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Mariya PECHERSKAYA
Institute of Materials Science, SPA Physics-Sun, Tashkent, Uzbekistan, mariya.pecherskaya@yahoo.com

Khakimjan BUTANOV
Institute of Materials Science, SPA Physics-Sun, Tashkent, Uzbekistan, khakimjan@yahoo.com

Suhrob A. IBODULLAEV
Institute of Materials Science, SPA Physics-Sun, Tashkent, Uzbekistan, Sukhrob9228@mail.ru

Olim RUZIMURADOV
Turin Polytechnic University in Tashkent, Tashkent, Uzbekistan, ruzimuradov@rambler.ru

Shavkat MAMATKULOV
Institute of Materials Science, SPA Physics-Sun, Tashkent, Uzbekistan, mi-shavkat@yandex.ru

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MODELING AND PERFORMANCE ANALYSIS OF SOLID OXIDE FUEL CELL

Mariya PECHERSKAYA*[1] *(mariya.pecherskaya@yahoo.com)
Khakimjan BUTANOV*[1] *(khakimjan@yahoo.com)
Suhrob IBODULLAEV*[1] *(sukhrob9228@mail.ru)
Olim RUZIMURADOV*[1,2] *(ruzimuradov@rambler.ru)
Shavkat MAMATKULOV*[1] *(mi-shavkat@yandex.ru)
[1]Institute of Materials Science, SPA Physics-Sun, Tashkent, Uzbekistan
[2]Turin Polytechnic University in Tashkent, Tashkent, Uzbekistan

A three-dimensional numerical model of the system configurations of various types of solid oxide fuel cells (SOFCs) is used and the effect of parameters on SOFC performance is numerically investigated using COMSOL Multiphysics. The effect of parameters such as support layer thickness, operating temperature, and electrode porosity are shown in the polarization and power curves for each model. The results of the study showed the advantages of the anode-supported SOFC compared to cathode- and electrolyte-supported SOFC.

Theoretical calculations demonstrate the highest output power density in the anode-supported SOFC at 900 °C, and reach a value of 0.585 W cm^{-2} *at a current density of 1 A cm*$^{-2}$*. For the cathode-supported SOFC at an operating temperature of 900 °C, the maximum output power density is 0.54 W cm*$^{-2}$ *at a current density of 0.9 A cm*$^{-2}$*. For the electrolyte-supported SOFC at 900 °C, the maximum output power density is 0.325 W cm*$^{-2}$ *at a current density of 0.58 A cm*$^{-2}$*.*

Keywords: solid oxide fuel cell, cathode, anode, electrolyte, model, I-V curves

МОДЕЛИРОВАНИЕ И АНАЛИЗ ПРОИЗВОДИТЕЛЬНОСТИ ТВЕРДООКСИДНОГО ТОПЛИВНОГО ЭЛЕМЕНТА

Мария ПЕЧЕРСКАЯ*[1] *(mariya.pecherskaya@yahoo.com)
Хакимжан БУТАНОВ*[1] *(khakimjan@yahoo.com)
Сухроб ИБОДУЛЛАЕВ*[1] *(sukhrob9228@mail.ru)
Олим РУЗИМУРАДОВ*[1,2] *(ruzimuradov@rambler.ru)
Шавкат МАМАТКУЛОВ*[1] *(mi-shavkat@yandex.ru)
[1]Институт материаловедения, НПО Физика-Солнца, Ташкент, Uzbekistan
[2]Туринский политехнический университет вТашкенте, Ташкент, Узбекистан

Представлены результаты построения трехмерной численной модели конфигураций системы различных типов твердооксидных топливных элементов (ТОТЭ) и численно исследовано влияние параметров на производительность ТОТЭ с помощью COMSOL Multiphysical. Влияние таких параметров, как толщина слоя подложки, рабочая температура и пористость электрода, показано на поляризационных и мощностных кривых для каждой модели. Результаты исследования показали преимущества ТОТЭ с анодом по сравнению с ТОТЭ с катодом и электролитом.

