POWERING A HOME WITH FUEL CELLS

Home-based electricity generation is possible using a fuel cell system. Panasonic Corporation applied simulation to help reduce the cost of these systems to make them more commercially feasible.

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A household fuel cell cogeneration system is a new way to generate electricity and heat. The system can be installed on-site at individual residences, and uses the electrochemical reaction between hydrogen and oxygen to produce energy. It is, essentially, an environmentally friendly power plant for the home. The hydrogen required can come from natural gas piped into residences, where available; the oxygen is provided by the ambient air. Such a system generates electric power with high efficiency even when the required electrical output is low, and is expected to help increase energy savings and decrease CO_2 emissions.

Panasonic Corporation is developing a household fuel cell cogeneration system called Ene-Farm. The company needs to overcome the challenges of system cost and reliability before widespread deployment. Reducing cost requires a better understanding of how hydrogen ions flow through the membranes in the membrane electrode assembly (MEA) that is the heart of a polymer electrolyte membrane fuel cell (PEMFC). The Panasonic engineering team used simulation software from ANSYS, along with some software they developed in-house, to model MEA for different materials and fuel cells. Simulation helps the team reduce the direct material cost for the Ene-Farm, while increasing efficiency and improving its commercial potential.

In the MEA, hydrogen atoms release their electrons on the anode side of the cell upon passing through a layer of anode material and then protons reach a layer of catalyst material. The

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TECHNICAL OVERVIEW OF FUEL CELL SYSTEMS: HOW COMPUTER SIMULATION IS USED TO REDUCE DESIGN TIME — WHITE PAPER
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electrons return to the anode current collector and travel through a load circuit to the cathode (air) side, thereby generating electrical energy. The remaining hydrogen ions then pass through the polymer electrolyte membrane and react with the electrons and the oxygen on the cathode side to produce water vapor, which is the final product of the fuel cell reactions.

$$2H_2 \rightarrow 4H^+ + 4e^- \text{ (anode)}$$
$$O_2 + 4H^+ + 4e^- \rightarrow 2H_2O \text{ (cathode)}$$

Though these reactions are relatively simple, the nature of the species transport (atoms, ions) through the different layers of the MEA is complex, and must be kept in the proper balance to maximize the performance of the PEMFC.

DEVELOPING ACCURATE GAS DIFFUSION MODELS

Simulation of diffusion through a thin membrane requires an approach that resolves both macroscale and microscale effects for optimization. The ANSYS Fluent fuel cell and electrolysis add-on model with full multicomponent diffusion was used for the macroscale simulation. To model at microscale, several options are available. Panasonic engineers chose to develop an algorithm called the multicomponent Lattice Boltzmann method (MC-LBM) to support multicomponent gas diffusion. After validating their microscale model by comparison to experimental results, the team modified the ANSYS Fluent fuel cell and electrolysis model using user-defined functions (UDFs) to incorporate MC-LBM.

An important parameter in gas diffusion models is the coefficient of permeability, which describes the degree of permeability of a porous material. Panasonic engineers computed the coefficient of permeability of various membrane materials using their microscale model and used these values as inputs to the CFD model. In this manner, they created effective models for each layer of the fuel cell, which is required to accurately predict the overall performance. In addition to the coefficient of permeability for porous materials, these models include other parameters such as effective electrical conductivity, effective thermal conductivity and effective diffusion coefficient. Though the engineers did compute all of these parameter values, the process for determining the effective diffusion coefficient for porous materials using Fluent and MC-LBM is highlighted here due to the importance of this coefficient to the PEMFC's performance.

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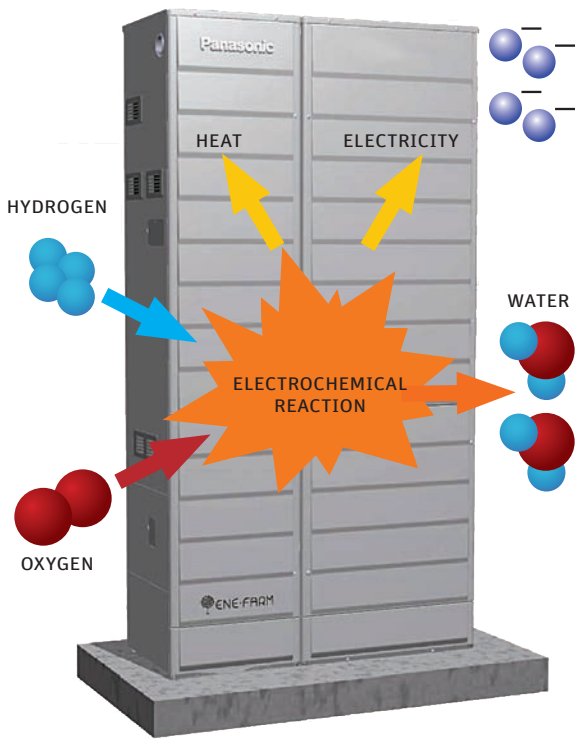
DETERMINING THE EFFECTIVE DIFFUSION COEFFICIENTS

