

# Modeling the Fuel Cell

FEATURE by Ed Fontes and Eva Nilsson

Virtual prototyping  
is a vital tool in  
the development  
of fuel cells

Several properties make fuel cells attractive for electricity production, but the strongest incentives are high efficiency and high energy density. The fuel cell provides a highly efficient conversion of the chemical energy in hydrogen, natural gas, or hydrocarbons into electrical energy. This is extremely beneficial for automotive applications and small-scale energy production for stationary uses. And because of their high energy density (energy per unit weight of the power source), fuel cells are superior to batteries in portable equipment.

Fuel cells may have their greatest environmental impact in motor vehicles. In most automotive engines, gasoline is converted into mechanical energy through heat produced during combustion. The efficacy of this process is limited by the efficiency formula for the Carnot cycle, which

describes the thermomechanical operation that takes place in a gasoline engine. The engine's operating temperature determines its efficiency, which is about 20% for an automobile.

In a fuel-cell-powered vehicle, the chemical energy in the fuel is converted to electrical energy and then to mechanical energy by an electric motor. The process bypasses the limitations of the Carnot cycle, such as the 20% engine efficiency. As a result, the theoretical efficiency of fuel cells is substantially higher than that of the combustion engine—around 90%. In practice, values reach about 50%. This

higher efficiency implies that fuel-cell-powered automobiles can travel more than twice as far as conventional cars using the same amount of fuel. Consequently, carbon dioxide emissions are lower, and the lower operating temperatures of fuel cells all but eliminate the production of nitrogen oxides ( $\text{NO}_x$ ) and sulfuric oxides ( $\text{SO}_x$ ).

The electronics industry is pursuing miniature fuel cells. Motorola has demonstrated a cellular telephone powered by a fuel cell whose operating time with one fuel cartridge is five times longer than that of a conventional battery with one recharge. Other likely applications include power supplies in laptop computers and portable video, audio, and entertainment equipment. Figure 1 shows a battery charger for cellular phones powered by a miniature fuel cell that was designed by Manhattan Scientifics, Inc. (New York, NY), and is driven by gas contained in an ampoule.

Fuel cells, which generated electrical power for the Apollo spacecraft during the U.S. lunar-landing program, have great potential for generating power in places without an electrical infrastructure. They can also serve as power sources in boats, portable construction tools, temporary traffic-control stations, mobile life-support units, and military applications.

In batteries, energy is stored as chemical energy in the battery itself. In fuel cells, chemical energy is stored in the fuel tank and electricity is produced on demand. This separation eliminates downtime for recharging—add a source of hydrogen, and the fuel cell can generate electricity in less than 1 min. Fuel cells also provide an uninterrupted power supply because there is no self-discharge, as occurs with batteries, an advantage that minimizes maintenance and maximizes the system's reliability. In addition, fuel cells have a higher energy density and therefore a higher power capacity per unit of weight.

The development of fuel-cell-powered equipment and vehicles has accelerated during the past five years (see *The Industrial Physicist*, February 1999, pp. 15–17). Competition among companies is growing, and the fight for a share of a potentially huge market has already started. Technology development is an important weapon at this stage, and small companies with technical skills in fuel-cell processes have become important partners to the large electronic and automotive companies.

In this rapidly developing and highly competitive market, the time from idea to prototype has shrunk. Therefore, tools for developing virtual prototypes have become exceptionally important. Optimizing a fuel cell's perfor-

