Optimal Design of a Solid Oxide Fuel Cell for Hybrid Vehicle Application

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ABSTRACT
This paper is focused on the possible design modification of a monolithic-type Solid Oxide Fuel Cell (SOFC) to be used as the prime mover for a hybrid vehicle. The SOFC power is selected in order to achieve the average power requirements of the vehicle. Reformed bioethanol is considered as a fuel.

A multi-objective optimization is performed in order to minimize the total volume of the fuel cell and to maximize its electrical efficiency. This results is obtained by using a full 3D model of the fuel cell, accounting for heat, mass and current transfer as well as chemical and electrochemical reactions. The model has been built in Fluent®. The selection of the design variables to be considered as the independent variables in the optimization procedure is selected on the basis of the analysis of the different contributions to the local entropy generation: viscous effects, mass transfer, heat transfer, coupling between heat and mass transfer and ohmic losses. The system optimization if obtained though iterative solution of the SOFC model driven by Modefrontier®. The final result is constituted by the Pareto front showing the optimal SOFC configurations.

INTRODUCTION
Hybrid vehicles constitute an interesting option to reduce emissions in transportation. They consists of a primary engine coupled with batteries in order to make it operating in optimal conditions and avoid fuel wasting during stops. High temperature fuel cells, as molten carbonate fuel cells and solid oxide fuel cells can be used as primary engines instead of internal combustion engines [1].

One of the big advantages of high temperature fuel cells resides in their theoretical efficiency [2]. Nevertheless, in real plants the registered efficiency is still far from the potential performance [3, 4]. One of the causes of this discrepancy is related with the geometries that determine non-uniformities in thermodynamic quantities as temperatures, concentrations, mass flow rates, etc. that causes inhomogeneous distributions in current densities and power production. This cause is investigated in this paper, together with possible improvements that can be achieved through changes in the fuel cell geometry. A tubular-like solid oxide fuel cell geometry, obtained considering a monolithic type fuel cell and adding an air injection tube, as shown in figure 1.
The fuel cell is composed of a solid electrolyte layer between a porous cathode and anode. Above and below this matrix there are two interconnections. Fuel and air flows in trapezoidal channels, but air is introduced through an injection tube located inside the cathodic channel. In this way, air flows from the top end of the cell to the bottom the end exchanging heat but without variations in chemical composition. Air exiting the tube flows in the trapezoidal air channels from the bottom to the top in co-current configuration with respect to fuel flow. Since anode is porous, the gases in the anodic channel permeate it. Hydrogen reacts with the oxygen ions coming from the cathode through the electrolyte, thus generating water:

$$H_2 + O^{2-} \rightarrow H_2O + 2e^- \quad (1)$$

Water produced in the reaction goes back to the anode channel and exits the cell, together with the other non oxidized gas species. The net result for the anodic side is a hydrogen flux from the channel to the anode-electrolyte interface and a water flux on the opposite side. At the cathode side, oxygen in cathodic channel permeate the cathode where ions form and migrate through the electrolyte:

$$\frac{1}{2}O_2 + 2e^- \rightarrow O^{2-} \quad (2)$$

The result for the cathode is one way flux from the channel to the electrode-electrolyte interface. The resulting overall reaction is:

$$H_2 + \frac{1}{2}O_2 \rightarrow H_2O \quad (3)$$

**MATHEMATICAL MODEL**

This fuel cell is analyzed using a CFD model, which provide a detailed description of physical phenomena taking place in fuel cells as well as the effect of the geometry of these phenomena. A three-dimensional CFD model accounting for heat and mass transfer as well as chemical and electrochemical reactions is used.

The following assumption are used in this model: steady state conditions, gas mixtures are considered as ideal gases, fluid flow is laminar and incompressible, porous electrodes are homogeneous and isotropic with uniform morphology proprieties such as porosity, tortuosity and permeability.

