Stack and cell modelling with SOFC3D: a computer program for the 3D simulations of solid oxide fuel cells

Michel Bernier, Raphaèle Herbin
Université de Provence, France,
Etienne Gehain,
Gaz de France, France

1 Introduction

SOFC3D is a computer program, which simulates the behaviour of a solid oxide fuel cell under permanent load. The computation of the local distributions of the electrical potential, the temperature and the concentrations of the chemical species is performed. The physics of the cell and the simplifying assumptions are presented, and a sketch of the numerical procedure is given. The numerical results show the behaviour of the potential, temperature and current distributions when certain parameters (geometry of the cell, electrolyte materials, temperature in the channels) are varied. Numerical simulation is also used to obtain an optimum for some geometry parameters such as cathode thickness or rib width. The radiation effects are taken into account. Some of the cell simulations are used in STACK3D, a 3D simulation code of the stack, which is currently being developed.

2 Numerical model of a cell

2.1 The mathematical model

A detailed cell model was obtained [9] by writing the conservation laws in the solid parts of the cell for heat, electrical current and mass, and the conservation of heat and mass in the air and fuel channels. The unknowns of the mathematical model are the temperature T at any point of the solid or the channels, the electrical potential Φ at any point of the solid part of the SOFC, and the molar fractions X_i of the various species ($i = O_2, H_2, H_2O, CO, CO_2, CH_4$) at any point of the channels and in the porous media of the solid part of the cell. Writing the constitutive laws for the various fluxes yields a coupled system of nonlinear elliptic equations, the detail of which may be found in e.g. [9], [5].

2.2 The numerical procedure

The necessary step in order to perform a numerical simulation of both cell and stack is to discretize the set of equations. The diffusion equations which hold in the solid part can be successfully discretized by any of the usual methods, i.e. finite differences, finite element or finite volumes. However finite volume discretization (see [8] for an introduction) was preferred over the finite element method because it is computationally cheaper, as can be seen in the results shown in [7]. It is also easier to take into account the coupling between the diffusion equation in the solid parts and the convective transport equations in the channels.

The discretization of the equations yields a nonlinear finite system, where the unknowns are the average values (over the control volumes) of T, Φ and X_i. The equations in T, Φ, X_i are coupled by the electrical conductivity (which depends on the temperature), the ohmic source terms and the interface source terms, both in T and Φ. A rather straightforward iterative method is used, which computes, for a given temperature, the solution to the mass and electric problems (X_i and Φ), and once convergence is obtained, solves the temperature problem. Note that the radiative terms imply an inner iteration for the solution of the 4th order nonlinearities in temperature.

2.3 Description of the computer program

The computer program consists of two parts. The first part is the computational kernel and database manager. It was written using the C language and contains 11000 lines. It has been used on several UNIX systems: Silicon Graphics, SUN, CRAY. The database input file contains the parameters which define the geometries (planar, cylindrical or tubular), the composition of the fuel (hydrogen or methane), the computational mesh and the set of operating conditions. A user-friendly graphic X interface has been developped. which includes a user-friendly mesh generator and a 3D-graphics post-processor. The results which are presented here were obtained on a INDIGO SG worksation with a 50MHz R4000 processor and 32 MB of real memory. The database file requires about 100 MB of disk memory.

3 Using the code as a design tool for the unit cell

We present here some uses which can be made of the code for the simulation of a unit cell. The code can simulate a cell using pure hydrogen only, or using methane with internal reforming. The operating parameters for both cases may be found in [9] or [5].