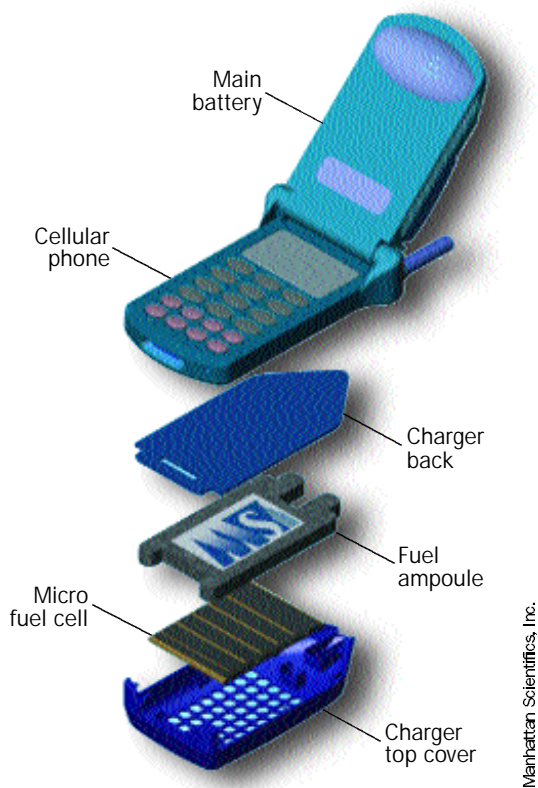


Figure 1. Prototype for a detachable fuel cell that could recharge a cell-phone battery multiple times from an ampoule of, say, methanol.

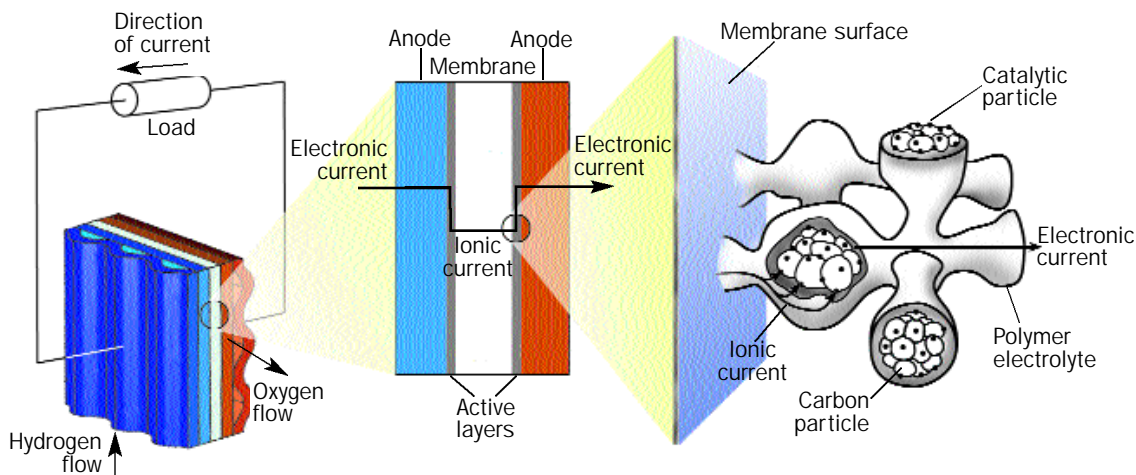


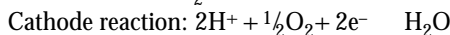
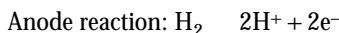
Figure 2. At the cathode of a unit cell in a proton-exchange-membrane fuel cell, protons travel through the membrane and unite with oxygen and the electronic current to form water.

mance in combination with its auxiliary equipment and operation of the electric motor requires a lot of mathematical puzzling. Thus, mathematical modeling, the basis of virtual prototyping, is a vital tool in the development of fuel cells. A combination of modeling and experimentation has reduced the cost and accelerated the pace of building and understanding prototype systems.

Modeling provides valuable insights into the electrochemistry of the fuel cell and the processes that take place in the heart of the fuel-cell system—the electrodes and electrolyte in the fuel-cell stack. These processes are described at the microlevel: single catalyst agglomerates; a unit cell consisting of an anode, a cathode, and the electrolyte between them; and as reactor models of the fuel processor in fuel cells for cars. Other important aspects include the design of the bipolar plates of the fuel cell, their influence on ohmic losses in the fuel-cell stack, and the use of modeling to optimize the design of fuel-cell systems.

