Multi-physics Simulation of a Circular-Planar Anode-Supported Solid Oxide Fuel Cell

Keyvan Daneshvar*[1], Alex Fantino[1], Cinzia Cristiani[1], Giovanni Dotelli[1], Renato Pelosato[1], Massimo Santarelli[2]

[1]Politecnico di Milano, Dipartimento di Chimica, Materiali e Ingegneria Chimica "G. Natta", Milano, Italy

[2]Politecnico di Torino, Dipartimento di Energetica, Torino, Italy

*Corresponding author: keyvan.daneshvar@mail.polimi.it

Introduction: A 2D isothermal axisymmetric model of an anode-supported Solid Oxide Fuel Cell (SOFC) has been developed. This model has the advantage of being able to deal with different operating parameters: the results shown here are based on a temperature of 1073 K, a pressure of 1 atm and Ni-YSZ/YSZ/LSM-YSZ as materials for the anode, electrolyte and cathode, respectively.

Figure 1. 3D representation of the geometry of the model in analysis

Computational methods: It is an axisymmetric geometry, so it means that, applying a revolution through the axis of symmetry, a 3D geometry is obtained (for more details see the paper).

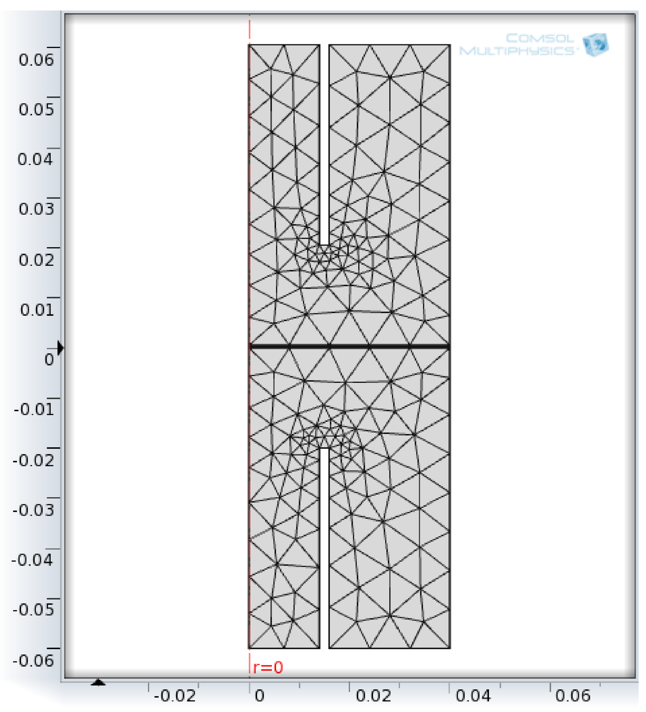

Figure 2. Axisymmetric meshed geometry of the setup

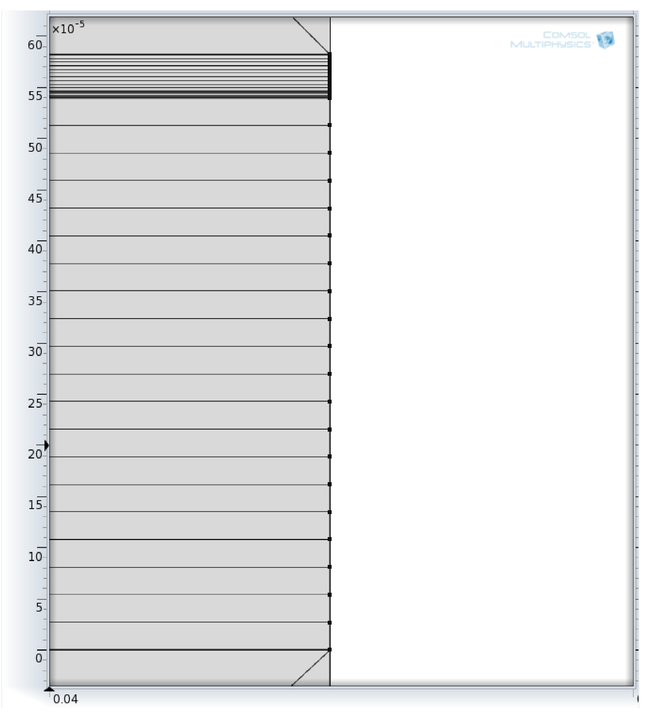

Figure 3. Mapped mesh of the cell, enlargement on the edge

In particular, for this model these features were used :

