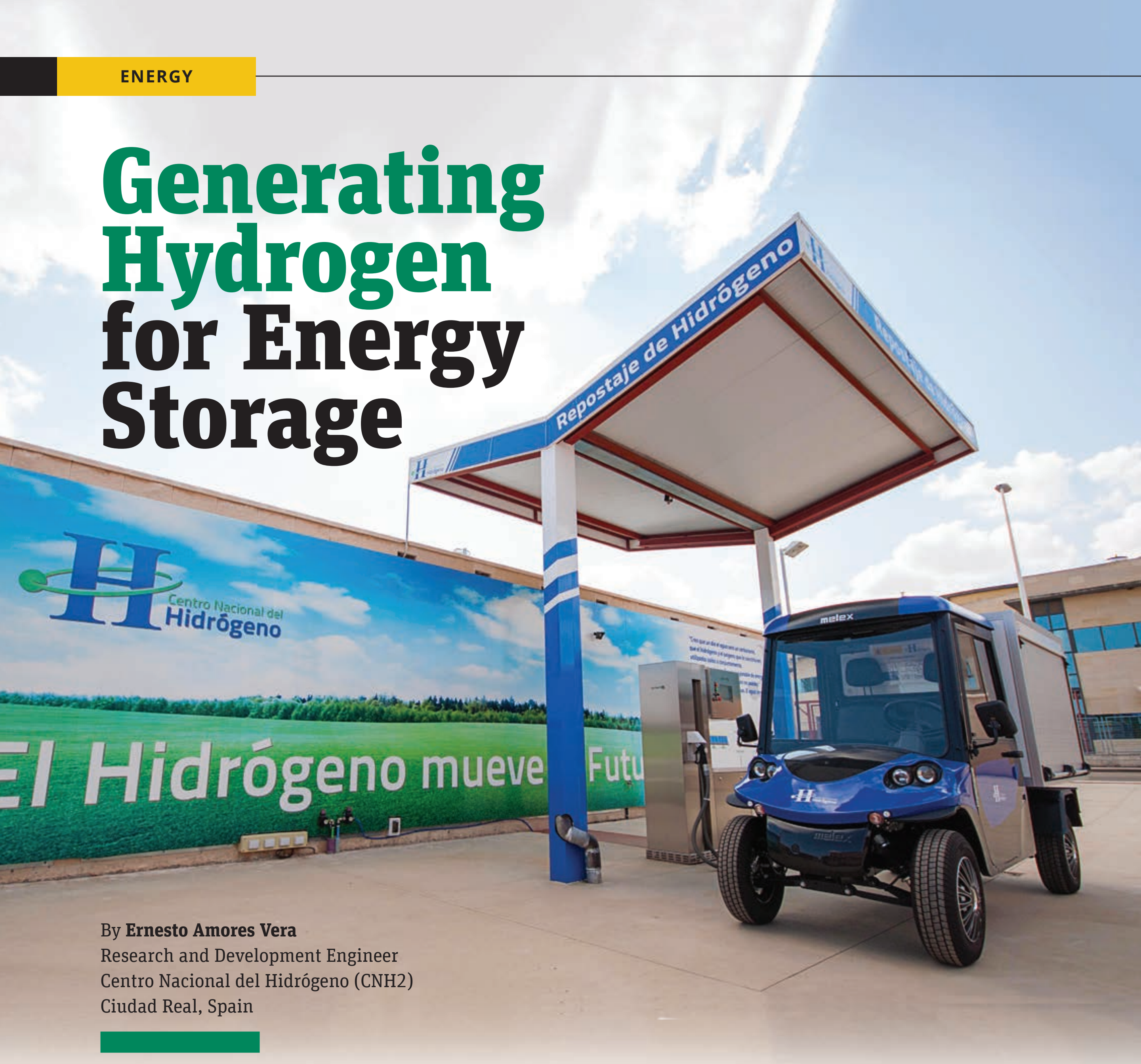
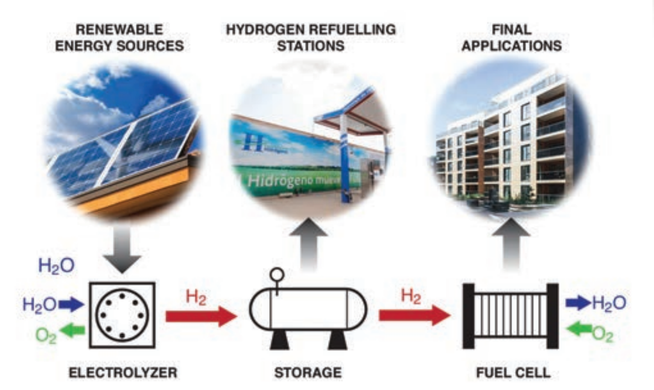