Теоретические расчеты демонстрируют наибольшую плотность выходной мощности в ТОТЭ с анодом при температуре 900 °С и достигают значения 0,585 Вт/см$^{-2}$ *при плотности тока 1 А/см*$^{-2}$*. Для ТОТЭ с катодом при рабочей температуре 900 °С максимальная выходная плотность мощности составляет 0,54 Вт/см*$^{-2}$ *при плотности тока 0,9 А/см*$^{-2}$*. Для ТОТЭ с электролитом при 900 °С максимальная выходная плотность мощности составляет 0,325 Вт/см*$^{-2}$ *при плотности тока 0,58 А/см*$^{-2}$*.*

Ключевые слова: твердооксидный топливный элемент, катод, анод, электролит, модель, I-V кривые линии

QATTIQ OKSIDLI YOQILG'I ELEMENTINI MODELLASHTIRISH VA ISHLASH TAHLILI

Mariya PECHERSKAYA*[1] *(mariya.pecherskaya@yahoo.com)
Xakimjan BUTANOV*[1] *(khakimjan@yahoo.com)
Suhrob IBODULLAEV*[1] *(sukhrob9228@mail.ru)
Olim RUZIMURADOV*[1,2] *(ruzimuradov@rambler.ru)
Shavkat MAMATKULOV*[1] *(mi-shavkat@yandex.ru)
[1]"Fizika-Quyosh" IICHB Materialshunoslik instituti, Toshkent, O'zbekiston
[2]Toshkent shahridagi Turin politexnika universiteti, Tashkent, O'zbekiston

Maqolada qattiq oksidli yoqilg'i elementlari (QOYOE) har xil turdagi tizim konfiguratsiyasining uch o'lchovli raqamli modeli qurilgan va QOYOE ishlash parametrlarning ta'siri COMSOL Multiphysical yordamida raqamli o'rganilgan. Taglik qatlamining qalinligi, ish harorati va elektrod g'ovakligi kabi parametrlarning ta'siri har bir model uchun polarizatsiya va quvvat egri chiziqlarida ko'rsatilgan. Tadqiqot natijalari katod va elektrolitli QOYOE bilan solishtirganda anodli QOYE ning afzalliklarini ko'rsatdi.

Nazariy hisob-kitoblar anodli QOYOEda 900 °C da eng yuqori chiqish quvvati zichligini ko'rsatadi va 1 A sm^{-2} *tok zichligida 0,585 Vt sm*$^{-2}$ *qiymatiga ega bo'ldi. Katodli QOYOE uchun 900 °C ish haroratida maksimal chiqish quvvati zichligi 0,9 A sm*$^{-2}$ *tok zichligida 0,54 Vt sm*$^{-2}$ *ni tashkil etdi. Elektrolitli QOYOE uchun 900 °C da maksimal chiqish quvvati zichligi 0,58 A sm*$^{-2}$ *tok zichligida 0,325 Vt sm*$^{-2}$ *ni tashkil etdi.*

Kalit so'zlar: qattiq oksidli yoqilg'i elementi, katod, anod, elektrolit, model, I-V egri

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Introduction

In the practice of solid oxide fuel cells (SOFCs) research, there is often a need for a preliminary analysis and creation of a functional model of a single cell. One of the first steps of the research is the modeling and calculation of the kinetic and thermodynamic parameters of electrodes and electrolyte systems based on previously obtained experimental results. A review of the calculation algorithms and data analysis of the given parameters makes it possible to optimize previously studied systems and create new models. Wang et al. [1], Kakach [2] and Andersson et al. [3] showed that numerical simulation of SOFC allows reducing the number of experimental tests to create single cell and only a minimum number of laboratory tests are required to verify the accuracy of the models.

Reducing the operating temperature of SOFCs while maintaining an acceptable level of the electrical characteristics increases their durability and reliability. The main task of modeling is to create a high-quality SOFC model with the maximum output power density and a relatively low operating temperature.

In order to decrease the operating temperature of SOFC, generally two approaches are used. The first one is to reduce the thickness of the electrolyte, and the other one is to use an electrolyte material with higher ionic conductivity at low temperatures. In both cases, it is necessary to comprehensively study the processes associated with the geometry and chemistry of the surface, charge transfer reactions, the physical representation of the electric potential stages, and other transfer phenomena. Each of these aspects follows a macroscale study.

The intermediate temperature of solid oxide fuel cell (IT-SOFC) is a relatively new area of research in the field of fuel cells, and correspondingly less modeled. A decrease in operating temperatures leads to an expansion of the choice of IT-SOFC materials, a low cost, and an increase of fuel cells capability. The most of the fuel cell modeling studies were performed by using the Comsol Multiphysics software.