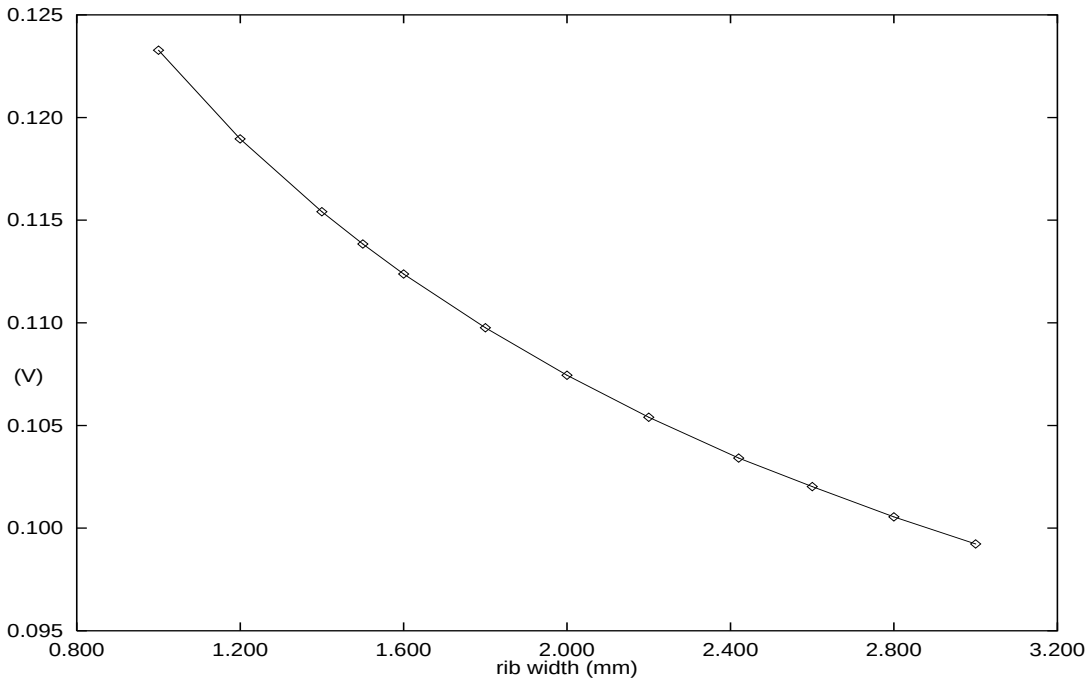

Figure 1: Ohmic loss vs rib width

3.1 Influence of rib width on overall efficiency

The conducting material between two channels is generally called the rib. The rib width seems to be an important parameter for the efficiency of the cell:

- on one hand, the wider the rib, the smoother the electrical current. Hence a wider rib will give a better conduction of the electrical current and less ohmic losses.
- on the other hand, the wider the rib, the narrower the channel; when the channel width decreases, the chemical species do not diffuse as well underneath the rib.

Therefore the numerical code can be used to check if an optimal value can be obtained for the rib width. The numerical results confirm the competing effects: when the rib width increase (with all other parameters fixed), the ohmic loss decreases (Figure 1), but the potential jump also decreases (Figure 2). With all other parameters fixed, an optimal rib width of 2.2 mm is obtained, as indicated on Fig. 3.

Influence of electrode thickness on efficiency

We study here the influence of the electrode thickness on efficiency of the unit cell. It is clear that a thicker interface electrode will be more resistant to the diffusion of