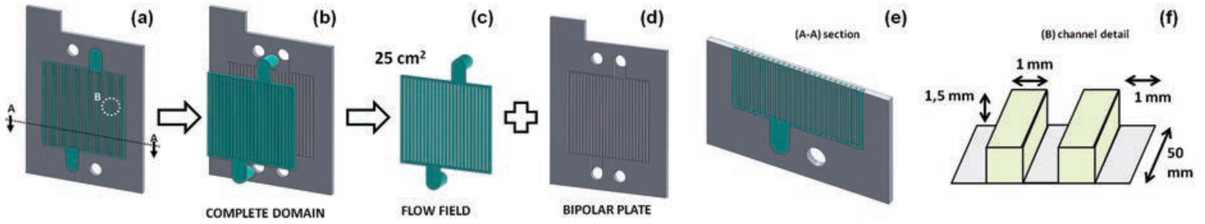
Generating Hydrogen for Energy Storage

By **Ernesto Amores Vera**
Research and Development Engineer
Centro Nacional del Hidrógeno (CNH2)
Ciudad Real, Spain

An increase in renewable energy production has fueled interest in proton-exchange membrane water electrolysis as a viable solution to generate hydrogen to store power. To optimize and improve proton-exchange membrane (PEM) cells, a national project called ENHIGMA uses ANSYS Fluent as the fundamental tool to simulate the flow field in these cells. The results from the simulations will help the future manufacture of more cost-competitive, efficient and durable PEM electrolyzers.



Hydrogen energy cycle: production, storage and transformation. Excess renewable energy production can be used by a water electrolyzer to produce hydrogen and oxygen. The hydrogen can be transported or stored in appropriate facilities, then when it is needed, hydrogen can be transformed into electricity using a fuel cell or it can be used as fuel in the mobility sector.



Geometry for the simulation model: (a) bipolar plate with the flow distribution channels; (b) complete domain; (c) parallel flow field; (d) bipolar plate; (e) section of the channels of the bipolar plate; (f) detailed dimensions of the channels

As demand for energy rises, the world requires more secure and reliable sources of electricity. This has accelerated innovation in energy production using many new technologies. However, many renewable energy sources (RES) such as solar, wind and others do not continuously produce electricity at a consistent rate. New and adequate energy storage is required to overcome the intermittency of RES and successfully integrate them into the power supply.

The storage capacity of batteries is often limited to hours or a few days. Hydrogen, an energy carrier, can be stored for indefinite periods. It can be produced from electricity generated by RES and, once stored, hydrogen can be transported and distributed for use, such as within hydrogen refueling stations in the mobility sector. It can also be reconverted to electricity with a fuel cell to power electric vehicles or a home, or be supplied to the grid.

Water electrolysis is one of the most environmentally friendly ways to produce hydrogen. In this electrochemical process, electricity is applied to split water, which produces hydrogen and oxygen. When the electricity comes from renewable energy sources, it is a zero-emission process.

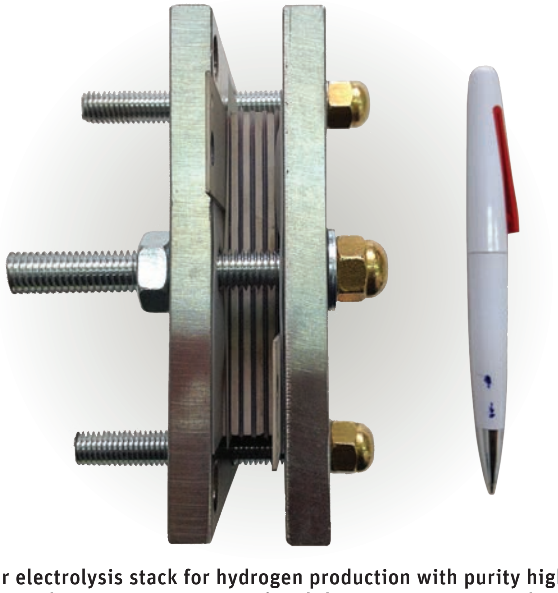
Among the different electrolysis processes, proton-exchange membrane water electrolysis (PEMWE) has become one of the most important. PEMWE systems can operate at high current densities (2,000 mA/cm^2) to generate hydrogen of high purity and high pressure. While there are large-scale commercial PEM electrolyzers in use today, various challenges, including high cost and durability, prohibit their widespread adoption.

“New and adequate energy storage is required to overcome the intermittency of renewable energy sources.”

