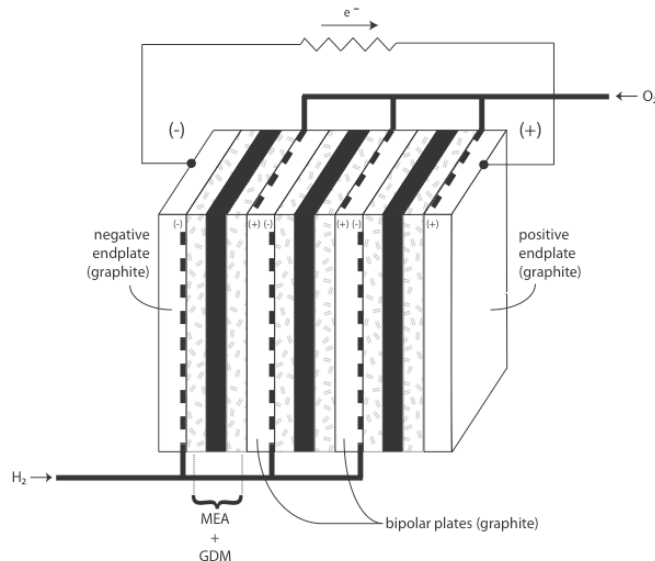


Figure 4. Simplified schematic of a three-cell fuel cell stack

Teaching Suggestions

GETTING STARTED

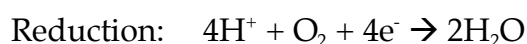
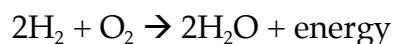
Step 1. Introduce redox reactions.

If students are familiar with the chemistry of batteries (from a previous electrochemistry unit, for example), it might be useful to begin by reviewing or explaining how batteries

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work. Explain that chemical reactions within the battery release (and accept) electrons, thus creating an electric current.

Introduce the term **oxidation-reduction** or **redox** to describe any reaction that involves the transfer of electrons. Explain that redox reactions are also responsible for generating electric current in a fuel cell. Write the synthesis reaction for water shown below and then explain how it can be split into two half-reactions: an **oxidation** reaction that releases electrons and a **reduction** reaction that accepts electrons.



Point out to students that in a balanced redox reaction, the number of electrons produced in the oxidation half-reaction must equal the number accepted in the reduction reaction. Thus, the oxidation reaction above must be multiplied by two. Then the two half-reactions can be added to yield the equation for the synthesis of water from hydrogen and oxygen gases.

INVESTIGATING

Step 2. Explore a computer simulation of a fuel cell.

Note: Ideally, students will do the computer simulation before working with the physical models. If that is not possible because of a lack of access to computers, the activities can be done in either order.

You may also wish to have them explore computer simulations of the internal combustion engine (ICE) cycle used by most automobiles before they answer Analysis Question 3. These simulations can be found on the HyTEC student page on the SEPUP website at sepuplhs.org/hytec.

Step 3. Model the redox half-reactions in a fuel cell.

Have students read the introduction and emphasize that **anode** describes the location where oxidation occurs and **cathode** describes the location where reduction occurs. Distribute the equipment and have students complete the Procedure.

If your students have had the opportunity to use both the computer model and the physical model, you can have them write about or discuss questions such as: “Compare the pros and cons of the physical and computer models.” or “Which did you find most helpful? Explain.”

Sample Responses

Procedure Questions, Part A, Questions 2–6

2. Click on “See Hydrogen Closeup.” Write the half reaction for what happens at the anode. Then write one or more sentences explaining what is happening.

At the anode, the following oxidation occurs : $\text{H}_2 \rightarrow 2\text{H}^+ + 2\text{e}^-$. A hydrogen molecule is oxidized, becoming two protons and two electrons.

3. Click on “See Oxygen Closeup.” Write the half reaction for what happens at the cathode. Then, explain what is happening in your own words.

At the cathode, the following reduction occurs: $4\text{H}^+ + \text{O}_2 + 4\text{e}^- \rightarrow 2\text{H}_2\text{O}$. Oxygen is reduced as it accepts two protons and two electrons to become water.

4. Click on “See Exchange Membrane.” Explain what would happen if the membrane were altered in a way that allowed electrons to pass through (in addition to protons).

If electrons could pass through the PEM, then they would not be forced to flow through the circuit, and no electricity would be generated.

5. Click on “See Electricity Closeup.”

What keeps electrons flowing through the circuit?

The input of hydrogen and its oxidation at the anode maintains the supply of the electrons.

What could cause the electric light to go off?

Answers will vary. Students will most commonly answer that if the hydrogen runs out, there will be no more electrons to flow through the circuit. If the PEM became permeable to electrons, current would also end.

6. Click on “See Exhaust Closeup.” Why are fuel cells potentially better for the environment than internal combustion engines?

The only exhaust product of a fuel cell is water.