The model consists of a set of partial differential equations and some constitutive equations in order to model the different phenomena. The partial differential equations are: the continuity equation, the momentum equation, energy conservation, the conservation of species and current conservation [5, 6]. The geometrical parameters are shown in Table 1, while model parameters are shown in Table 2.
Table 1. Geometrical parameters

<table>
<thead>
<tr>
<th></th>
<th>Anode</th>
<th>Cathode</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thickness (mm)</td>
<td>1.4</td>
<td>0.4</td>
</tr>
<tr>
<td>Axial length (mm)</td>
<td>17</td>
<td>17</td>
</tr>
<tr>
<td>Thickness (mm)</td>
<td>Electrolyte</td>
<td>0.1</td>
</tr>
<tr>
<td>Axial length (mm)</td>
<td>17</td>
<td></td>
</tr>
<tr>
<td>Length (mm)</td>
<td>Fuel channel</td>
<td>100</td>
</tr>
<tr>
<td>Cross section</td>
<td></td>
<td>90</td>
</tr>
<tr>
<td>Cross section</td>
<td>Air channel</td>
<td>100</td>
</tr>
<tr>
<td>(mm²)</td>
<td></td>
<td>80</td>
</tr>
<tr>
<td>Diameter (mm)</td>
<td>Injection tube</td>
<td>10</td>
</tr>
</tbody>
</table>

Table 2. Model parameters

<table>
<thead>
<tr>
<th></th>
<th>Anode</th>
<th>Cathode</th>
</tr>
</thead>
<tbody>
<tr>
<td>Porosity</td>
<td>0.3</td>
<td>0.3</td>
</tr>
<tr>
<td>Tortuosity</td>
<td>Anode 3</td>
<td>3</td>
</tr>
<tr>
<td>Pore size (m)</td>
<td>Anode $1 \times 10^{-5}$</td>
<td>1 \times 10^{-5}</td>
</tr>
<tr>
<td></td>
<td>Cathode $1 \times 10^{-12}$</td>
<td>$1 \times 10^{-12}$</td>
</tr>
<tr>
<td>Permeability (m²)</td>
<td>Anode $1 \times 10^{-12}$</td>
<td>$1 \times 10^{-12}$</td>
</tr>
<tr>
<td></td>
<td>Cathode $1 \times 10^{-12}$</td>
<td>$1 \times 10^{-12}$</td>
</tr>
<tr>
<td>Exchange current</td>
<td>Anode $1 \times 10^{3}$ A m⁻²</td>
<td>$5 \times 10^{0}$ A m⁻²</td>
</tr>
<tr>
<td></td>
<td>Cathode</td>
<td></td>
</tr>
<tr>
<td>Activation energy</td>
<td>Anode 120 J mol⁻¹</td>
<td>120 J mol⁻¹</td>
</tr>
<tr>
<td></td>
<td>Cathode</td>
<td></td>
</tr>
<tr>
<td>Electrical conductivity (Ω⁻¹ m⁻¹)</td>
<td>Anode 3.3 \times 10^{5}</td>
<td>7.9 \times 10^{5}</td>
</tr>
<tr>
<td></td>
<td>Cathode</td>
<td></td>
</tr>
<tr>
<td>Thermal conductivity (W m⁻¹ K⁻¹)</td>
<td>Anode 6.23</td>
<td>1.15</td>
</tr>
<tr>
<td></td>
<td>Electrolyte</td>
<td></td>
</tr>
<tr>
<td>$S/K$ (m⁻¹)</td>
<td>Anode 1000</td>
<td>Cathode 1000</td>
</tr>
</tbody>
</table>

Fluid flow is computed through continuity equation (4) and momentum equation (5).

\[ \nabla \cdot (\rho \vec{v}) = 0 \]  

\[ \rho \cdot (\vec{v} \cdot \nabla) \vec{v} = -\nabla p + \mu \cdot \nabla^2 \vec{v} - \frac{\mu}{K} \vec{v} \]  

where \( \rho \) is the fluid density, \( \vec{v} \) the velocity vector, \( p \) the pressure, \( \mu \) the fluid viscosity, \( K \) is the permeability of the porous media.

