Multi-scale Modeling Methodology for Computer Aided Design of a Solid Oxide Fuel Cell Stack

Diego Larrain, François Maréchal, Nordahl Autissier, Jan Van herle, Daniel Favrat
Lab. for Industrial Energy Systems (LENI), Institute of Energy Sciences, Faculty of Engineering. Federal Institute of Technology (EPFL). CH-1015 Lausanne, Switzerland.

Abstract
This paper presents the multi-scale modeling strategy developed for the design of a solid oxide fuel cell (SOFC) stack. Around the main models which are the repeat element model (in simplified 2D and CFD), specific model for experiments have been developed to identify key parameters for the main models. Features of the different models used are presented. The CFD model and the simplified 2D model are compared in their sensitivity on transport properties and operating parameters. Results of the multi-objective optimization performed on the repeat element design parameters are presented.

Keywords: multi-scale model, design optimization, solid oxide fuel cells

1. Introduction
Conception and development of a solid oxide fuel cell stack is a challenging task involving many aspects such as materials, assembly, fluid flow, thermal management. In fact, a stack and its base component, the repeat element, is essentially a chemical reactor which can be optimized and improved. Materials improvement and processing is not discussed here. Design goals are to reach good performance (power density) and reliability (ie. limited risk of failure and degradation) under some constraints. This problem, involving multiple physical phenomenon, different scales (from the pores of the catalyst to the interactions of the fuel cell with the system), is addressed with a multi-scale modeling approach.

In the following, the methodology and main features of the models are presented, then a comparison of the outputs from the simplified 2D model and the CFD model is performed and finally first optimization results of a repeat element configuration are shown.

First, the basic principle of a fuel cell system and repeat element is presented.

1.1. The SOFC planar stack
A solid oxide fuel cell is essentially a membrane based chemical reactor on which electrochemical reactions allow production of electric power. The cell is composed of three layers (the two electrodes and an electrolyte): on the cathode oxygen from air is reduced to oxygen ions, the electrolyte is a gas tight ionic conductor, on the anode fuel (either carbon monoxide or hydrogen) is oxidized. This redox reaction involves a charge transport and therefore a current, the useful operating potential is essentially related to the electrolyte and electrode quality.

A solid oxide fuel cell stack is an assembly (connected in series) of a base element called repeat element. The repeat element is composed by different layers: a metallic interconnect, a gas channel for the fuel, a cell on which the electrochemical reaction occurs, a gas

1Author to whom correspondence should be addressed: diego.larrain@epfl.ch
channel for the air, and finally a second metallic interconnect. A scheme in 2D of our repeat element is shown on figure 1, the general pattern is a counter-flow, the non reacted fuel is burned at the fuel outlet.

2. Methodology and tools developed

A fuel cell stack is a complex system involving several phenomena such as electrochemical reactions, fluid flow in the two gas chambers, heat transfer between the different layers of the stack by convection, radiation and conduction, and interactions with the surrounding environment and system components. Dimensions of the element are of different order of magnitude as channel are in the order of 1mm, the length of the cells around 10 cm.

A single model handling the complete geometry and all the phenomena is unmanageable with the current state of the art (Gubner et al. [2003]) and leads to extremely long CPU time. The problem can then be tackled with several complementary models (see on figure 2). The main model developed is the repeat element model (ie. the basic element of a fuel cell stack), this model has been developed with two different tools, gPROMS and Fluent (Autissier et al. [2004]). Essential information on the kinetic parameters is provided by experiments which have been modeled to perform parameter identification (Larrain et al. [2003]).

Other simple models are designed for specific experiments to identify other parameters (like Darcy coefficient for the fluid flow). As the repeat element itself is part of a stack, a stack model is used essentially to define more realistic boundary conditions than the usual adiabatic conditions. CFD models in 2D are used to solve the flow distribution through the height of the stack. The simplified 2D model of the repeat element is finally used to
run multi-objective optimization with the Queuing Multi Objective Optimizer (QMOO) algorithm (Leyland [2002]).

2.1. The repeat element models
The simplified model is developed with the gPROMS package. The model is based on a simplified description of the flow pattern in 2D (which is necessary with punctual inlet configuration). Fuel and air side have their own description of the flow field (Larrain et al. [2004]). Energy equations for the fluids and solids allow computing of the temperatures. The solid is considered as monolithic with volume averaged transport properties. Electrochemical reactions are computed with parameters identified from experiment. Boundary conditions applied are radiation on the side of the cell and no heat transfer in the height of the cell. This model allows to compute an operating point in 1 minute and to carry out sensitivity study (with ca. 20 points) with CPU time below 15 minutes on a regular P4 (1.4GHz) computer under Linux. The CPU time is highly dependent on the mesh used. The CFD model has been developed in Fluent with a mesh of ca. 100 000 cells for the solid and the fluid parts. The electrochemical reactions are computed with user defined functions. This model allows simulation of an operating point in 10 to 20 minutes once initialized. The bottleneck in CFD is essentially on the mesh preparation which is time consuming.

The figure 3 shows the output of hydrogen concentration given by the simplified 2D model. Figure 3(b) shows the temperature field for an adiabatic case.