To compute the coefficient for a porous material, Panasonic engineers created a flow domain model where the material was sandwiched between two

FUEL CELL SYSTEM BODY

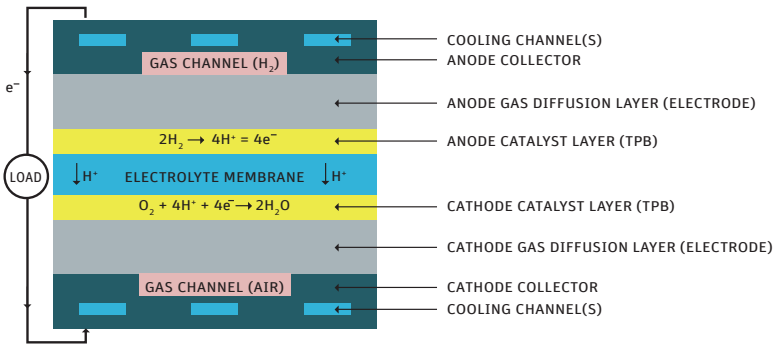
▲ Panasonic's Ene-Farm household electricity system employs a fuel cell stack to generate power.



$2H_2 + O_2 \rightarrow 2H_2O + 4\bar{e}$

▲ How a fuel cell generates energy

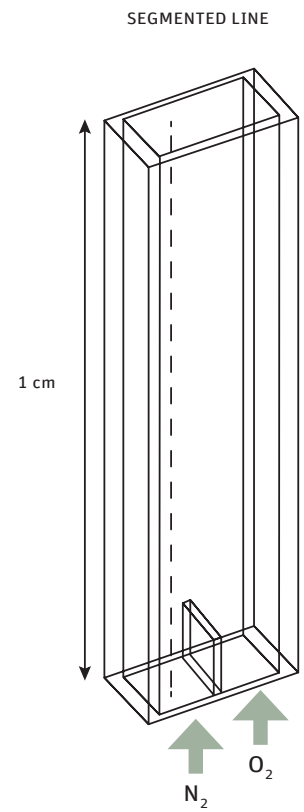
The ability to quickly, efficiently and accurately model fuel cells will eventually lead to decreased production costs and wider deployment of household fuel cell cogeneration systems.



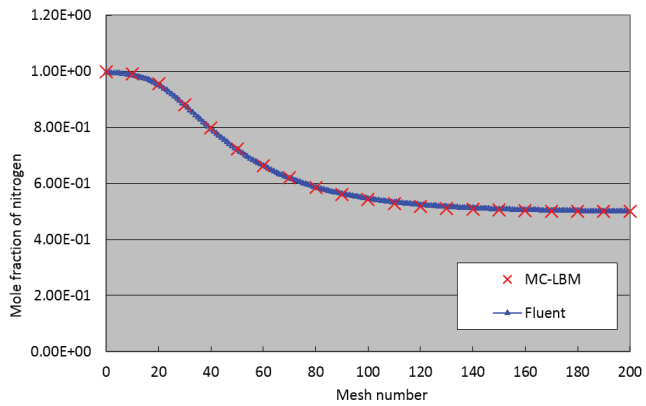
▲ Schematic of a PEMFC showing the different layers that comprise the membrane electrode assembly (MEA)

flow channels that allow the different gases to flow in through each side. They performed a simulation using their in-house microscale algorithm to compute the value of the mole fraction of each gas at the outlet section of the channel.

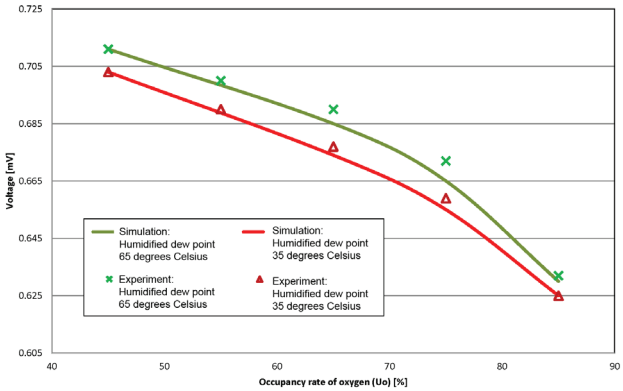
Next, the engineers used the fuel cell and electrolysis model with full multicomponent diffusion. For each material layer, the team set a homogeneous (bulk) diffusion coefficient for the porous material section and used this as a variable to compute the value of the effective diffusion coefficient for that layer. The team varied the bulk diffusion coefficient value in the CFD software until the mole fraction of each gas species matched the results from the in-house microscale simulation. The computed effective diffusion coefficient values ranged from approximately 10 to 80 percent of the diffusion coefficient for the bulk material. In PEMFC simulations, a model with an effective diffusion coefficient that is proportional to the porosity and a value approximately 60 to 80 percent of the bulk material is