1. The Secondary Current Distribution.
2. Transport of Concentrated Species.
3. Free and Porous Media Flow

Charge balance equations

$$\nabla \cdot \mathbf{i}_k = Q_k$$

$$\mathbf{i}_k = -\sigma_k \nabla \phi_k$$

Charge transfer kinetics equations

$$i_{a,ct} = i_{0,a}\left[\frac{c_{h2}}{c_{h2,ref}}\exp\left(\frac{0.5F}{RT}\eta\right) - \frac{c_{h2o}}{c_{h2o,ref}}\exp\left(\frac{-1.5F}{RT}\eta\right)\right]$$

$$i_{c,} = i_{0,c}\left[\exp\left(\frac{3.5F}{RT}\eta\right) - x_{o2}\frac{c_t}{c_{o2,ref}}\exp\left(\frac{-0.5F}{RT}\eta\right)\right]$$

Maxwell-Stefan equation

$$\rho\frac{\partial}{\partial t}(\omega_i) + \rho(\mathbf{u}\cdot\nabla)\omega_i = \nabla\cdot\left(\rho\omega_i\sum_{k=1}^{Q}\tilde{D}_{ik}\mathbf{d}_k + D_i^T\frac{\nabla T}{T}\right) + R_i$$

Navier-Stokes equations

$$\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot\left[-p\mathbf{I} + \mu\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right) - \frac{2}{3}(\nabla\cdot\mathbf{u})\mathbf{I}\right]$$

$$\nabla\cdot(\rho\mathbf{u}) = 0$$

Porous gas diffusion catalyst layers equations

$$\left(\frac{\mu}{\kappa} + Q\right)\mathbf{u} = \nabla\cdot\left[-p\mathbf{I} + \frac{\mu}{\varepsilon}\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right) - \frac{2}{3}(\nabla\cdot\mathbf{u})\mathbf{I}\right]$$

$$\nabla\cdot(\rho\mathbf{u}) = Q$$

Results: Figure 4 shows the trend of the cell potential. Figures 5 shows the mass fractions of the present species in channels and cell. Figure 6 shows the polarization and the power density curves versus current density obtained from both the experimental data (Santarelli M., private communication) and modeling. Figure 7 and 8 show how the increase of the cell radius and anode thickness have a negative influence on the performance of the cell.