## Fuel-cell system

A fuel cell works through the principle of separating the oxidation of a fuel, such as the oxidation of hydrogen and the reduction of oxygen. The oxidation and reduction processes take place at the anode and cathode, respectively; electrons are released to an outer circuit at the anode and received through the same circuit at the cathode. The following reactions occur in two types of fuel cells, the proton-membrane-exchange and phosphoric acid fuel cells. Solid-oxide, molten-carbonate, and alkaline fuel cells have different but similar reactions.



The outer circuit is completed through an external load, and the transport of protons in the electrolyte completes the circuit inside the fuel cell (Figure 2).

From an environmental point of view, the optimal fuel in a fuel cell is hydrogen produced by means of renewable sources such as solar power (see *The Industrial Physicist*, February 2001, pp. 13–14). However, hydrogen is difficult to store efficiently, despite the extensive

research put into technologies such as metal hydrides and nanofibers.

Alcohols, such as methanol, and hydrocarbons offer the most effective hydrogen storage available today. The process that separates hydrogen from a fuel is called the reformation reaction. In miniature applications such as cell phones, methanol is reformed to hydrogen in the fuel cell itself. For applications that require higher power outputs, such as cars, methanol can be reformed in a device—essentially a tubular reactor—that is located

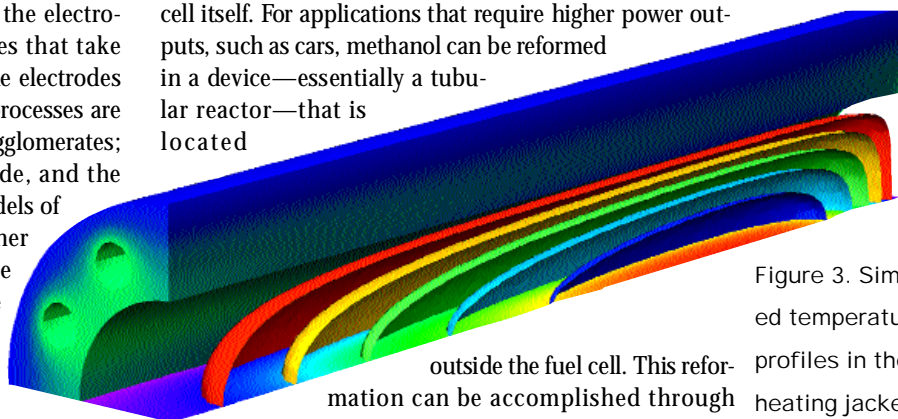


Figure 3. Simulated temperature profiles in the heating jacket and core of a tubular steam-reforming reactor, using different color scales.

outside the fuel cell. This reformation can be accomplished through steam reforming or partial oxidation.

The design of the tubular reactor, which is called a reformer, is important to the performance and efficiency of the total system. The reformer should be able to work at low and high loads and at high, sudden outputs. Its weight and space should be minimized, and the heat-management system optimized for different operating conditions, such as low outputs at constant speed and high outputs when sudden acceleration is required.

Figure 3 shows the result of a simulation of the temperature distribution in a tubular reactor used for reforming methanol to hydrogen using the steam-reforming reaction. A jacket heats the reformer—a part of the fuel processor—and reactions in its core consume the heat. The curved surfaces in the core represent isothermal surfaces. Because temperature differences are larger in the reformer core, different color scales are used for the heating jacket and for the core. The heat is exchanged from the heating channels in the jacket, through the highly conductive jacket material, and into the core. We can calculate the temperature profile in the reformer by setting up a heat balance that assumes that heat transfer takes

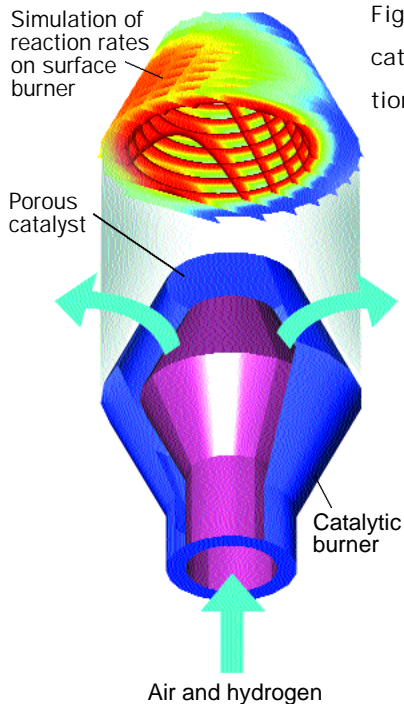


Figure 4. When hydrogen combines with oxygen on the nonuniform, porous catalyst surface of this burner, a simulation can be used to show the reaction rate distribution, from high (red) to low (blue).

place by conduction and convection.