Sample Responses

Procedure Part B, Questions 2 and 6

2. *Examine your models. Describe how the bonds in your O₂ and H₂ molecules are represented.*

The bonds are shown as complementary or matching puzzle pieces.

6. *Using the shapes of the molecular models and the picture of the fuel cell as a guide, create a storyboard of at least four frames depicting the chemical reactions that happen inside a fuel cell to create electricity. Be sure to label all parts as needed.*

Answers will vary, but storyboards should include the break up of hydrogen into protons and electrons at the anode, the migration of protons through the PEM, the movement of electrons through the circuit, and the reaction of oxygen with protons and electrons to form water at the cathode.

SYNTHESIZING

Step 4. Evaluate the possibility of using fuel cells to replace internal combustion engines on buses.

Ask student groups to share their diagrams of a fuel cell bus with the class. You might consider making these into posters and having each group present their ideas.

Sample Responses and Discussion of Analysis Questions

1. *With your group, draw a diagram of a fuel cell bus on poster paper. Indicate parts, such as hydrogen storage tanks, fuel cell, electric motor, hydrogen and oxygen intakes, the exhaust pipe, and any other necessary parts with clear labels. Try drawing the bus from the side, the top, and the inside. Be prepared to share your diagram with the class.*

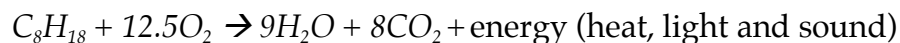
Answers will vary. Diagrams should convey an understanding that

- Hydrogen will have to be stored on the vehicle, and will be fed into the fuel cell anode.
- Oxygen will come from the air, and will be fed into the cathode.
- The fuel cell will not directly power the bus, but will provide the electricity to drive an electric motor.

- d. The exhaust will be water.
2. *Note that oxygen for fuel cell vehicles is obtained from the surrounding air. Why do you think this is?*

Oxygen is sufficiently abundant in the air to supply what's needed for the reaction. Carrying pure oxygen on board the vehicle would take up more room, add more weight, and add more cost. Although fuel cells operate more efficiently on pure oxygen, it is more practical and economical to use oxygen from the surrounding air.

3. *Gasoline internal combustion engines release chemical energy through the combustion reaction shown below.*



- a. *What are the main similarities between the H₂ fuel cell reaction and this internal combustion engine reaction?*

Both this reaction and what happens in a fuel cell are redox reactions. Both consume oxygen and produce water. They also release energy.

- b. *What are the main differences between the H₂ fuel cell reaction and this internal combustion engine reaction?*

The oxidation of gasoline occurs through an explosive combustion reaction. The fuel for the internal combustion engine (ICE) reaction is a much larger molecule that includes the element carbon in addition to hydrogen. Because of the presence of carbon in the fuel, carbon dioxide is a product in addition to water. The ΔG is also larger, which indicates that each mole of fuel consumed in the ICE releases more energy than each mole of H₂ consumed in the fuel cell (but keep in mind that a mole of octane has a much greater mass than a mole of hydrogen).

Extensions

1. Contrast the chemistry of a fuel cell with the chemistry of a battery. You can learn about the chemistry of a battery in almost any chemistry textbook, or by visiting the HyTEC student page of the SEPUP website at sepuplhs.org/hytec.

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2. Fuel cells are more efficient at converting chemical energy to useful energy than are the internal combustion engines in our automobiles. You can learn more about the properties and operation of internal combustion engines and how they differ from fuel cells by visiting the HyTEC student page of the SEPUP website at sepuplhs.org/hytec.

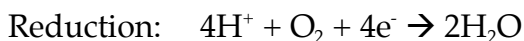
Activity 4 Modeling the Fuel Cell Reaction

In the previous activity, Mariyah saw fuel cells in action. Now it's time for her to learn the details about how they work.

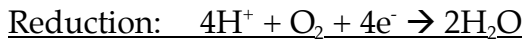
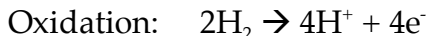
In the preceding activity, you used a proton exchange membrane (PEM) fuel cell. This type of fuel cell is already in use in buses, cars, and power generators, and may be widely used in the future. Like a battery, a fuel cell converts chemical energy into electricity. Unlike a battery, a hydrogen fuel cell continues to provide electricity as long as it is supplied with hydrogen and oxygen.

The chemistry of fuel cells has been understood since the 1830s. Like batteries, fuel cells create electricity through chemical reactions that involve the transfer of electrons. Chemists call these reactions **oxidation-reduction**, or **redox**, reactions. Redox reactions can be split into two parts, the oxidation half and the reduction half. Half-reactions that release electrons are called **oxidation reactions**; half-reactions that accept electrons are called **reduction reactions**.

Inside a PEM hydrogen fuel cell, electric current is generated using the two chemical half-reactions shown below.



