Reforming a Fuel Cell Modeling Process

Coupling flow simulation with complex chemistry tools brings a united front to analyzing leading-edge energy systems.

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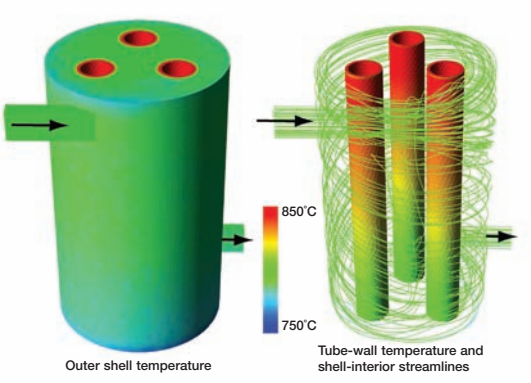
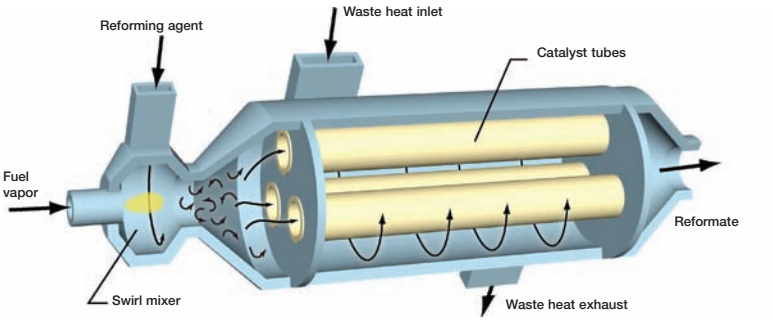
Since its basic principle was first demonstrated in the early nineteenth century, fuel cell technology has evolved into many different variations. The underlying mechanism common to all fuel cells is conversion of chemical energy into electricity by means of reforming the fuel into hydrogen along with the subsequent electrochemical oxidation of hydrogen into water. Depending on the type of fuel cell and its application, the fuel can be lighter hydrocarbons — such as natural gas, propane or methanol — or heavier liquids, like diesel or jet fuel. The key advantages of fuel cells over systems that burn fossil fuels include fewer moving parts and overall reduced pollutant emissions. Some of the challenges in developing fuel cells for more widespread use are the high cost of catalyst or other fabrication materials, the difficulty of hydrogen storage, and very complex chemistry.

Solid oxide fuel cells (SOFCs) in particular have been the subject of much research in recent decades: They have the ability to reform many different fuels, and their high operating temperatures offer the side benefit of using the exhausted heat energy. With support from the U.S. Office of Naval Research, a team from the Colorado School of Mines (CSM) has been working with ANSYS simulation tools to model the chemistry, electrochemistry and fluid mechanics of an SOFC stack system. Such a system — for example, an auxiliary power unit (APU) used by a Navy vessel — commonly comprises a shell-and-tube design that includes internal or external reformers, depending on the fuel. The endothermic steam-reforming operation is supported by circulating the exhausted heat energy from the exothermic electrochemical oxidation within the fuel cell. The complex catalytic chemistry is confined within the tubes, while the three-dimensional fluid mechanics of the air flow surrounding the tubes is complex but does not involve chemical complexity.

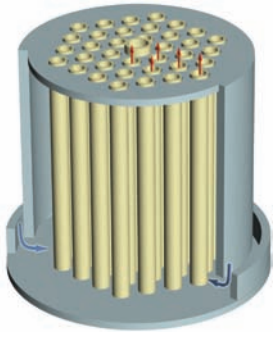


Results from the simulation of a shell-and-tube reformer simulation for the catalytic partial oxidation of propane in which an ANSYS FLUENT model of three-dimensional fluid flow and heat transfer is coupled with a CHEMKIN-based plug-flow model. Shown are the temperatures on the outside of containment shell (left) and catalyst tubes (right).

To evaluate the full anode-supported SOFC stack configuration — in which the anode side is the tube side and the cathode side is the shell side — the CSM team needed to couple the complex chemistry with the three-dimensional fluid mechanics. On the shell side, researchers considered the fluid flow



Conceptual configuration for a shell-and-tube reformer



Configuration of a 36-tube anode-supported SOFC stack

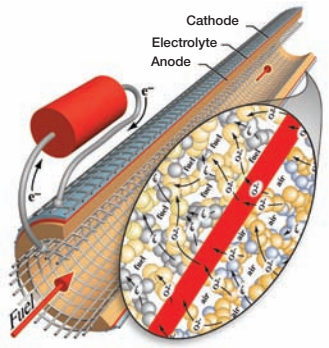
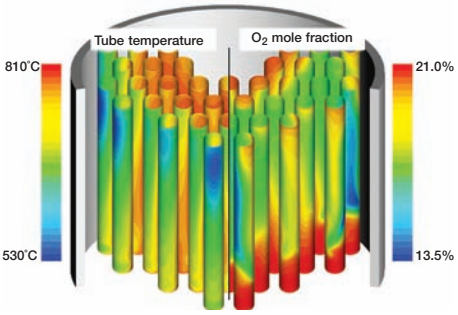


Illustration of a single anode-supported SOFC tube. Electric current is generated on the inside of the tubes (anode) and is discharged on the tube exterior (cathode). The balloon shows the essential microscale electrochemical phenomena in the porous composite electrode layers.