A surplus of fuel is usually fed to the cell to avoid a buildup of byproducts from fuel processing, such as inert gases and reaction products, and to optimize the operation of the cell at both constant and accelerating speeds. The cell's exhaust—carbon dioxide, other carbon species, and water—is fed into a catalytic burner. The heat produced in combusting the waste is subsequently used in the fuel processor, including as the heat source for the reformer jacket. Using a catalytic burner at low temperature minimizes the production of  $\text{NO}_x$ .

Figure 4 shows the simulated reaction distribution in a catalytic burner. In this case, we assume that one of the burner's porous walls was accidentally made too thin during the manufacturing process, which results in a nonuniform flow through the porous catalyst and uneven combustion. The red color signifies areas with a higher combustion rate due to a larger convective flow of fuel. This flow pattern might eventually lead to an uneven temperature distribution and the ignition of the hydrogen and other gases. The simulation shows that safety and "what if?" scenarios can be successfully studied with modeling.

## Electrodes

In the fuel cell, hydrogen is oxidized at the anode. This oxidation takes place at the active sites of the catalyst and serves as the charge-transfer reaction between electronic and ionic currents. This reaction requires the transport of hydrogen gas through pores in the anode to the active sites at the catalyst surface.

At the cathode, protons react with electrons supplied by the solid catalyst and oxygen to produce water. The oxygen is supplied to the reaction site through pores in the polymer electrolyte incorporated in the catalytic layer of the cathode. Modeling can detect problems in electrode design that result in less than optimal performance. At the cathode, oxygen has to diffuse to the reaction site and the polymeric electrolyte must transport the protons to the same site at the same time. To minimize transport resistance, the oxygen's path through the poly-

mer must be as short as possible, but the system also requires enough polymer material to reduce resistance for the ionic current transported by protons.

Figure 5 shows the oxygen concentration inside and around catalyst agglomerates. Substantial concentration gradients arise in the polymer electrolyte inside the electrode at high loads. The figure shows a projection of two catalyst agglomerates, which are covered by a thin film of polymer electrolyte. The agglomerates form a neck where the polymer electrolyte forms a meniscus, the soft overlap of the electrolyte between the two particles. This structure results in an increasing resistance for oxygen transport. The model is highly idealized, but the

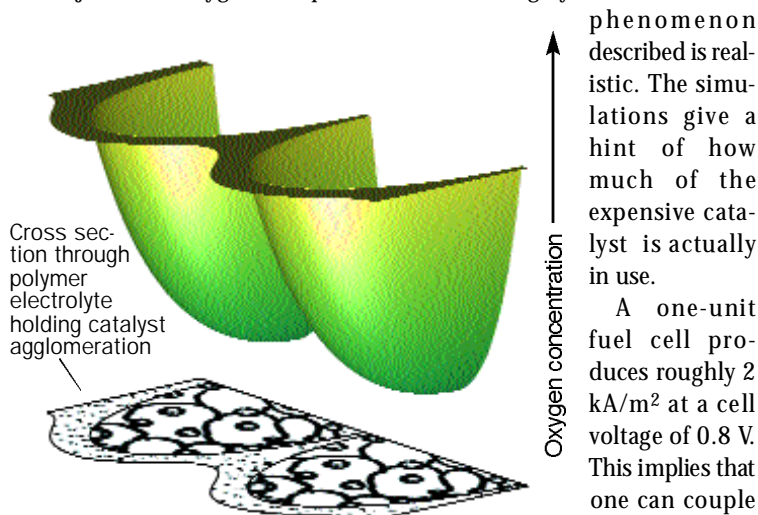


Figure 5. This simulation shows that the oxygen concentration in the polymer electrolyte of the fuel-cell cathode is highest before it reacts in the catalyst region inside.

phenomenon described is realistic. The simulations give a hint of how much of the expensive catalyst is actually in use.