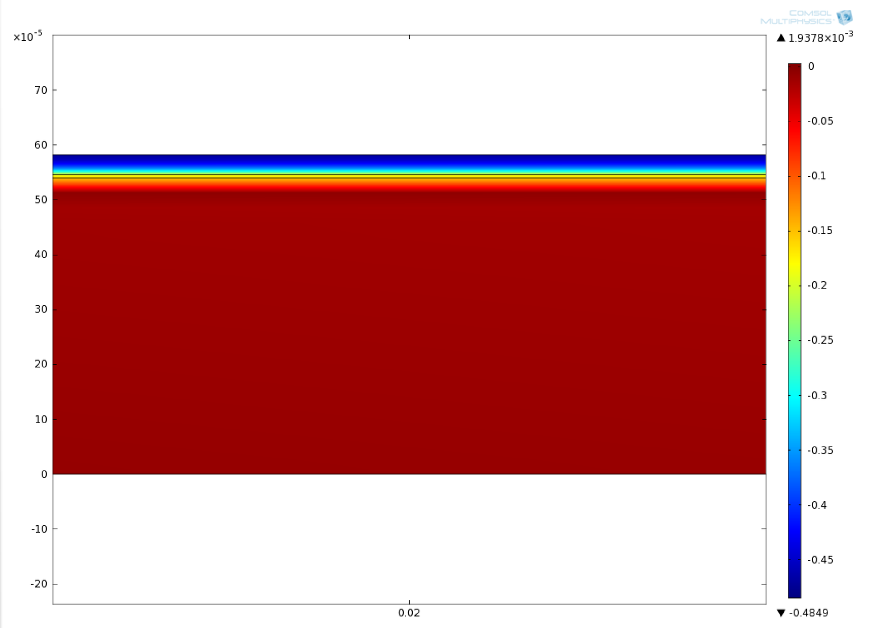

Figure 4. Side view of the cell potential

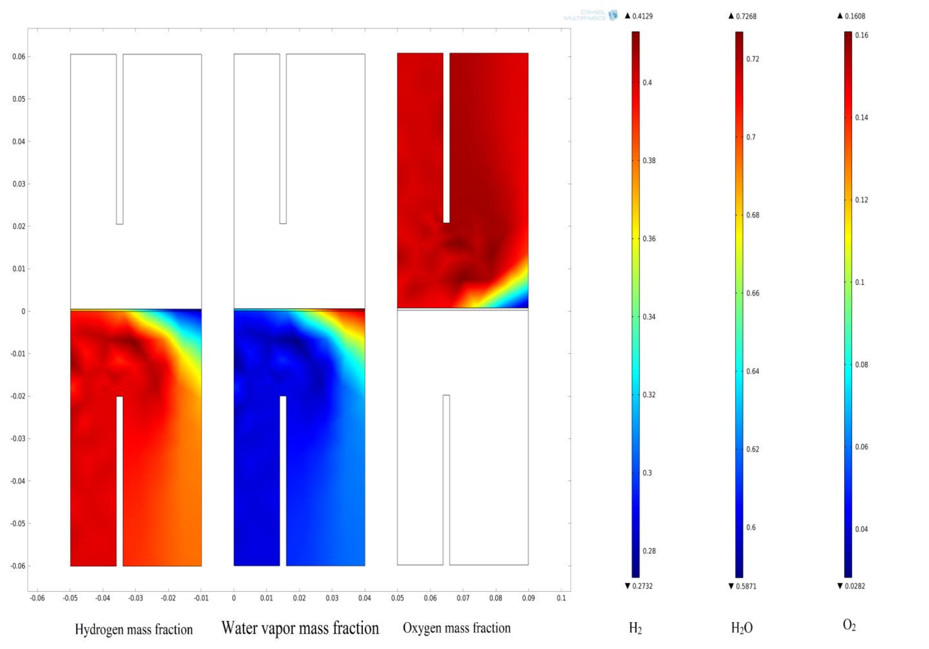

Figure 5. Hydrogen, water vapor and oxygen mass fraction

Operating pressure (Pa)	101325
Inlet temperature (K)	1073
Faraday Constant (C/mol)	96500
Gas constant (J/mol. K)	8.314
Anode ionic conductivity (S/m)	3.34*10⁴ exp (-10300/*T*)
Cathode ionic conductivity (S/m)	3.34*10⁴ exp (-10300/*T*)
Anode electronic conductivity (S/m)	2*10⁶
Cathode electronic conductivity (S/m)	42*10⁴ exp (-1150/*T*)/T
Electrolyte ionic conductivity (S/m)	3.34*10⁴ exp (-10300/*T*)
Porosity ($\mathcal{E}$)	0.4
Particle diameter (m)	2*10⁻⁶
Tortuosity	$((3-\mathcal{E})/2)^{0.5}$
Permeability	$\mathcal{E}^3 d^2/150(1-\mathcal{E})^2$
Inlet velocity (m/s)	0.1
Viscosity of H2 (Pa*s)	9.27*10⁻⁶
Viscosity of O2 (Pa*s)	16.27*10⁻⁶
Anode exchange current density (A/m²)	5300
Cathode exchange current density (A/m²)	2000
Specific surface area (1/m)	1.025*10⁵