One of the earliest SOFC modeling was fulfilled on the basis of the Butler-Volmer equation, without parameters of the Tafel equation [4]. Patcharavorachot et al. [5] developed a strictly electrochemical reaction model, where mass and heat transfer, fluids flow, and internal reforming reactions were ignored. Bessler et al. [6] studied the electrochemistry of SOFC anodes focusing on the nickel-doped yttrium-stabilized zirconium oxide (Ni/YSZ) materials, where the electrochemical reactions were described in several steps using the Arrhenius equations. Also, the Butler-Volmer equations are often used to describe the dependence of overvoltage on current density. However, a more detailed approach was developed by Bessler et al. [7]. All of these models of fuel-side electrochemical reactions based on pure hydrogen, i.e., it is assumed that carbon monoxide and methane are completely converted to hydrogen before the electrochemical reactions. However, alternative fuels usage was investigated in the works of Hajimolana et al. [8].

Moreover, Huang et al. [9] and Khazaee et al. [10] studied the effects of various designs of gas supply channels on the flow field and flow uniformity. The results showed a large flow non-uniformity between the inner and outer flow channels. A higher performance was observed with rectangular channel geometry compared to triangular and trapezoidal, where it provides more efficient fuel transportation, reducing the local current density in the downstream region. Unfortunately, in these works, the physicochemical characteristics of the materials were not well studied.

Additionally, in the development of the SOFC design, planar type designs are well studied because of the higher power densities compared with tubular type designs.

A planar type of anode-supported SOFC with a very thin electrolyte drastically decreases the ionic transport resistance and allows operation at intermediate temperatures and reduces material problems of SOFC.

This work is focused on the modeling of a single SOFC with planar construction, study of the reaction kinetics and calculation of the important electrochemical characteristics of the SOFC by optimizing their parameters. The numerical modeling was carried out by the finite element method. The planar SOFC design includes the most widely tested materials, such as the porous cathode – an oxide semiconductor compound of lanthanum manganite $La_{0.8}Sr_{0.2}MnO_3$; dense electrolyte - ZrO_2 doped with Y_2O_3 (8% YSZ); and the porous anode, NiO/YSZ based cermet. Analysis of the effect of the parameters such as operating temperature, geometry (thickness of SOFC components) and porosity shows that anode-supported SOFC is the more suitable construction type to achieve a high SOFC performance for the further experimental work.

SOFC Simulation

Electrochemical model

The macrokinetic processes in the SOFC components were studied using numerical modeling. As shown in Figure 1, the development of 3D model of a single planar SOFC calculations was performed using COMSOL Multiphysics 6.0 [22].

It is extremely important to understand and build an electrochemical model to determine the

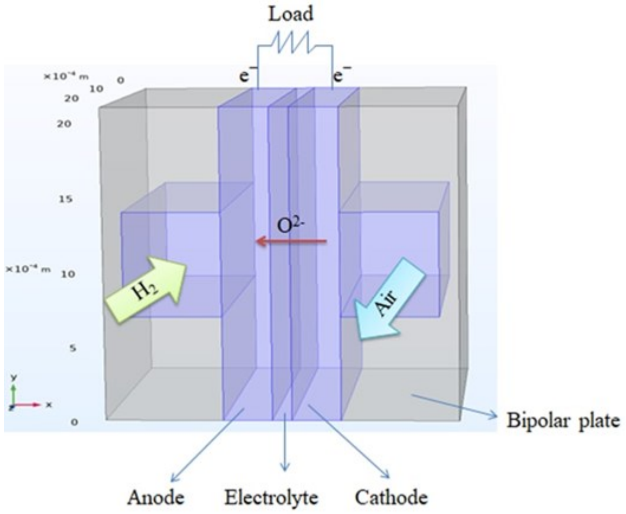


Figure 1. 3D model of the constructed planar SOFC.

kinetic parameters and to evaluate the possible mechanisms of SOFC reactions, which includes calculation of the following processes (free and porous media for gas flow):

- Study of electronic and ionic charge balance (using Ohm's law);
- Kinetics of charge transfer (described by the Butler-Volmer equation);
- Mass balance in gas-diffusion electrodes and gas channels (diffusion study based on the Maxwell-Stefan equation and convection);
- Flow distribution in gas channels (using the Navier-Stokes equations);
- Flow in porous gas diffusion of electrodes (using the Brinkman equations).

