MODELING OF CROSS-FLOW STACK: SENSITIVITY TO THERMAL PROPERTIES OF THE MATERIALS

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ABSTRACT
LENII activities in SOFC are focused on the development of a new planar stack concept based on anode supported cells in collaboration with the company HTceramix SA. Modeling of repeat element, stack and systems is starting in parallel. This work presents a model of a SOFC stack in cross flow configuration. Concentrations, temperature and current density fields are computed, with a focus on sensitivity study for thermal parameters, while operating parameters are kept constant for the different cases. The main parameter considered was the thickness of the metallic interconnect and the related thermal conductivity. Stack height and cell size effects are presented as well. Importance of the temperature field on the design point and degradation behavior is briefly discussed.

INTRODUCTION
In stack development, modeling can play an important role, allowing comparison of different configurations (in terms of materials, cell size) and aid the decision in choosing one option from another. In the framework of a stack development project (1), a stack model aiming to represent the behavior of the repeat elements and stacks is being defined. The cross-flow configuration model is a first step towards that goal as it allows comparison of results with the available literature (2-4). A model for our repeat element configuration is in preparation.

Adiabatic boundary conditions are assumed most of the time for the repeat element model. The validity of this assumption will be discussed here using stack results. From the cross-flow repeat element model, the third dimension has been added to be able to compare different stack heights and thermal transport properties. Results for stack previously published (5) show that adiabatic conditions on the middle cell are reached for a 10-cell stack. Comparison between a stack with ceramic bipolar plate and a one with metallic bipolar plate shows this is the case for a ceramic bipolar plate (2) but not for the metal plate case.

Our repeat element is based on anode supported cells, The temperature range allows to work with Fe/Cr steels as bipolar plates. With the aim to reduce the repeat element
volume and the cost, the interconnect thickness tends to be reduced. This work presents how the temperature field on the cells vary with a change in interconnect thickness.

Before presenting the results obtained on several stack heights and cell sizes, the base equations of the model are presented.

MODEL

Energy Balance Equations:

The model is based on the well known cross-flow design (2). It has been implemented in gPROMS modeling environment (6). The model is based on a set of energy and mass balance equations. Each of the fluids (i.e. fuel and air) has its own energy balance equation. The solid is considered as monolithic and the transport properties are averaged on the volume. As we consider a stack with several cells (from 11 to 51 cells), the energy equation for the solid takes account of heat conduction through the height of the stack (z direction). For the moment, the case with hydrogen/water mixture is considered on the fuel side.

The energy equation for the solid describes a local balance based on the heat conduction equation with source terms:

\[ \lambda_{st} \frac{\partial^2 T_{solid}}{\partial x^2} + \lambda_{sx,y} \left( \frac{\partial^2 T_{solid}}{\partial x^2} + \lambda_{st} \frac{\partial^2 T_{solid}}{\partial y^2} \right) + \sum \dot{Q} = 0 \]  

where \( \sum \dot{Q} \) is the sum of the volumic sources: the heat of reaction released, the electric power removed and the heat transfer to the gases. The thermal transport properties \( \lambda_{st} \) and \( \lambda_{sx,y} \) (in \( \text{W/mK} \)) are averaged on the volume.

The thermal property of the cell itself is computed using a model for the thermal conductivity of the anode cermet (7). The thermal properties of the cermet Ni/YSZ are very sensitive to composition and porosity. Between 32 vol\% Ni and 44 vol\% Ni, and the corresponding porosities, the cell conductivity varies between 4.4 \( \text{W/mK} \) and 10 \( \text{W/mK} \). For the anode supported cell, as the electrolyte is much thinner than the anode (by a factor of ten as least), the cermet dominates the heat conduction (conductivity of the yttria-stabilized-zirconia YSZ is only 2.8 \( \text{W/mK} \)).

The energy equation for the gases is implemented with the same idea performing a local enthalpy balance and considering heat transfer with the solid. The general equation is:

\[ \sum \chi_i C_{pi} \left( v_x \frac{\partial T_{gas}}{\partial x} + v_y \frac{\partial T_{gas}}{\partial y} \right) = \frac{h_{gas}}{L} (T_{solid} - T_{gas}) \]  

where \( \chi_i \) is the molar fraction of the species, \( C_{pi} \) the heat capacity of the species, \( v_x \) and

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Figures 1 and 2 show the temperature profiles for the mid cell of a 21 cells stack with low and high conductivity, respectively. The gas velocity, \( v \), and the gas channel height, \( L \), are indicated.