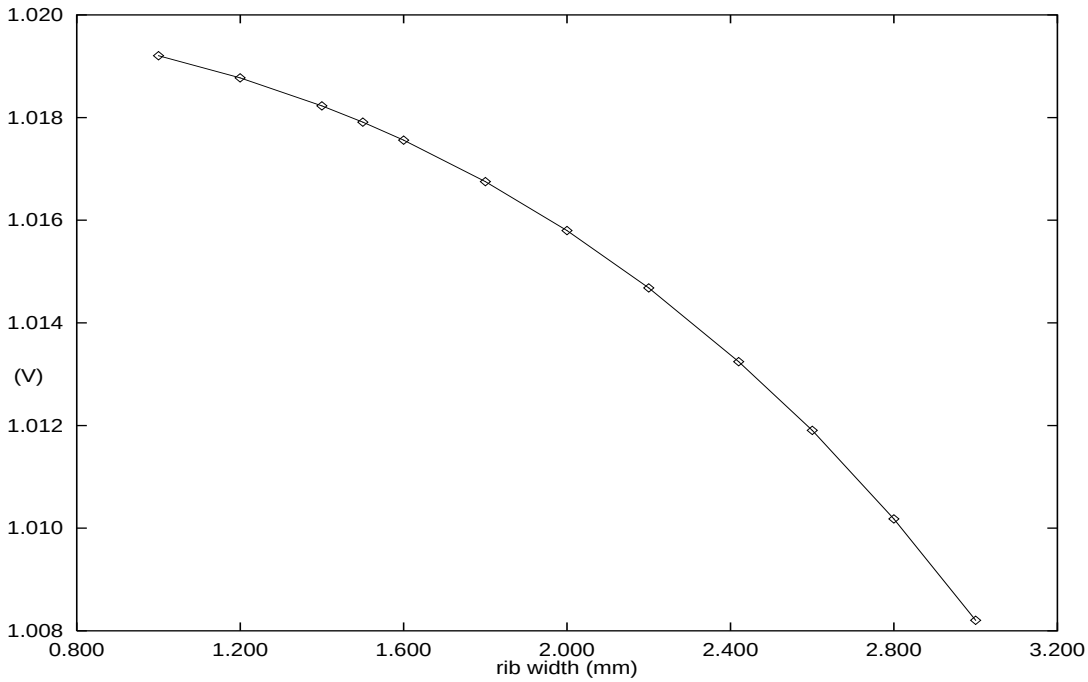

Figure 2: PEN potential jump vs rib width

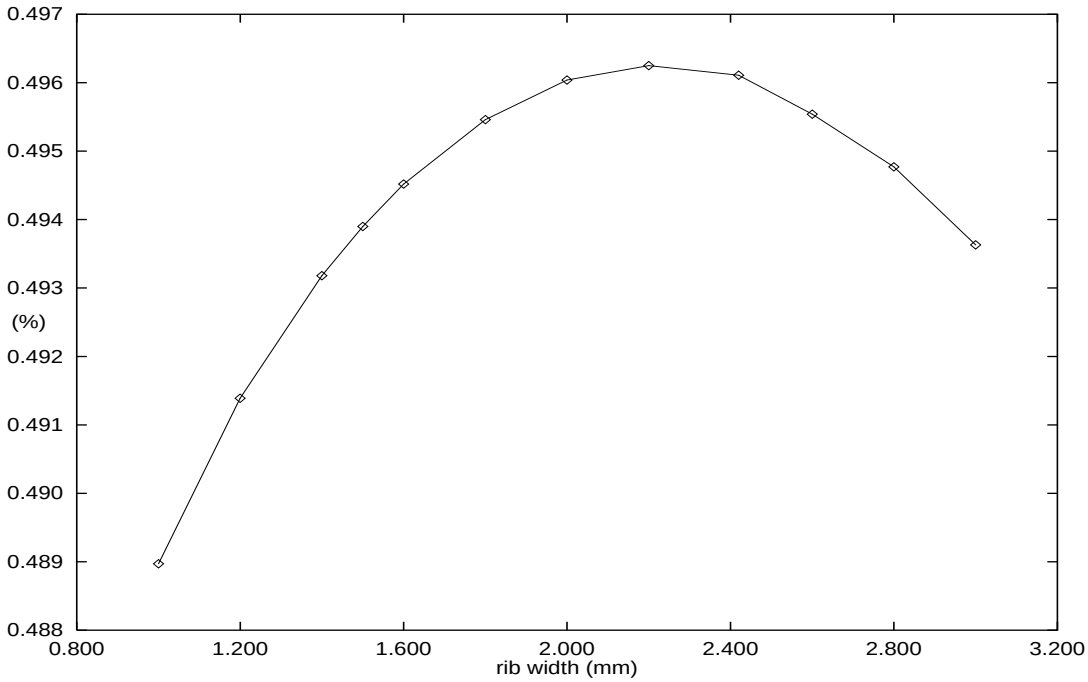

Figure 3: Efficiency vs rib width, pure H_2 model

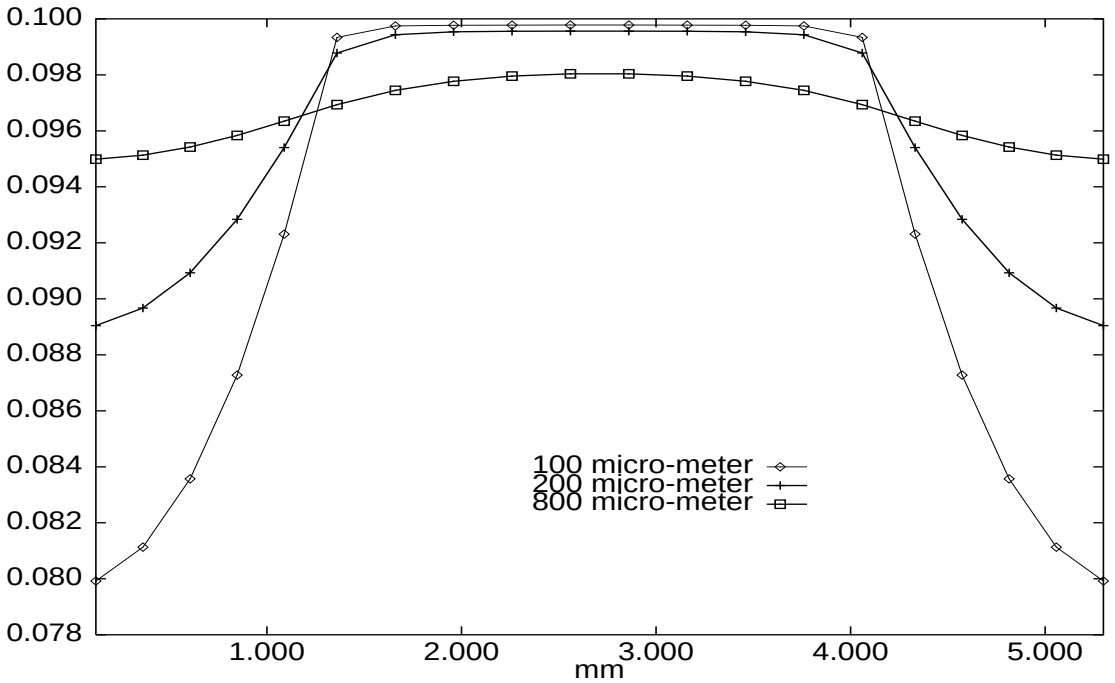

Figure 4: H_2 molar fraction profile, anode thickness 100, 200, 800 μm

the gaseous species; in order to study the significance of this effect we use the 2D pure hydrogen model for a co-flow geometry. It is clearly seen from Figure 4, which represents the hydrogen concentration profile for various anode thicknesses, using pure hydrogen as a fuel, that the hydrogen concentration at the electrode/electrolyte interface is much lower away from the channel than close to it.

Figure 3.1 represents the PEN potential jump computed with the Nernst law w.r.t. the molar fractions in the channels, at the interface electrode/electrolyte, and with the maximum value of the molar fraction at the electrode/electrolyte interfaces. Taking this last value is in fact assuming a 1D diffusion in the porous electrode. It is clear from Figure 3.1 that the 3D effect in the diffusion loss is quite important, and that it can in fact become dramatic in the case of a narrow anode.

In the case where methane is used, above results will be altered since the methane reforming rate increases with the anode thickness (and the amount of the catalyst), assuming a volumetric reforming reaction. There are now several competing effects which play a role in the optimization of the anode thickness:

- the diffusion of gas is better for a relatively thin anode (but not too thin, as observed in Figure 3.1),
- the production of methane by volumetric reforming increases with the thickness

