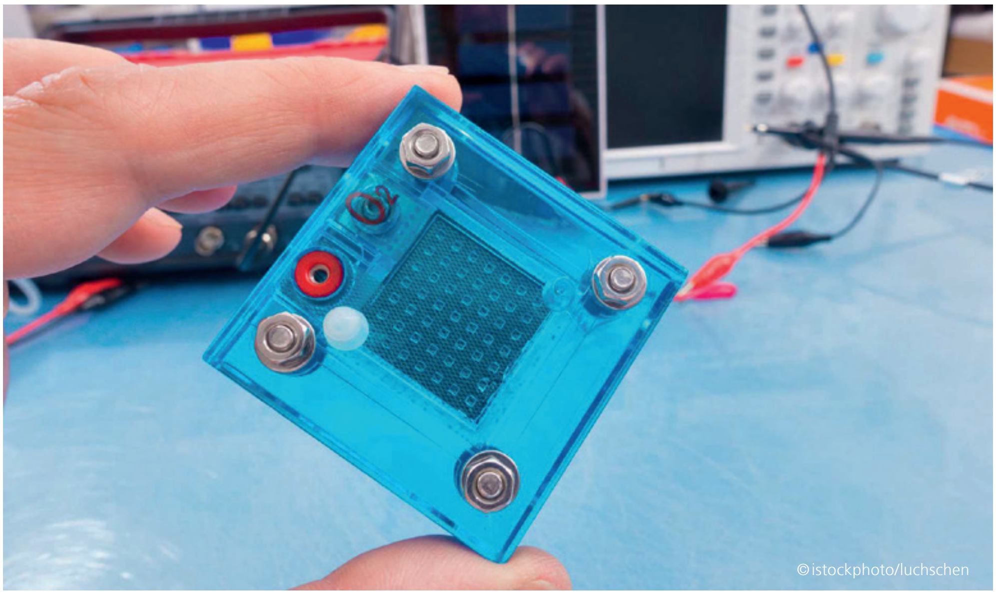
Understanding Hydrogen Electrolysis on a Small Scale – Achieving Big Things for Greener Energy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Hydrogen technologies are seen as paving the way for climate-neutral mobility and as holding out hope for the climate-neutral design of the energy industry and the chemical industry. But to achieve this, the chemical processes of the cells need to be better understood. A team from the "Transport Processes" department supports the design and optimization of the cells with novel shape optimization methods.

The fuel cell seems to be the ideal vehicle drive: quiet, clean and independent of oil. The hydrogen required for this can be obtained from green electricity via electrolysis. An electrolysis cell is similar to a fuel cell, except that the entire process is reversed: Using electrical energy, hydrogen is obtained by splitting water into hydrogen and oxygen. Among other things, a cell consists of two metallic plates (bipolar plates) and a membrane. "The flow dynamics of the bipolar plate are quite crucial for the performance of the cell ," says Dr. Christian Leithäuser from the "Transport Processes" department. "We want to design these in such a way that the oxygen produced is discharged sufficiently quickly to make the cell more efficient. To do this, we simulate a multiphysics problem and use shape optimization methods."

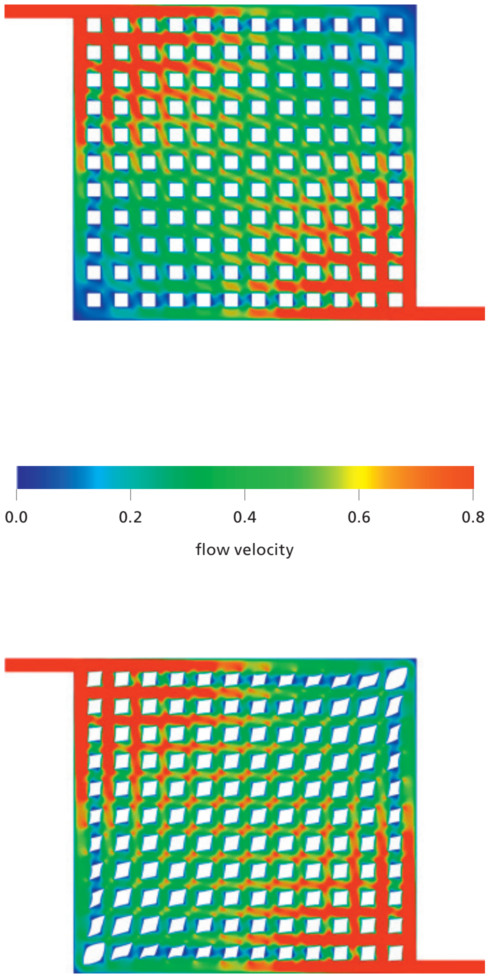
PhD thesis results in simulation tool CASHOCS for design

This topic of "designing bipolar plates for hydrogen electrolysis" was investigated in more detail by his colleague Sebastian Blauth in his doctoral thesis: "An open-source software package called CASHOCS was created based on my work," Blauth reports. This stands for "Computational, Adjoint-Based Shape Optimization and Optimal Control Software". "CASHOCS has since become a generic tool that we now use for the design of chemical reactor components." Similar issues arise in fluid dynamic stack design. Here, too, it is important that all cells are flowed to as uniformly as possible and without major pressure losses.

Example PEM electrolysis: Optimize free of dead zones

In Proton Exchange Membrane (PEM) electrolysis, water is supplied via the bipolar plate on the anode side. This is also split into hydrogen (H_2) and oxygen (O_2) by the supply of energy. The hydrogen migrates through the membrane and is collected on the cathode side. The resulting oxygen must be removed via the bipolar plate on the anode side so that the cell efficiency does not drop.

The bipolar plate should therefore always have an even flow – without so-called death zones from which the oxygen does not escape quickly enough. The graphic on the right illustrates the design with the CASHOCS tool. The reference design is shown above with the inlet in the upper left corner and the outlet in the lower right corner. The flow velocity is illustrated by the color scheme. In the lower left and upper right corners of the reference bipolar plate are death zones with poor flow. The bottom graph shows an already optimized bipolar plate. The tool's algorithm cleverly manipulates the reference geometry until the best possible uniform flow is achieved. The optimized bipolar plate is then free of dead zones.



Optimized stack design: Two bipolar plates before and after shape optimization. Blue areas are death zones with insufficient flow (reference above, optimization below).

In particular, such an approach with a digital twin opens up a detailed insight into the complex processes within the microstructures that would not be possible at all purely experimentally. Looking to the future: Implementation of the new design is now easily possible using additive manufacturing processes. The development results will thus flow into the next generation of electrolysis cells.

More about the focus "Fluid Dynamics Process Design"
www.itwm.fraunhofer.de/tv-process-design

More about the CASHOCS tool: www.pypi.org/project/cashocs/

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