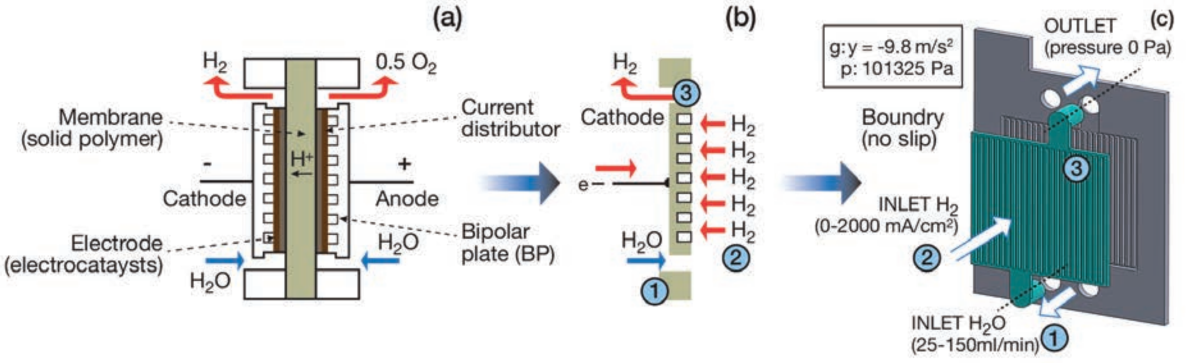
The Centro Nacional del Hidrógeno (CNH2) (the Hydrogen National Center) in Spain carries out research into future technologies like hydrogen and fuel cells. CNH2 is the technical coordinator of the ENHIGMA project (2016–2019) and, with other research centers and companies, is investigating ways to develop a low-cost, durable and energy-efficient PEM electrolyzer.

VITAL COMPONENT IN THE DESIGN

The bipolar plates (BPs) are some of the most important components in a PEMWE. Providing structural strength, these metal



A PEM water electrolysis stack for hydrogen production with purity higher than 99.995%. The active area is 25 cm^2 and the maximum current density of 2,000 mA/cm^2.



Model setup for the flow field in a PEM water electrolysis cell: (a) simplified scheme of a complete cell; (b) domain of the cathodic chamber considered in the model; (c) phenomena considered in the channels of the cathode

plates separate each membrane–electrode assembly (MEA) in a PEMWE stack. They feature machined flow channels that distribute the water inside the cell and carry the generated gases (H_2/O_2) to the outlets. They are also essential for sufficient electrical conduction to the reaction points and for the dissipation of heat. BPs account for approximately 50% of the costs of PEMWE due to the materials and manufacturing method used, so improving PEMWE requires the optimization of this component.

Computational fluid dynamics (CFD) simulation is fundamental in obtaining information about the flow distribution in the BPs. The ENHIGMA research team used ANSYS Meshing and then ANSYS Fluent to solve the various complex CFD simulations. With CNH2's high-performance computing license (ANSYS HPC), the research team could divide the various calculations among the eight cores it has in-house for parallel processing to solve the complex CFD simulations quickly and cost-effectively.

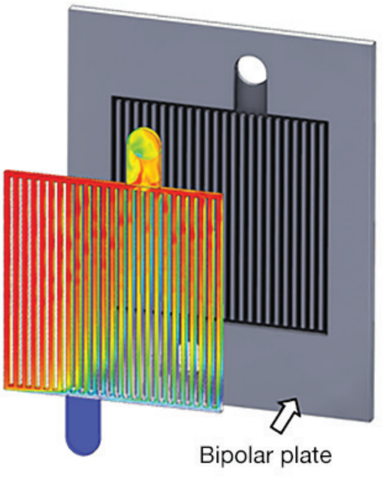
“These results will help contribute to the future manufacture of better-performing, lower-cost, energy-efficient and durable PM electrolyzers.”

DEVELOPMENT OF THE MODEL

A variety of possible flow field configurations can be used for the water flowing in a PEMWE cell, but the straight parallel channel geometry is often considered the best design for flow distribution due to its simplicity. The project team chose this configuration to model in the simulations. To simplify the models, they analyzed the flow distribution only in the cathode chamber using the ANSYS Fluent PEMWE model. ANSYS Fluent also has other fuel cell models, including those for PEM and solid oxide fuel cells (SOFC).

The first step in the process was to perform a mesh independence study in ANSYS Meshing to determine the optimal number of nodes for the simulation. Seven meshes were evaluated to determine the best discretization, with the optimal number being 1,901,570 nodes.

ANSYS Meshing easily enabled researchers to mesh complex geometries so they were able to create suitable meshes for different zones in the same model. For example, they used a hexahedral mesh for the channels and a tetrahedral mesh for the inlet/outlet of the BPs.



Hydrogen fraction in an electrolysis cell when straight parallel channels are used in a bipolar plate. The flow distribution is deficient in the middle channels. As a result, hot spots and inefficient hydrogen production can occur in the lateral channels.