The heat transfer coefficient, \( h_{gas} \), is computed from the Nusselt number for a laminar flow. As this paper focuses on the thermal gradient and its sensitivity to some geometric parameter, the kinetic model is kept simple with an overall resistance taking into account the sum of the activation and ohmic losses. This resistance is a function of temperature. The local current density is computed from the Nernst equilibrium potential and the actual cell potential with the equation:

\[
U_{cell} = U_{Nernst} - R_{ohm}j
\]

[3]

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This equation is applied to each cell in the stack. As the total current is conserved on the height of the stack, the potential of each cell is computed to obtain the same current integral on each cell. Temperature fields on the middle cell of a 21 cell stack are shown in Figures 1 and 2.

**Boundary Conditions**

The boundary conditions assumed have an influence on the temperature profiles. On the sides of the stack, radiation to the environment is assumed. This same condition is applied to the top and the bottom cell of the stack. In real test set-up, the stack is held between two flanges; then, the repeat elements stack bottom and top are not directly exchanging heat with the environment. As the flanges are made of Inconel, they are conductive enough and the error introduced by this assumption may not be too important. The gas inlet temperature on both air and fuel side is set to the environment temperature and is the same for all the cells of the stack. This simplification, with the symmetric boundary condition, leads to a symmetric temperature profile on the height of the stack. Modeling of preheating of the gases, as well as consideration of the top and bottom flanges, will be implemented in further work.

**CASE STUDY**

This section aims to study the sensitivity of the thermal profile of the stack to the interconnect thickness, which plays a major role in the thermal transport properties of the solid (the properties being volume averaged). In the plane direction, the cell and the interconnect share the heat conduction process, as the interconnect becomes thicker compared to the cell the conductivity increases. The variation is high in the plane (by a factor close to 2.5). In the z direction, the conduction is dominated by the nipples that are machined in the interconnect, which represent at least 50% of the path length in this direction, this explains that the conductivity in z direction is less sensitive to the interconnect thickness (25% variation). Some values are summarised in Table 1.

The effect of the contact interfaces on conduction is neglected, and as for electronic conductivity, those interfaces play a major role. This may lead to overestimation of the thermal transport properties.

**Table 1. Conductivity in plane x,y and in z direction depending on interconnect thickness.**

| Thickness in mm | \( \lambda_{x,y} \) in W/mK | \( \lambda_{z,z} \) |
|-----------------|-----------------------------|--------------------|
| 0.3             | 2.85                        | 5.65               |
| 0.7             | 4.65                        | 6.15               |
| 1               | 5.75                        | 6.55               |
| 1.5             | 7.15                        | 7.10               |

Comparing stacks of different height and different cell sizes may not lead to useful results if attention is not paid to the modeling cases. The following approach has been used: for...
each of the simulated case, the same average current density (0.3A/cm²) and fuel utilization (77%) has been fixed, this is made by adapting the current and flow rate per cell in the input values for the model. For the cell size of 100 cm², cases have been run for stacks from 11 to 51 cells. For the other cell sizes, comparison is made on the basis of the 31 cell stack. Table 2 summarizes the different cases and inputs to the model.

The dimensions of the repeat element are:

- anode, electrolyte and cathode respectively of 250, 6 and 50 μm thick; both electrodes are 50% porous
- the current collectors are square nipples of 1000 μm height, the surface coverage is 30%
- interconnects are Fe/Cr steels sheets of 0.3 to 1.5mm thick.

Table 2: Model parameter variation.

| Parameter         | Case                        |
|-------------------|-----------------------------|
| air excess        | λ=5                         |
| env. temperature  | 1000 K                      |
| hydrogen flux     | 1.28e-4 mols, 2e-4 mols, 2.88e-4 mols |
| current           | 19.2 A, 30 A, 43.2 A        |
| number of cells   | 31, 11, 21, 31, 41, 51      |

RESULTS AND DISCUSSION

This section summarizes the results for the numerous cases that have been simulated. First, sensitivity to the thermal properties and height of the stack is presented.