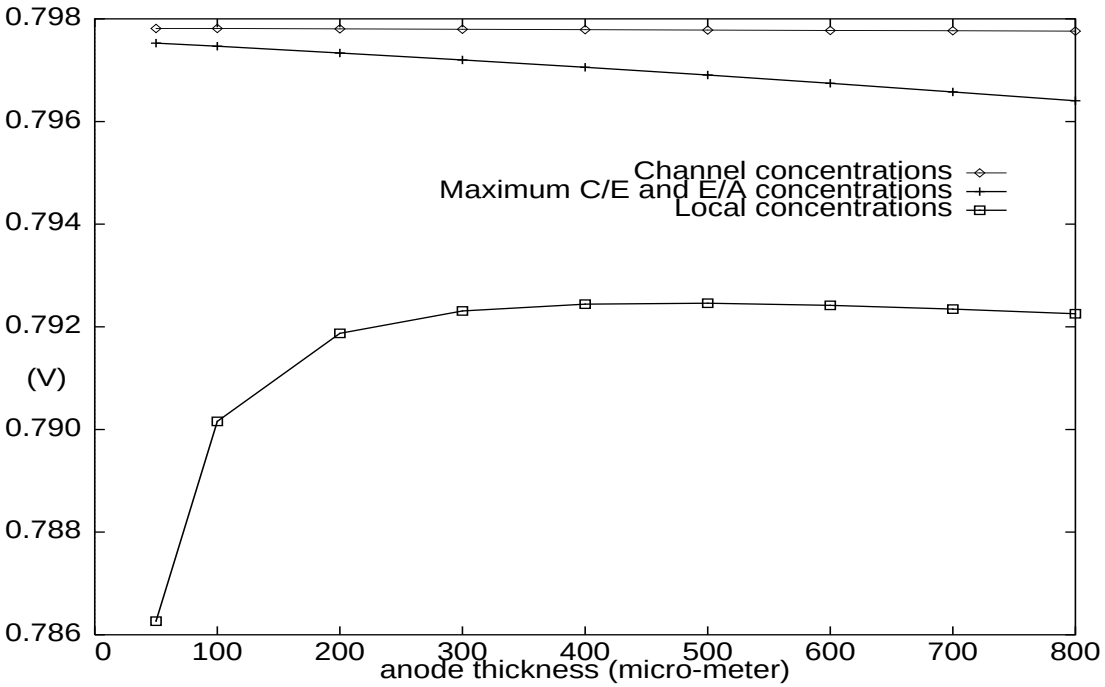

Figure 5: PEN potential jump vs anode thickness

of the anode (see Figure 6);

- the methane reforming is an endothermic reaction, so that when the methane production increases, it decreases the temperature;
- the ohmic loss increases with the anode thickness, which tends to increase the temperature.

The numerical code simulating the 3D model for methane in the planar geometry was used to study this phenomenon. The input parameters were set as [9], with a fixed inlet fuel flux($= 0.0385\, mol/h$). The thickness of the anode was varied from $50\,\mu m$ to $800\,\mu m$. In fact for a anode thickness of $50\,\mu m$, there is not enough hydrogen produced by reforming for the requested produced current, and the numerical code cannot reach a solution.

The results (figure 7) show that for a planar geometry, a thickness of $200\,\mu m$ seems to be optimal with respect to the efficiency (defined as the ratio of the electric power over the chemical power of the inlet gas). It was observed [5] that the Nernst potential increases steadily with the anode thickness, but so do the ohmic losses and the polarization losses.

The minimal temperature may go below the inlet temperature of the fuel because of the endothermic characteristic of the reforming reaction, as may be seen in Figure