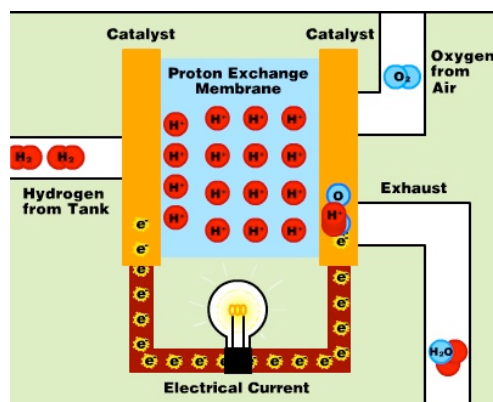
These equations can be added to obtain the complete equation. But first the oxidation reaction must be multiplied by two, so that the number of electrons in the reactants balances with the number of electrons in the products.



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Inside the fuel cell are two electrodes. Each electrode has a platinum catalyst that speeds up the redox reaction.

The electrode where oxidation occurs is called the **anode**. At the **anode**, hydrogen is oxidized and electrons are delivered to an external electrical circuit. In the previous activity, this circuit provided the power that let the electric motor turn the propeller. The electrons travel through this external circuit to the **cathode**. Reduction occurs at the cathode, where oxygen is reduced and the reactants combine to form water.



A *proton exchange membrane* separates the two electrodes. This membrane conducts protons through to the cathode, but blocks electron transport. Electrons are forced to flow through an external circuit and generate current. At the cathode, these protons join in the reduction reaction to form water.

Since we can't see the electric current or the chemical reactions inside a fuel cell, using models and computer simulations can help us understand what is happening.

Challenge

How do the redox reactions in a fuel cell generate electricity?

Materials

For each group of two students

fuel cell molecular modeling set (11 pieces)

PEM fuel cell diagram

computer with access to HyTEC Fuel Cell simulation

Procedure

Part A: Computer Simulation of a Fuel Cell

1. The simulation of a fuel cell is available at the HyTEC student page of the SEPUP website at sepuplhs.org/hytec. Open the simulation on your computer

screen and view the entire process. After clicking on “See Catalyst” and “See Exhaust Closeup,” click “Run Animation” and discuss the following with your partner or group.

- a. Identify the anode and the cathode.
 - b. Describe what happens to the hydrogen and oxygen.
 - c. Explain how water gets generated at the exhaust port.
2. Click on “See Hydrogen Closeup.” Write the half-reaction for what happens at the anode. Then write one or more sentences explaining what is happening.

 3. Click on “See Oxygen Closeup.” Write the half-reaction for what happens at the cathode. Then, explain what is happening in your own words.

 4. Click on “See Exchange Membrane.” Explain what would happen if the membrane were altered in a way that allowed electrons to pass through (in addition to protons).

 5. Click on “See Electricity Closeup.”
 - a. What keeps electrons flowing through the circuit?

 - b. What could cause the lightbulb to go off?

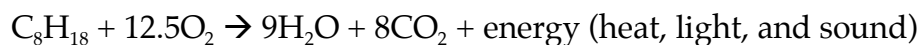
 6. Click on “See Exhaust Closeup.” Why are fuel cells potentially better for the environment than internal combustion engines?

Part B: Modeling the Fuel Cell Reaction

1. Working with a partner, use the appropriate pieces of the modeling set to build two hydrogen gas (H_2) molecules and one oxygen gas (O_2) molecule. In your notebook, draw each molecule.
2. Examine your models. Describe how the bonds in your O_2 and H_2 molecules are represented.
3. Place the two H_2 molecules on the anode side of the fuel cell diagram and the O_2 molecule on the cathode side.
4. Model the break up of H_2 at the anode. Move the broken pieces along the appropriate paths on the fuel cell diagram. Electrons should go through the circuit with the light bulb. The protons pass through the membrane.
5. Model the creation of water at the cathode. In your notebook, draw one of the two water molecules that are created.
6. Using the shapes of the molecular models and the picture of the fuel cell as a guide, create a storyboard of at least four frames depicting the chemical reactions that happen inside a fuel cell to create electricity. Be sure to label all parts as needed.

Analysis

1. With your group, draw a diagram of a fuel cell bus on poster paper. Indicate parts, such as hydrogen storage tanks, fuel cell, electric motor, hydrogen and oxygen intakes, the exhaust pipe, and any other necessary parts with clear labels. Try drawing the bus from the side, the top, and the inside. Be prepared to share your diagram with the class.
2. Note that oxygen for fuel cell vehicles is obtained from the surrounding air. Why do you think this is?
3. Gasoline internal combustion engines release chemical energy through the combustion reaction shown below. Octane (C_8H_{18}) is a major constituent in gasoline.



- a. What are the main similarities between the H_2 fuel cell reaction and this internal combustion engine reaction?
- b. What are the main differences between the H_2 fuel cell reaction and this internal combustion engine reaction?

Key Vocabulary

anode, cathode, oxidation reactions, oxidation-reductions, redox