Results from modeling a 66-tube SOFC stack operating on a mixture of hydrogen, carbon monoxide and methane, which are produced by reforming hexadecane. The right-side tubes show gas-phase oxygen mole fraction on the tube surfaces. The left-side tubes show tube surface temperatures.

and heat transfer, including thermal radiation among all tubes and the containment shell. For this task, the team chose ANSYS FLUENT software (a component of the ANSYS Academic Research CFD product bundle) to model the complex, but nonreactive, fluid mechanics.

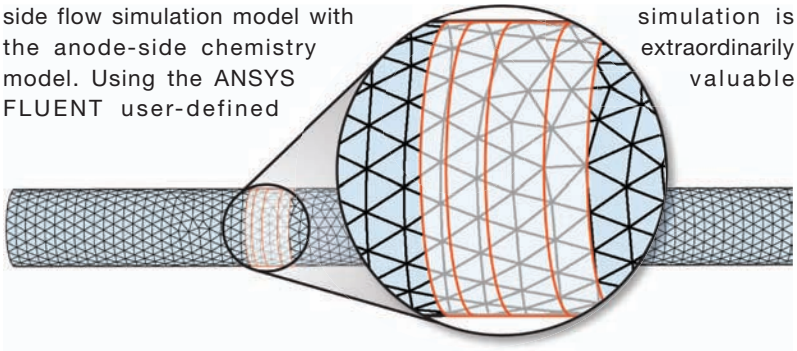
On the tube interior (anode) side, the simulation of chemical kinetics for reforming practical military logistics fuels — diesel in the case of an APU — demands hundreds of surface reactions and thousands of gas-phase reactions. One-dimensional chemistry tools such as CHEMKIN™ or CANTERA can handle the reaction kinetics and charge transfer, as long as the fluid mechanics can be modeled simply. In this case, the fuel reforming chemistry and charge-transfer electrochemistry inside the tubes are all complex, but the fuel flow is indeed simple enough and can be modeled in a one-dimensional tool as a plug flow.

The next aspect of the overall simulation process was coordinating the iterative coupling of the cathode-side flow simulation model with the anode-side chemistry model. Using the ANSYS FLUENT user-defined function (UDF) capability, the research team automated the process of averaging three-dimensional temperature and oxygen mole fraction data from the shell-side simulation and mapping it onto the tube-side band mesh. Additionally, the UDF directed the tube-side chemistry model to supply heat flux and oxygen mass flux boundary conditions from each of the tubes back to the shell-side fluid flow model.

Results of the simulations revealed that there can be significant temperature variations between different tubes. The tubes were generally cooler at the bottom, which was caused by a combination of internal fuel reforming and heat transfer to the shell-side air. Because the outer tubes acted as radiation shields, the inner tubes generally operated at higher temperatures. Shell-side air was introduced from below and exhausted at the top, and, therefore, the oxygen decreased from bottom to top.

When designing and optimizing a tubular SOFC stack, simulation is extraordinarily valuable because it is important for all tubes to deliver similar performance. The coupled model is useful for investigating the effects of design considerations, such as tube packing and air-flow alternatives, on the overall performance of the stack. However, since the tube interior geometries were not fully resolved in this research due to their complex microstructure, extensions to the work under consideration include performing detailed three-dimensional ANSYS FLUENT simulations of the charge transport through the porous anode material on representative tube volume sections to calculate the effective electrical conductivity. This microscale-effective conductivity could then be used as an input for the full one-dimensional tube-side simulation to further improve transport modeling inside the tubes, thus enabling the beginnings of a multiscale analysis.

The capability to couple complex flow and heat transfer using flow simulation with complex chemistry and electrochemistry is a powerful new tool for certain classes of reacting-flow problems. The CSM team developed the ANSYS FLUENT UDFs to be sufficiently general so that a range of one-dimensional chemistry tools could be incorporated. This approach to modeling tubular configurations can be useful beyond fuel cells, as it is directly applicable to geometrically related layouts, such as battery packs, nuclear fuel rods or cracking furnaces.



A three-dimensional ANSYS FLUENT face mesh on an SOFC tube with an overlying one-dimensional band mesh