SIMULATING THE FLOW FIELD

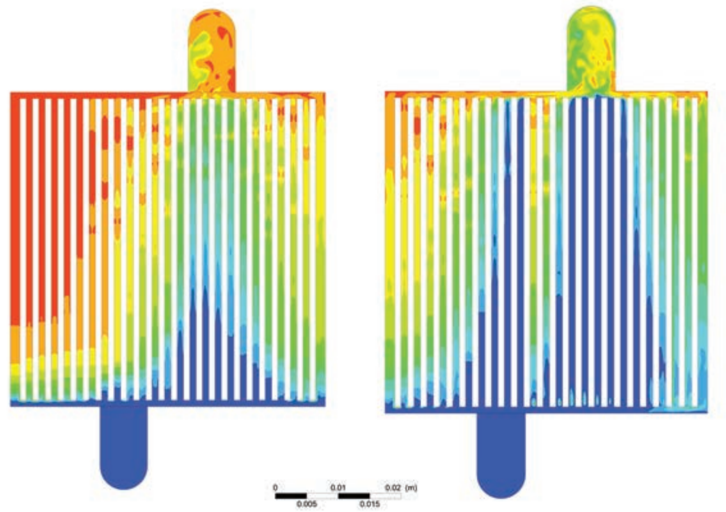
The team used ANSYS Fluent software to simulate the flow field in the models of interest. To predict the flow of water as it enters the cell and is distributed through the channels, Fluent solved equations for conservation of momentum, continuity and energy.

Using Faraday's law of electrolysis, the team then calculated the hydrogen generation rate as hydrogen flowed from the membrane-electrode assembly (MEA) to the channels when a potential difference was applied between the electrodes (auxiliary equation). This equation is introduced into the model as a velocity boundary condition (current density versus hydrogen flow rate).

Next, as the water and hydrogen generated moved in the channels to the cell outlet, the team needed to calculate multiphase flow. In a PEMWE, there is a main phase (water) and a second phase (small hydrogen bubbles) dispersed within the main phase. Calculating multiphase flow is complex as several phenomena occur in a liquid–gas mixture. Instead of using a full Eulerian multiphase model, the team created a mixture model in ANSYS Fluent. This is a simpler model that performs as well as a full multiphase model while requiring a smaller number of variables. Typical applications include bubbly flows where the gas volume fraction remains low. Using this mixture model method, the volume fraction equation for liquid and gas phases was obtained.

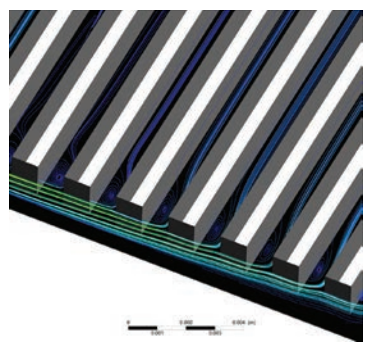
RESULTS FOR IMPROVED DESIGNS

With the simulations complete, the research team could then analyze the results. When looking at the hydrogen volume fraction in an electrolysis cell at different flow rates, the results showed that when the water flow increases from 25 to 100 mL/min for a given current density, the flow distribution was deficient in some channels. The same was true with the results for mixture density, with channels being increasingly blocked when the current density increases. The results revealed that when the current density changes from 500 to 2,000 mA/cm^2 for a given flow rate, the hydrogen produced tends to fill the channels having a relatively lower flow velocity, blocking the passage of water in those channels.



Hydrogen fraction in an electrolysis cell at different flow rates with straight parallel channels. When the water flow increases from 25 (left) to 100 (right) mL/min for a given current density, the flow distribution is deficient in some channels.

Although a straight parallel channel configuration in the BPs is often considered the best configuration for the flow field, the results obtained using CFD simulation in ANSYS Fluent revealed that this is not the case. There are significant weaknesses in the proposed design, especially at high currents and high flow rates, which causes hot spots and reduces the efficiency of the process. A new flow distribution configuration had to be proposed.



Streamlines at the closest part of the bipolar plate to the channel inflow at 500 mA/cm^2 and 100 mL/min. In some channels, when the flow rate is high, vorticity phenomena may occur. This limits the water flow in each channel so that the hydrogen generated in the cell accumulates, reducing the efficiency of the process.

CONTRIBUTING TO A HYDROGEN FUTURE

The goal of the ENHIGMA project is to obtain results that will improve the commercial feasibility of PEM electrolyzers. Fundamental to this is the optimization of a key component, the BPs. Through various CFD simulations of this component in ANSYS Fluent, the research team has gained conclusive preliminary results of the flow field in PEM water electrolysis. These results will contribute to the future manufacture of better-performing, lower-cost, energy-efficient and durable PEM electrolyzers.

Comprehensive Numerical Simulation of PEM Fuel Cells
ansys.com/pem