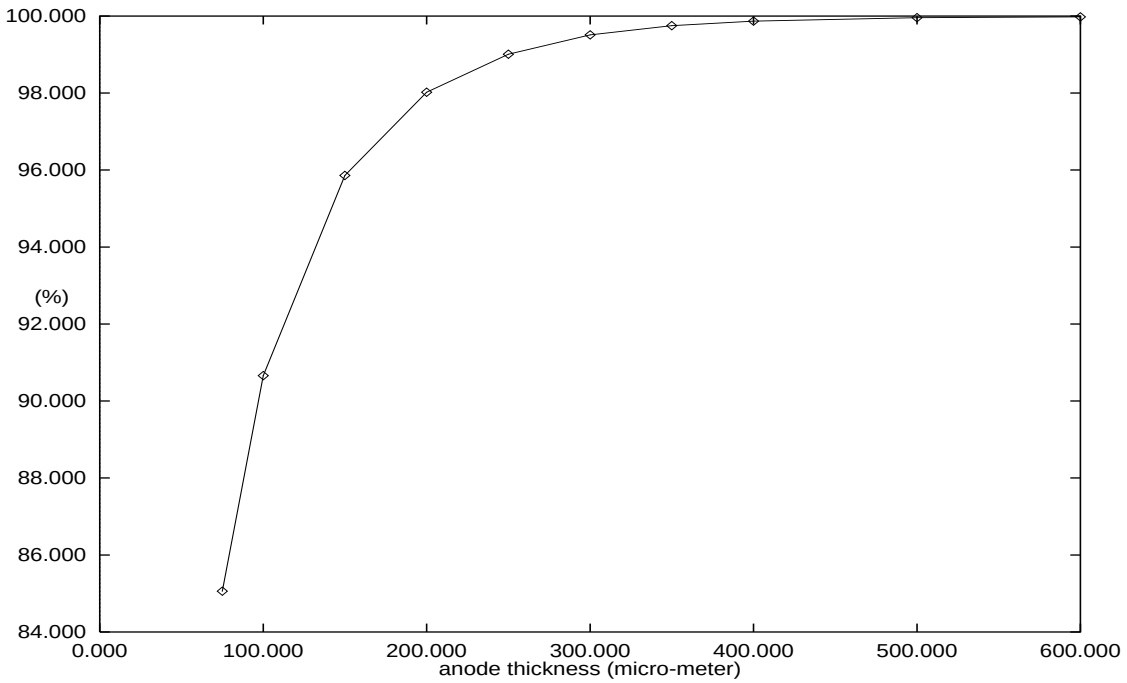

Figure 6: Methane conversion vs anode thickness

8. This is in agreement with the remarks on a "cold cell" of [11].

4 Stack simulation

Because of computer memory requirements, it is hopeless to try and simulate a whole stack using the local balance approach which we developed in SOFC3D for the detailed simulation of a unit cell. Hence the neccessity of a "macro" model, which uses balances over larger areas than one unit cell. Our approach is based on the homgeneization theory which is used for instance for the study of the macroscopic behaviour of composite materials.

From some previous theoretical studies [2], we deduce a macroscopic model for the stack which may be written in terms of the temperatures T_a and T_f of the channels, the temperature T of the solid part, the electric potential Φ and the concentration species X_i in the channels. In this model, the diffusion effects of the chemical species is taken into account through a sink term depending on the X_i in the channels, and deduced from the cell calculations performed with SOFC3D. A numerical code based on this macroscopic model and using the finite volume method for the discretization of the partial differential equations is being developed. The computation of the temperature in the solid parts is deduced from computations of the temperature a