Table 1. Material properties and operating conditions used in this simulation

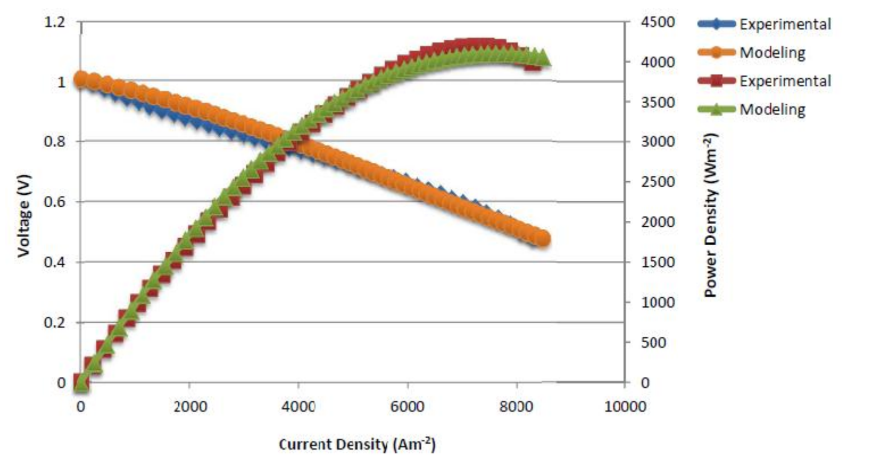

Figure 6. Polarization and power density curves vs current density

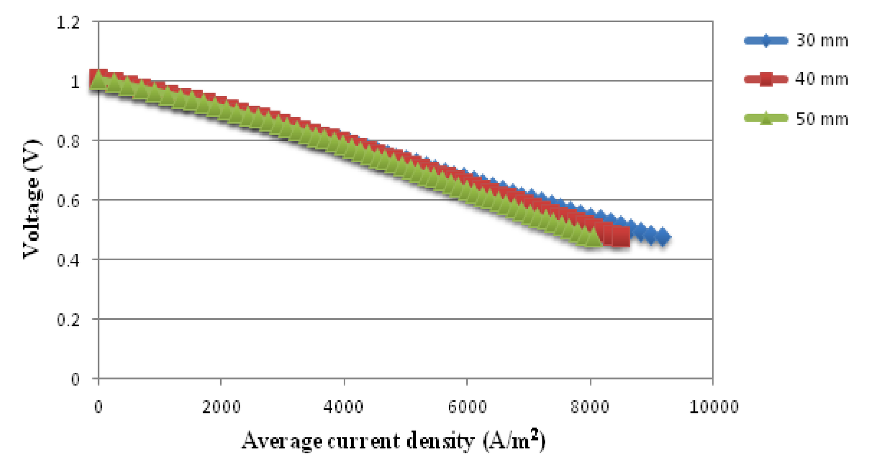

Figure 7. Influence of the cell radius on the polarization curve

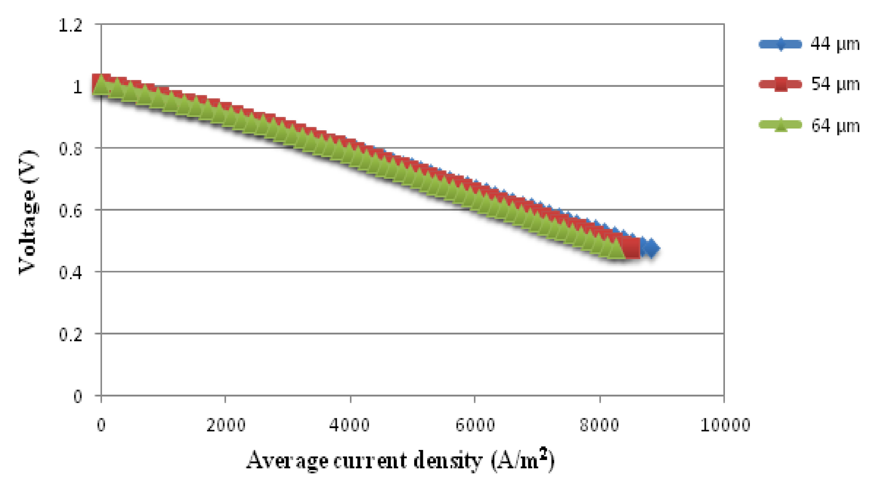

Figure 8. Influence of the anode thickness on the polarization curve

Conclusions: A model of SOFC was analyzed via COMSOL, comparing the results with experimental data: the good agreement between the results has ensured the effectiveness of the model. It was then carried out a parametric study to see the influence of parameters on the model. Future studies will take into account thermal analysis in a more accurate way.

References:
1.Yixiang Shi, Ningsheng Cai et al, Numerical modeling of an anode-supported SOFC button cell considering anode surface reaction, Journal of Power Sources,164,639-648(2007).
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