In the air and fuel channel the last term of momentum equation is absent and it is written in the form Navier-Stokes equation, in porous electrodes it is in the form of the Brinkman-extended Darcy equation being the inertial terms negligible [7].

The conservation of species is written by considering the gas species and the mixture of gases. The equation for the general species \( i \) is written as
\[ \nabla \cdot (\rho \cdot \nabla \cdot \omega_i) = -\nabla \cdot \vec{J}_i + S_i \tag{6} \]

where \( \omega_i \) is the mass fraction of component \( i \), \( \vec{J}_i \) is the diffusion flux of species \( i \), and \( S_i \) is the source term due to chemical reactions (steam reforming and water gas shift reaction). The diffusive mass flux \( \vec{J}_i \) is modeled as

\[
\vec{J}_i = \rho D_{j,\text{eff}} \nabla \omega_i + \frac{\rho \omega_i}{M} \sum_j D_{j,\text{eff}} \nabla \omega_j - \nabla M \sum_j D_{j,\text{eff}} \omega_j \tag{7} \]

The first term on the right-hand side represents the Fick diffusion due to concentration gradients. The last three terms are the corrections to enforce the Stefan-Maxwell equations for the multi-component diffusion term. Solid structure in porous media reduces the diffusion rate as it limits the flow rate, to account for this effect the effective binary diffusivity in porous media is calculated as follow [8]:

\[
D_{ij,\text{eff}} = \frac{\varepsilon_T}{\tau} D_{ij} \tag{8} \]

where \( \varepsilon \) is the porosity, \( \tau \) the tortuosity and \( D_{ij} \) the mass diffusion coefficient calculated through the Fuller-Schettler-Gidding correlation:

\[
D_{ij} = \frac{0.143 \cdot 10^{-6} \cdot T^{1/2}}{M^{1/2} (\mu_i + \mu_j)^{1/2}} \tag{9} \]

\[
M_{ij} = 2 \left(1/M_i + 1/M_j \right)^{-1} \tag{10} \]

where \( M \) is the molar mass, \( T \) the local temperature and \( \mu_i \) the binary diffusion coefficients. These coefficients are 6.12 for hydrogen, 18.5 for nitrogen, 16.3 for oxygen, 13.1 for water [9].

Generation and destruction of species due to electrochemical reactions (1)-(3) taking place at the triple phase boundary are set as boundary conditions on the surfaces between electrolyte and electrodes. These terms are expressed through the Faraday law.

In the case of fuel constituted of a mixture of \( \text{H}_2, \text{H}_2\text{O}, \text{CO}, \text{CO}_2 \) and \( \text{CH}_4 \), the methane steam reforming reaction and the water gas shift reaction take place as well. In this case proper source terms should be considered [10].

When a multi-component gas mixture is considered, equation (6) is written for \( n-1 \) species. In this case, the mass fraction of the \( n \)th species is calculated as

\[
\omega_n = 1 - \sum_{i=1}^{n-1} \omega_i \tag{11} \]

Energy equation is written in the form

\[
\nabla \cdot \left( \rho \vec{V} \left( \rho E + p \right) \right) = \nabla \cdot \left( k_{\text{eff}} \nabla T - \sum_i h_i \cdot \vec{J}_i \right) + S_p \tag{12} \]

where \( k_{\text{eff}} \) is the effective conductivity, which is the gas conductivity in the channels and the weighted mean conductivity of gas conductivity and solid matrix conductivity. In the porous matrix the local thermal equilibrium hypothesis between the gas and the solid matrix is formulated.

The first two terms on right-hand side represent energy transfer due to conduction and diffusive species transport.

\[
E = \frac{h}{\rho} + \frac{v^2}{2} \tag{13} \]
\[ h_i = \int c_{p,i} \cdot dT \quad (14) \]

Since the gas mixture is assumed to behaves as an ideal gas, the enthalpy \( h \) of the mixture is calculated as

\[ h = \sum_{i=1}^{n} \omega_i \cdot h_i \quad (15) \]

The source term \( J_s \) accounts for Joule heating effect due to ohmic resistance. Heating contributions due to reversible heat associated with the electrochemical reaction and the activation overpotential are set as boundary conditions on the surface between electrolyte and electrodes.