A one-unit fuel cell produces roughly 2  $\text{kA}/\text{m}^2$  at a cell voltage of 0.8 V. This implies that one can couple several cells in series to increase the voltage to usable levels. In a fuel-cell stack, bipolar plates

serve as both separators and current conductors between adjacent anodes and cathodes and also supply gas to the electrodes through channels in their structure. In addition, the edges of the plates serve as manifolds for the fuel-cell stack.

The design of the bipolar plate in systems that require high power output is vital to the performance of the fuel-cell stack. The plate must be capable of effectively distributing gas to reduce transport resistance while providing the path for electronic current. Figure 6 shows the potential distribution in the contact area between the electrode and the bipolar plate. Contact resistance should be minimized and, if the bipolar plate is made of a metallic material, it is important that low-conducting oxide layers are not formed between the electrode and plate. The color scales in the figure are different for the

Bipolar metal plate separates anode and cathode and carries gas flow

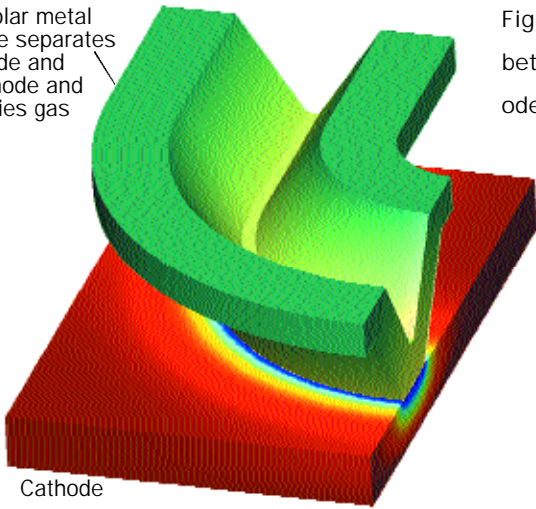


Figure 6. Voltage distribution at the contact zone between a bipolar plate (green to yellow) and the cathode (blue to red) in a fuel cell stack.

likely that some of the buses and cars in our urban areas will soon be fuel-cell-driven.

## Further reading

Appleby, A. J.; Foulkes, F. R. *Fuel Cell Handbook*; Krieger Publishing: Malabar, FL, 1989; 790 pp.

Kordesch, K. *Fuel Cells and Their Applications*; VCH Verlagsgesellschaft: Weinheim, Germany, 1995; 375 pp.

Larminie, J.; Dicks, A. *Fuel Cell Systems Explained*; John Wiley & Sons: West Sussex, United Kingdom, 2000; 308 pp.

Los Alamos National Laboratory provides an online fuel-cell tutorial at <http://education.lanl.gov/resources/fuelcells/fuelcells.pdf>.<sup>[1]</sup>

plate and electrode because of a large difference in conductivity between the two materials. We can use models such as this to investigate the influence of bipolar plate design on fuel-cell performance.

The use of fuel cells for electronic and portable equipment is on the verge of commercialization. Today, fuel-cell-powered automobiles are exhibited as concept cars. Unfortunately, the cost of the materials presently used for fuel cells is too high for mass production. The large automotive companies, however, have shown a commitment to solving these problems, and they forecast production at an industrial scale within three years. It is

## B I O G R A P H Y

Ed Fontes is product manager at COMSOL AB, an engineering software development company in Stockholm, Sweden ([ed@comsol.se](mailto:ed@comsol.se), [www.comsol.com](http://www.comsol.com)). Eva Nilsson is a consultant in battery and fuel-cell technology at Catella Generics AB in Stockholm ([eva.n@cgr.se](mailto:eva.n@cgr.se), [www.cgr.se](http://www.cgr.se)).