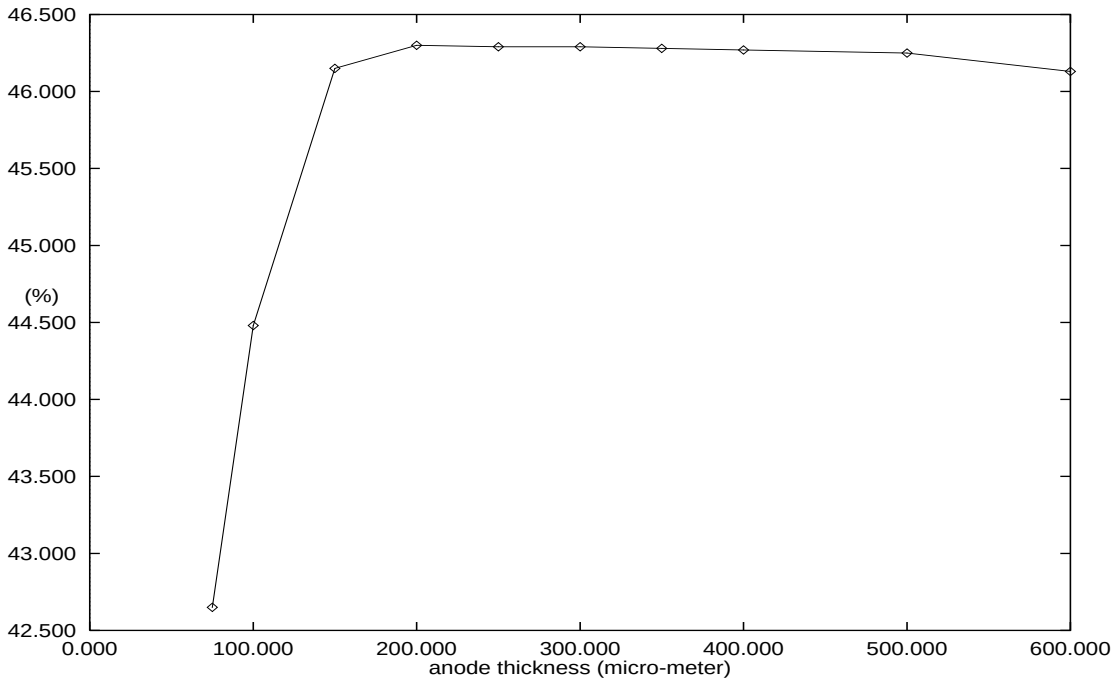

Figure 7: Efficiency vs anode thickness

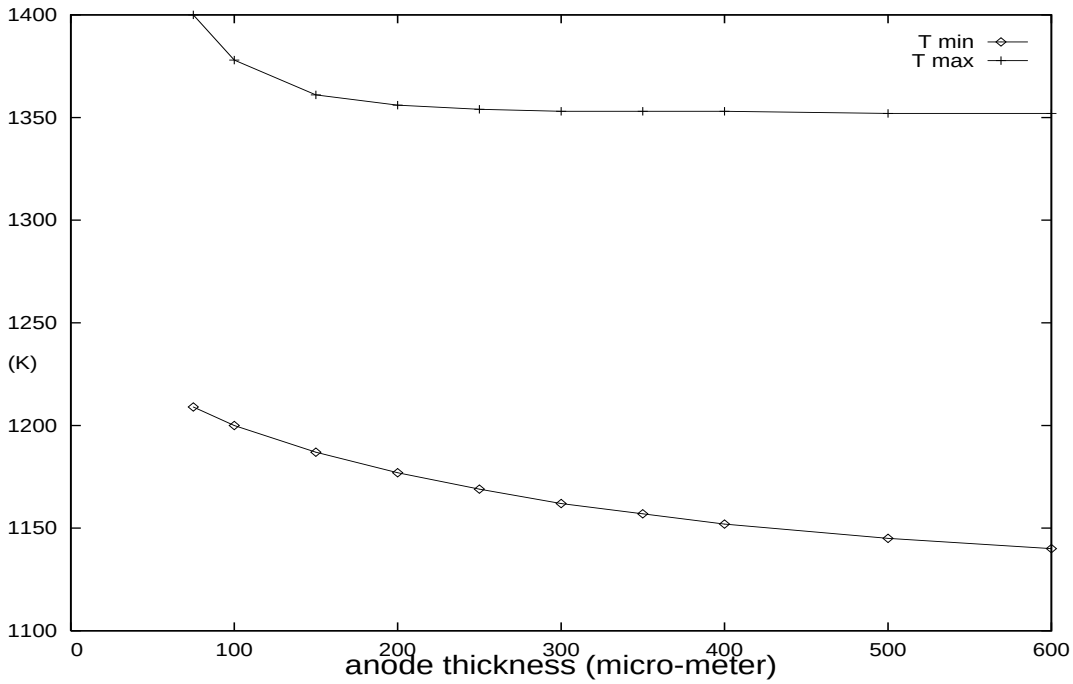

Figure 8: Maximum and minimum temperatures vs anode thickness

tthe cell level, for given channel temperature.

5 Conclusion

A 3D numerical code was developped for the numerical simulation of solid oxide fuel cells and stacks. The results show that the code which was written for the simulation of the unit cell may be used as a design tool for the unit cell, but also as a tool for the input data of a stack model. Note that both computer codes (cell and stack) can be used for various geometries (see e.g. [9].

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