In the electrolyte, equation (12) becomes a Poisson equation, as only the conductive term and the source term survive.

Last equation to solve is the charge conservation, which is written in the form:

\[ \nabla^2 \phi = 0 \quad (16) \]

where \( \phi \) is the electrical potential. The current density \( \vec{i} \) can be obtained from electrical potential through Ohm’s law:

\[ \vec{i} = -\sigma \cdot \nabla \phi \quad (17) \]

where \( \sigma \) is the electrical conductivity. The conversion between electronic and ionic current takes place on the triple-phase boundary, i.e. the surface between electrodes and electrolyte. On these surface current density is related with the activation overpotential through the Butler-Volmer equation [11, 12]:

\[ i = i_0 \left( e^{\frac{\beta \eta_{act} F}{RT}} - e^{\frac{(1-\beta) \eta_{act} F}{RT}} \right) \quad (18) \]

where \( \eta_{act} \) is the activation overpotential, \( \beta \) and \( n \) are the transfer coefficient \((\beta = 0.5)\) and the number of electrons participating in the reaction \((n = \frac{1}{2} \text{ on cathode side and } n = 2 \text{ on anode side})\), respectively. The exchange current density \( i_0 \) depends on the partial pressure of the reacting gas composition and the temperature [13, 14]. On the anode side,

\[ i_0 = \gamma_A \cdot \left( \frac{P_{H_2}}{P_{ref}} \right)^{1.25} \cdot \left( \frac{P_{H_2O}}{P_{ref}} \right) e^{\frac{E_0}{RT}} \quad (19) \]

On the cathode side

\[ i_0 = \gamma_C \cdot \left( \frac{P_{O_2}}{P_{ref}} \right)^{0.25} e^{\frac{E_0}{RT}} \quad (20) \]

The activation overpotential is related with the overall cell potential through the following equation:

\[ V_{cell} = V_{rev} - \eta_{electrode} - \eta_{electrolyte} - \eta_{act} \quad (21) \]

where \( V_{rev} \) is the reversible potential between the electrode and the electrolyte, and can be computed with the Nernst’s equation as follow
\[ V_{rev} = -\Delta G^0 \frac{n_e \cdot F}{n_e \cdot F} + R \cdot T \cdot \ln \left( \frac{p_{H_2} \cdot p_{O_2}^{0.5}}{p_{H_2O}} \right) \]  

(22)

MODEL RESULTS

The model introduced in the previous section couples electrochemical calculation with computational fluid dynamics. The Navier–Stokes equation, transport equations and boundary conditions are discretized by using the finite volume method (FVM) to obtain velocity field, temperature and mass fractions in the fuel cell. The local current density is then computed and sources term for species and energy equation are determined. This procedure is repeated until convergence is reached. Finally, local and global entropy generation are calculated and stored. In the equations, the convective terms are modeled by second order upwind scheme while the diffusive terms are modeled by the central difference scheme. The numerical solution procedure adopts the semi-implicit SIMPLE algorithm [15].

Figure 2 shows the velocity path lines inside the cathode channel. The air flows in the tube from the top of the cell to the bottom. At the closed end of the channel two vortexes take place. This is typical of tubular fuel cell. Air flows back from the bottom end to the top in the cathode channel. It is interesting to observe that in the lower part of the channel the velocities are higher; this is due to a smaller cross-section below the air tube.

In the porous electrodes the flow is mainly driven by diffusion phenomena: in the anode the net flow is directed to the fuel channel. This is due to the production of water because of electrochemical reaction. At cathode side, oxygen is consumed, thus the air flows from the channel to the cathode.

