COMPLETE MODELING OF kW-RANGE SOFC STACKS

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ABSTRACT

As planar solid oxide fuel cell (SOFC) stack development progresses and moves on from Watt-range single cells to commercially more interesting kW-range SOFC stacks, a need for adequate modeling capabilities arises to simulate these SOFC stacks properly. Commercially available tools for 3D modeling like Computational Fluid Dynamics (CFD) programs nowadays allow unstructured meshing for coding even complex design topologies. At the Forschungszentrum Jülich, the transition to the CFD tool Fluent was made. Initial stack models were composed of repeating single-cell units. This contribution also proposes a strategy for speeding up simulations of complete power plant cycles involving the CFD model and a spun-off 1D simplification.

INTRODUCTION

The development of the planar solid oxide fuel cell (SOFC) technology has been progressing over recent years worldwide. The aim of development becomes more and more to scale up the technology from the laboratory-type Watt range to the commercially much more relevant kiloWatt range. At the Forschungszentrum Jülich, an anode substrate-supported planar concept is under development featuring 20 cm by 20 cm (7.9 in. by 7.9 in.) cells with a metallic interconnector made of ferritic steel. It was possible to assemble and operate stacks as tall as 40 cells yielding 9.2 kW on hydrogen fuel and 5.4 kW on methane fuel, respectively (1). This progress brings about an increased need for modeling capabilities for large stacks so that their behavior can be studied and subsequent stack design improvements and SOFC plant operation optimization can be introduced more efficiently. Because modeling is a service that contributes to the overall system engineering efforts, modeling must be able to follow the way to larger stacks so it will remain able to deliver the required solutions. Within the scope of modeling must be both the stack and the power plant. Here the difficulty arises that it seems necessary to have a three-dimensional (3D) model of the stack, which requires so much CPU time that using this 3D model as a component in the flowchart of the overall power plant does not seem feasible. The present investigation proposes a strategy for looping a CFD-based concept for stacks and a corresponding one-dimensional (1D) spinoff to be used as a component for more rapid flow chart simulation of the entire SOFC system.
THE OBJECTIVES OF SOFC MODELING IN JÜLICH

The role of modeling in the overall design process from single-cell development to the design of fully operable kW-range SOFC systems at the Forschungszentrum Jülich is defined by the value it can add to the design and engineering activities of complete kW-range SOFC systems. Viewing SOFC modeling this way makes it very clear that it must meet the following requirements:

• Ability to reproduce laboratory results.
• Ability to meet demand rapidly—low turnaround time.
• Ability to perform transient simulations of full-scale kW-range stacks in three spatial dimensions.

While the first bullet is a necessity that does not require further discussion, it may be helpful to explain that the ability to turn around simulation inquiries (i.e., by the SOFC system engineering department) rapidly is important so that a parameter study can be finished in a reasonable amount of time. This will minimize the risk of creating a bottleneck in the overall engineering process.

The third bullet outlines that it is seen as inevitable at the Forschungszentrum Jülich to have a model that can simulate multicell stacks in the kW range in three spatial dimensions (3D) and the time. Hence it is not difficult to conclude that high computing time requirements of kW-range 3D SOFC stack models are not practical for use in power plant system simulations in which the SOFC is only one component. At the Forschungszentrum Jülich, it is planned to build and operate a 20-kW SOFC system and to use modeling extensively during the design and test phases, so ways to arrive at a lower turnaround time must be found. This paper proposes a co-simulation approach using a 3D structural model and a 1D behavior model.

STRATEGY FOR SIMULATING BOTH kW-RANGE STACKS AND SYSTEMS

It was decided to use the CFD package Fluent by the company Fluent Inc. at the Forschungszentrum Jülich in 1999. The decision to use a CFD package like this one was driven by the wish to be able to model the electrochemical performance of a kW-range stack, including its flow distribution in the manifolds. A CFD package like Fluent is able to model those flow fields in the cell planes as well as in the manifolds without further modification. However, the SOFC typical part of the model, which is the electrochemical kinetics and the internal reforming process, needed to be included separately. For customizations like this, Fluent provides an interface to include user-defined functions (UDFs), which must be written in the C programming language.

The availability of a model for complete stacks meant the door to modeling full-sized stacks—and even SOFC power plants—swung open. Because it became possible to model complete stacks, it could be justified to spin off a 1D simplification that made it possible to bring down CPU time to 10 to 30 seconds. This 1D model loses the information on the 3D structure of the SOFC stack, but, because it still contains the same equations and parameters (gradients simply reduce to simple derivatives in the x-direction, which stands for the flow direction in the gas channels), it can describe the
behavior of a Jülich-made SOFC stack accurately enough. This is why the 1D model is called "behavior model" and the 3D model implemented in Fluent is called "structural model" in Jülich. The behavior model can be used in flow chart software or plant simulation tools to efficiently screen operating parameters, flow chart design variants, etc., to find the best powerplant design for a given application. After that has been done, a simulation of the stack using the structural model with the interface results found by the power plant optimization can restore the integrity of the 1D simulation and the structural model.