Sensitivity to the Interconnect Thickness

As the conductivity of the cell changes, the temperature profile changes, the maximum temperature decreases (see Figures 2, 1) and the location of this maximum tends to be closer to the center of the cell when conductivity increases. To compare the different cases, the temperature on the center of the cell has been reported for the whole range of thermal conductivity and different stack heights (Figure 3). The temperature at the same location is reported for a 31 cell stack to determine the difference between a border cell, an intermediate cell (# 7) and the middle cell (figure 5). Figure 5, together with Figure 4, show that even for a 51 cell stack, with such a conductivity on the z axis, no adiabatic boundary conditions are found. The maximum temperature profiles show no region of constancy within the height of the stack.

In the plane, the situation is different, the maximum temperature difference from edge to center of the middle cell amounts to 120, 80 and 50 K respectively for a 51, 31, and 21 cell stack. Bearing in mind that the minimum temperature is around 1025 K, the maximum temperature difference changes from 250 to 130 K for a cell within a 51 cell stack by varying the interconnect thickness. In other words, an increase by a factor 2.5 in thermal conductivity decreases the thermal gradient by 50%.

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Figure 3. Sensitivity of temperature to the thermal conductivity.

Figure 4. Maximum cell temperature depending on z (right half is for low conductivity, the left half is for high conductivity).
Temperature sensitivity to the position in Z

Figure 5. Sensitivity of temperature to the conductivity, for 3 different stack cells in a 31 cells stack.

Sensitivity to cell size

Cell size is also of importance for the thermal gradient. The larger the cell, the larger the amount of energy (both electric and thermal) produced per cell. For a given cell size change, the area changes with square of the length change, but not the area that exchanges energy with the environment (the edges). This leads to an increase in maximum temperature found in a larger cell. To try to quantify the variation, Figure 6 represents the temperature profile on the coordinate passing through the cell center and following the fuel path for a 31 cell stack in the case with low conductivity. Profiles are quite similar in shape, but the maximum temperature changes significantly with 1170, 1230 and 1260 K for the 64, 100 (reference size) and 144 cm² cell size respectively. An increase of around 50% in the cell size increases the maximum temperature difference at least by 20%.

Figure 6. Temperature profiles for 3 cell sizes.
Discussion

From the previous section, some important elements can be highlighted. First, for the dependence on stack height, this study shows that for the cases simulated here, stacks are not adiabatic and short stacks (11 cells) have low temperature gradients. Second, the thickness of the interconnect is an important parameter in the conception of a stack, together with the cell size, the operating point and the air ratio. It determines the thermal gradients and maximum temperature.

The study shows results for a quite moderate average current density (of 0.3 A/cm²). Of course the effect of current density is extremely important and will have to be quantified. Nevertheless, the trends that have been revealed would be the same for other current densities. The number of parameters that affect temperature profiles is important and sensitivity studies should be carried out on each one of them. To compare the effect of most of them, a repeat element model with adiabatic boundary conditions or boundary conditions derived from the present study gives enough information and uses less CPU time (the sensitivity on interconnect thickness for the 51 cell stack takes a few hours to be performed). Formal optimization could be a way to a solution, but this requires the definition of an objective function, which is not obvious.

The limit to the thermal gradient that cells can stand is not known precisely, and a value is therefore difficult to fix. Another phenomenon affected by temperature differences is the degradation of materials and particularly the metallic interconnect. This phenomenon may be easier to quantify. To achieve the goal of low performance degradation on long term operation, this aspect will have to be studied.

CONCLUSIONS

A model for a stack in cross flow configuration has been developed and has allowed to carry out a sensitivity study of the temperature profile to the thickness of the metallic interconnect for several stack heights and cell sizes. The results have confirmed the interest in the concept of anode supported cells with metallic interconnect, in terms of stacking possibility: a 50 cell stack has no adiabatic cell and thermal management is easier than in an electrolyte supported cell stack. The cell size has to be considered carefully with other parameters and it has a strong influence on temperatures profile.

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