![Figure 2. Velocity path lines inside cathode channel.](image)

Figure 3 shows the hydrogen concentration at anode side along several transversal cross sections. It is clear that hydrogen mass fraction has strong gradient in streamwise directions, and this profile is characterized by the rate of consumption of hydrogen due to electrochemical reactions. From figure it is also evident that a concentration gradient takes place also in transversal direction. This is the result of hydrogen diffusion process from bulk flow to the three-phase boundary, in particular this effect is stronger in the lower zone of the anode, where hydrogen mass fraction is smaller.
In figure 4, the oxygen mass fraction in the cathode channel is depicted. Since air flows inside the tube first, the higher oxygen concentration is localized in the bottom part of the cell. As in the case hydrogen, oxygen mass fraction presents variation both in streamwise direction and in the x-y plane. In particular the oxygen cannot reach easily the upper plane of the cathode, this occurs because the porous matrix on cathode side represents an obstacle to the air flow.

Figure 4. Oxygen mass fraction.

Figure 5 shows the temperature distribution in the fuel cell.

Since the electrochemical reactions are exothermic, an overall increase in the cell temperature is expected with respect to the inlet conditions. However, temperature distribution shows different features at anode side respect to cathode side. In the fuel channel temperature initially increases along z direction and reaches a maximum value of 1063 K at 60% of cell length, then temperature decreases up till the outlet section. On the
other hand, in the cathode channel the outlet temperature of air is close to the inlet temperature. Air temperature increases monotonically from outlet tube section to the inlet tube section.

![Figure 5. Temperature distribution in the fuel cell.](image)

It is interesting to notice that temperature is much higher in the region below the air tube at cathode side. There are significant temperature gradients along the cross sections, in particular in the electrodes. This is due to the small convection in the porous matrix.

**SOFC OPTIMIZATION**

SIMPLEX optimization algorithm is used to iterate the previously CFD computations for different cell geometries in order to study how the power density is affected. This is performed using the software Modefrontier®. The design variables, X scaling factor and Y scaling factor, are selected on the basis of the main irreversibilities that take place on the cell. These have been studied in [16].

The largest irreversibilities are due to heat transfer. The effect of scaling factors on convection heat transfer irreversibilities are shown in figure 6 and on conduction heat transfer irreversibilities are shown in figure 7.
The shape of the channel is let free to change in the optimization procedure in order to obtain a reduction mainly in the irreversibilities due to convection. The initial value of the scaling factors (figure 3a) is assumed as equal to 1. The x and y scaling factors are allowed to vary in the range 0.8-2.0, while the z scaling factor can vary from 1 to 1.5.

In the optimization procedure the total active surface has been constrained to a fixed value. Thus, the total TPB sites for electrochemical reactions are constant for all the examined geometries. This means that the free design variables in the optimization are actually 2, since the third dimension is calculated so that the active surface of the cell is kept constant.
The SIMPLEX algorithm moves the initial value of scaling factor in order to reach the optimal objective, i.e. the maximization of power density. The optimal configuration is identified by $X$ scale = 1.4 and $Y$ scale = 0.8, therefore it turns out to be stretched along $x$ direction and smaller than the initial design in $y$ direction. Figure 8 shows the initial geometry and the optimal geometry.
Another important technical parameter to be considered is the volume of the device. Figure 9 shows some results obtained by performing the optimization using the power density as the objective function to be maximized. On the left side of the diagram, it is possible to notice that a small reduction in the power density (from about 3640 W/m² to about 3615 W/m²) allows a significant reduction in the fuel cell volume, about 20%.

**CONCLUSION**

In this paper, geometry optimization of a tubular solid oxide fuel cell for possible application in hybrid vehicles is performed. A numerical model built using Fluent® accounting for fluid flow, mass transfer, heat transfer, current transfer as well as chemical and electrochemical reactions is presented. Scaling factors are considered as the design parameters free to vary. The optimization is driven using the software Modefrontier®, which allows one to iteratively modify the design parameters and run the corresponding simulation in order to maximize the power density.

With respect to the initial design, the power density is increased of about 10%. Another benefit that can be achieved in the optimization consists in the reduction of fuel cell volume.

**BIBLIOGRAPHY**