The 1D Behavior Model

The 1D behavior model is obtained by omitting the width and height coordinates of the structural model. This leaves only the coordinate along the gas channel. It is obvious that the internal manifolds and the spatial orientation of the fuel and air supply and exhaust pipes cannot be modeled any more, so it is assumed that the contribution of the overall heat transfer in the stack mostly comes from the flow through the gas channels and that the manifolds can be neglected. It is because of this rather crude simplification that the 1D behavior model can be questioned quite easily if it is not backed up by a structural model. The possibility to spin off such a greatly simplified 1D model hinges on the fact that the stack design is either a co- or a counterflow one. In case of a similar cross-flow design, the behavior model must be at least two dimensional. As mentioned above, the set of differential equations needed to describe the electrochemical and chemical reactions stays the same, which makes the structural and behavior models consistent. The big simplification is that the spatial derivatives need only be taken in the gas channel direction. As of October 2002, a stationary 1D behavior model for the Jülich design is available as a Matlab implementation, and the next goal is to extend that to a transient model as well. The current Matlab-based stationary behavior model typically runs between 20 and 30 seconds. This model can certainly be implemented in other programming languages as well. To accelerate the runtime of the system simulation even more, the SOFC behavior model could be rewritten in compiler-based programming languages like C or Fortran. At the Forschungszentrum Jülich, the NAG library is available for Fortran 77, 90, and C under different Unix systems including Linux. This option is currently evaluated for creating programs executing very rapidly on different platforms.

RESULTS AND VERIFICATION

Comparison of Five-Cell Stack Simulations with a Test Run

Figure 1 compares a modeling run based on the CFD model, denoted by the solid line, and experimental results, denoted by the boxes and circles. The experiment was conducted in December 2001 using the standard Jülich anode-supported cell design with a ferritic steel interconnector plate. The so called E-design stack consisted of 10 cells, 20 by 20 cm. Holes for thermocouples were drilled in the interconnector plates #3 (circles) and #8 (boxes), where the enumeration started at the top of the stack. The stack operated with 35 L/min of hydrogen containing 3% water vapor at a furnace temperature of 825°C. The cathode was supplied with 100 L/min of air. For convenience of computing time, the experimental data of the 10-cell stack was modeled with a five-layer stack simulation.
As shown in Figure 1, the results agree quite well with the measurements. It is certainly desirable to improve the agreement between the measurements and the simulation runs further, but the point to be made here is that it is possible to simulate planar SOFC stacks using the described CFD-based model and verify the results with measured values.

Application of the 1D Behavior Model

Figure 2 illustrates a run of the stationary 1D behavior model. While a complete run of a 3D Fluent simulation takes several hours, the 1D behavior model finishes its run in 20 to 30 seconds. The simulation was based on data that could be representative of a 20-kW unit running on a fuel mixture of methane and steam. The corresponding steam-to-carbon ratio was 2 moles steam per mole of methane assuming complete internal reforming. The current density was assumed to be 300 mA/cm² at a fuel utilization of 80%. This resulted in a calculated terminal voltage of 0.71 V. The methane-steam mixture flows from left to right, entering at 550°C while it is being internally reformed (dashed-dotted line), and the air flows from right to left (dashed line), also entering at 550°C. The air excess ratio related to the methane in feed was 2.5, and the operating pressure was 100 kPa absolute (0 kPa gauge). The solid line is the temperature of the bipolar plate. Additionally, lines for the minimum temperature of the bipolar plate, 685°C, its mean temperature of 779°C, and its maximum temperature of 836°C were included, emphasizing the fact that considerable temperature differences may exist along the gas channel length. As well, whereas the temperature of the bipolar plate is at least 685°C, the supply gases can enter the SOFC much colder even if all the methane is to be reformed internally (in this case 550°C was assigned to both the fuel mixture and the air, as mentioned above). This simulation also shows that the flow of cool air streaming in from the right at a stochiometric air-to-fuel ratio of 2.5 cools the stack more than the internal reforming reaction on the left. Toward the middle of the gas channel, a temperature maximum of about 836°C is reached by the bipolar plate through the heat production due to the electrochemical oxidation of CO and H₂. This maximum temperature must be compared.
with the exit temperature of the air, roughly 730°C, and the exit temperature of the (depleted) fuel mixture, 685°C. This shows that the temperature of the interconnector may be locally much higher, so the air flow and both the fuel and the air entrance temperatures must be carefully chosen to avoid damaging the stack by local overheating.

The local overheating effect can be amplified by using interconnector materials with lower heat conductivity or using thinner interconnector plates. This result cannot be obtained by thermodynamic energy balance calculations because that cannot deliver the spatial resolution. Hence, a simple 1D SOFC model may be preferable over just energy balance-based approaches even for stationary power plant simulations. Figure 3 shows the species concentration profile (corresponding to Figure 2) along the gas channel. It can be seen that the initially present CH₄ is reformed quite rapidly, leading to a steep increase in the H₂ mole fraction. The H₂ peak is then shaped by the electrochemical oxidation that starts shaving off hydrogen.
CONCLUSIONS

The development of planar SOFCs has been progressing for the last couple of years so that assembling kW-range stacks has become possible. The technology is now reaching a stage where kW-sized prototype systems are being developed. SOFC modeling has always delivered an important contribution to the overall R&D efforts. As the technology is advancing from R&D to the engineering stage, it becomes increasingly important that SOFC modeling can simulate these new kW-range stacks consisting of 60 cells and do it more efficiently. As a result, the computational effort can become so great that simulation runs may become inefficient because the grid size of the resulting models becomes too big. This paper has shown that it is possible to reach a high turnaround frequency of simulation runs by a spun-off 1D behavior model designed for use in flow chart simulation tools to enable rapid design and operability screening for complete SOFC systems. It is the vision at the Forschungszentrum Jülich that this efficiency increase will help ensure that rapid SOFC development progress can be maintained in the future.

REFERENCE

1. A New Milestone in Fuel Cell Research was Reached, Press Release, Forschungszentrum Jülich GmbH, April 2002.