![Figure 3. Model outputs, all cases @ 1045K operating temperature, 28A total current and 70% fuel utilization](image)

The model used for parameter estimation of the kinetics is adapted from the repeat element model. The algorithm used for parameter estimation is included in the gPROMS package. However, the future use of genetic algorithm is been considered. Optimization of the repeat element is performed with the simplified 2D model. The interfacing between the model and the QMOO optimizer has been realized with a c++ code. The model used is the regular repeat element model with a lower mesh definition. Simulation of each case takes around 20s. The total time for optimization is then quite important as 3000 to 6000 simulations are required for sufficient convergence. Attention must be
paid to the model developed; simplification is a way to reduce CPU time but one has to verify whether trends and responses to each of the optimized variables remains the same.

3. Results

3.1. Comparison of CFD and gPROMS models

Electrochemical performance of the repeat element predicted by both models is close, not surprisingly as both use the same kinetic parameter. Comparison on other outputs such as temperature profiles and sensitivity to parameters important for the energy balance is presented here.

The first case is the comparison of response to the air stochiometric ratio change of the 2 models. This has been tested at two different operating points: at 200 ml/min hydrogen with 14 A of total current and at 300 ml/min hydrogen with 23.5 A of total current. Temperature of operation was set to 1023 K. The cell surface assumed was 52cm². The air excess ratio has been varied from 1.5 to 6.

The temperature profiles along the symmetry axis show a satisfactory agreement (see on

![Figure 4. Temperature profile comparison along the symmetry axis and sensitivity air flow rate](image)

(a) profile comparison for the 2 models  
(b) sensitivity to air flux

Figure 4. Temperature profile comparison along the symmetry axis and sensitivity air flow rate

As CFD has a finer mesh (ca. 600 nodes versus 36 on that axis), details of the inlets are more accurately described. The simplified model underestimates the temperature of ca. 10K.

Figure 4(b) and 5(a) shows the results for the sensitivity to the air flux and the change of the maximum temperature point coordinate. The response to the flux change is quite similar whereas for the position of the maximum temperature point, the simplified model overestimates the change in position. This comes from the inlet region definition. Sensitivity to the interconnect conductivity is presented in the figure 5(b). The response of both model is the same but the temperature is underestimated by the simplified model.

This comparison gives confidence on the use of the simplified gPROMS model for sensitivity studies and optimization of design parameters as the trends simulated by both models are the same. Therefore, the use of CFD could be focused on the optimization of fluid pattern and its detail while the general flow pattern, thermal parameters and operating point can be explored with the simplified model in gPROMS.
3.2. Optimization results

Goals of solid oxide fuel cell research and development are performance increase (in terms of efficiency, power density) and limitation of degradation. These goals are conflictive as power density tends to increase temperature gradients and maximum temperature, and that most of the degradation processes are accelerated with temperature. The trend between these two objectives could be shown performing a sensitivity study on each of the variables. However, in order to find the best solutions for all decision variables, an optimization algorithm is required.

Optimization has been performed on a counter-flow repeat element configuration with two sets of objective functions. The first set is: maximize the power density per unit volume and minimize temperature difference. The second set is: maximize the power density and minimize the maximum temperature on the cell.

The constraint on the problem is a power output of 18W. The design variables are the cell area, the interconnect thickness, the pressure drop target on the air side, the aspect ratio of the cell, the air ratio. The operating variables are the operating temperature and the fuel flow.

The Pareto optimal front obtained in the 2 cases is presented on figure 6. It is interesting to notice that it is feasible to have a quite high power density (higher than 1W/cm³ with a reasonable temperature gradient, or maximum temperature.

On the characteristics of the optimum solutions for the case minimizing temperature gradients, it is worth noting that all the solutions except the very compact ones uses an operating temperature at the higher bound. This can be explained as increasing the temperature reduces the resistances to reaction and leads to more homogeneous distribution of current and temperature. Fuel flow is mostly on the upper bound as well as here the constraint is on the power output and not on the efficiency, again running the cell at higher fuel flow gives less gradients. Having the efficiency as the constraint would probably give different result. Finally, it appears that optimization is a tool which allows to determine
Figure 6. Pareto optimal fronts for a repeat element delivering 18W with pressure drop on the air side in the range 20 to 30 mbars and for 2 sets of objective functions

the best configuration for some given parameters, but the answer is strongly dependent on the goals and definition of the problem.

4. Conclusion

The use of a multi-scale modeling approach for SOFC repeat element design allows to simulate performance and predict behavior of existing systems, run sensitivity studies, and optimize design and operating parameters with a simplified 2D model. This model has demonstrated consistency and good behavior comparing the outputs with a more detailed CFD based model for the same situation.

The 2D model, is now extended to other configurations, to transient behavior modeling and to the modeling of indicators for degradation during operation. The CFD model will be extended to explore further details on fluid patterns and to be combined with a solids model for stress analysis, which cannot be performed with the output data coming from the simplified model as the spatial resolution is too low. To reduce the computing time, parallel computing is being applied to the CFD model and optimization.

References