▲ Macroscopic flow channel of approximately one centimeter used to compare ANSYS Fluent results to a multicomponent Lattice Boltzmann method (MC-LBM) simulation using an in-house simulation tool



▲ Comparison of ANSYS Fluent and MC-LBM computed mole fractions for gas flow rates of 0.1 meter/second for both nitrogen and oxygen



▲ Experiment and simulation results to validate the accuracy of battery performance predictions

	Material A	Material B	Material C	Material D
Measurement results (m^2)	1.52 E-15	1.15 E-15	6.8 E-12	5.7 E-12
Simulation results (m^2)	1.49 E-15	1.17 E-15	6.6 E-12	5.6 E-12
Accuracy (Simulation vs. measurement)	0.98	1.01	0.97	0.98

▲ Coefficient of permeability results from permeometer test measurements and MC-LBM calculations

generally adopted. However, these computed results indicated that modeling an effective diffusion coefficient that is simply just proportional to porosity is inadequate.

Finally, the Panasonic team applied the in-house microscale MC-LBM algorithm to the fuel cell and electrolysis model using UDFs to create an improved simulation for each layer of the PEMFC. They validated the accuracy by checking the voltage behavior of the cell with straight flow channels under specific conditions.

PREDICTING THE CELL VOLTAGE BEHAVIOR

To complete the study, the team predicted the cell voltage behavior for two conditions of fuel cell oxygen utilization (Uo): humidified dew points of 65 C and of 35 C. Oxygen utilization is the percentage of available oxygen used to generate electricity. A lower oxygen utilization value indicates a higher amount of supplied oxygen and vice versa. By changing the utilization value, the concentration of oxygen within the fuel cell will change, and an increase or decrease in cell voltage can be predicted. The PEMFC's voltage behavior for a specific oxygen utilization value can be obtained from experiment and compared to the simulation results to indirectly validate whether the gas diffusion that occurs within the fuel cell is accurately modeled. The Fluent predictions agreed very well with the experimental results for the dependency of oxygen utilization on the humidified dew point.

By using highly accurate simulation software, Panasonic has improved the accuracy of predicting PEMFC characteristics. This has greatly contributed to improving the process efficiency in developing fuel cell stacks. The ability to quickly, efficiently and accurately model fuel cells will eventually lead to decreased production costs and wider deployment of household fuel cell cogeneration systems.

Fuel Cell Design Solutions

While fuel cell developers advance this renewable energy source technology for transportation, stationary power, material handling machinery and other distributed power applications, they must refine the reliability, performance and durability of fuel cell systems and components. Fuel cell operation requires continuous access to a fuel source (typically hydrogen) and, for many types of fuel cells, the fuel can be reformed on-site to be consumed. Fuel cells have no moving parts and generate less emissions (including the conversion of required hydrocarbon used to generate hydrogen) than fossil-based power sources.

There has been more significant advancement in the development of fuel cells for stationary power because of simpler logistics and infrastructure than, for example, those for the automotive industry. However, continuous innovation and incremental improvement are required for both industries to expand on success for stationary power generation and encourage broad acceptance for the transportation industry.

One focus area for research and development, and design, is the fuel cell membrane. ANSYS continues to develop solutions for modeling solid-oxide fuel cells (SOFC) and proton exchange membranes (PEM), as well as other types. For PEM full cells, the focus has been on a complete 3-D model that resolves catalyst layers and membrane separately, rather than assuming that the membrane electrode assembly (MEA) is one infinitesimally thin flat surface. Ability to resolve 3-D effects within the MEA enables better understanding of spatial variation of key parameters. Engineers use this insight to choose materials, determine the performance of different fuels, assist with water and water vapor management, resolve the effects of mass transfer and phase change, and ascertain the influence of temperature variation on exchange current density.

Other areas of development focus are individual chemistry models, as well as the ability to combine chemistry, electrochemistry and fluid mechanics to obtain an accurate understanding of how interactions affect the entire fuel cell. This capability is of special interest to developers of SOFC stack systems, which are used for auxiliary power units and to generate electricity for data centers or for distributed power applications. ANSYS solutions can be employed to study individual components or full fuel cell stacks to optimize the stack design, improve electrical resistance, and design the entire power-unit system.

— **Ahmad Haidari,** Director, Energy Industry Marketing, ANSYS