General electrochemical reactions in SOFC

The main electrochemical reaction of hydrogen oxidation proceeds with the release of water vapor and the formation of two electrons (Equation 1). On the anode side of the SOFC, at the three-phase boundary (TFB) such as solid electrolyte/electrode/gas, the fuel is oxidized by the atmospheric oxygen, which is ionized at the TFB with the cathode and passes through the solid electrolyte in the form of a doubly charged ion.

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

On the cathode side, oxygen is reduced to its ionic form by electrons supplied from an external load, the reaction is represented as follows:

$$O_2 + 4e^- \rightarrow 2O^{2-} \qquad (2)$$

The overall cell reaction is:

$$2H_2 + O_2 \rightarrow 2H_2O \qquad (3)$$

Kinetics of electrochemical reactions on electrodes

The kinetics of the charge transfer reactions described by the Butler–Volmer equation includes the calculation of the charge transfer current density.

The distribution of the current density and voltage for a single cell are calculated after the flow distribution for both fuel and air has been determined here. At this step, firstly need to calculates the corresponding local current density for each electrode.

Local exchange current density generated by electrochemical reactions at the anode $i_{loc,a}$, calculated by the following equation:

$$i_{loc,a} = i_0\left\{\exp\left[\frac{\alpha_a F\eta}{RT}\right] - \exp\left[-\frac{\alpha_c F\eta}{RT}\right]\right\}, \qquad (4)$$

where, $\alpha_c = n - \alpha_a$ is the charge transfer coefficient for the process in the cathode α_c and in the anode α_a and n is the number of electrons involved in the process.

The parameters of the gas mixture before the electrochemical reaction were calculated by determining the partial pressures of hydrogen and oxygen. The partial pressure of water vapor was taken from the main electrochemical reaction in SOFC.

Based on the partial pressure of hydrogen and water vapor reacted at the anode, the charge transfer kinetics equation is indicated as follows:

$$i_{loc,a} = i_{0,ref,a}(T)\left\{\frac{p_{h2}}{p_{h2,ref}}\exp\left[\frac{0.5F\eta}{RT}\right] - \frac{p_{h2O}}{p_{h2O,ref}}\exp\left[-\frac{1.5F\eta}{RT}\right]\right\}, \qquad (5)$$

where, $p_{h2,ref}$ and $p_{h2O,ref}$ - the initial value of the partial pressure of hydrogen and water.

The exchange current density for the reduction reaction proceeding at the cathode $i_{loc,c}$, calculated by using partial pressure of oxygen, as given in the following form:

$$i_{loc,c} = i_{0,ref,c}(T)\left\{\exp\left[\frac{3.5F\eta}{RT}\right] - \frac{p_{O2}}{p_{O2,ref}}\exp\left[-\frac{0.5F\eta}{RT}\right]\right\}, \qquad (6)$$

where, $p_{O2,ref}$ - initial value of oxygen partial pressure.

Temperature dependent initial value of the local current density $i_{0,ref}(T)$ was calculated separately for both anode and cathode.

$$i_{0,ref,a}(T) = RTk_a \exp\left(-\frac{Eact_a}{RT}\right)/2F \quad , (7)$$

$$i_{0,ref,c}(T) = RTk_c \exp\left(-\frac{Eact_c}{RT}\right)/4F \quad , (8)$$

where, $Eact_a$ and $Eact_c$ are activation energy of the charge transfer process at the anode and cathode.

The parameters for calculating the above expressions are given in Table 1 [5, 11].

Table 1

Parameters for calculating the exchange current density

Element	$k_{a,c}$	$Eact_{a,c}$ (kJ/mol)	n
Anode	6.54×10^{11}	140	2
Cathode	2.35×10^{11}	137	4

The total value of the current density is calculated by using the following equation:

$$i_v = a_v i_{loc} , \quad (9)$$

where, a_v - active surface area and i_{loc} - local exchange current density.

When current is supplied from the fuel cell, the operating voltage or actual voltage of the fuel cell (E) is less than the open circuit voltage, is given in this equation:

$$E = E_{вq} — (\eta_{act} + \eta_{ohm} + \eta_{conc}) \quad (10)$$

This is due to internal resistance and overvoltage losses associated with electrochemical reactions at the electrode/electrolyte interface. Ohmic losses η_{ohm} occur due to the electrical resistance of the electrodes and resistance to the flow of ions in the electrolyte. These losses are important for all types of fuel cells and proportional to the current density (i). Ohmic losses are described by the following equation:

$$\eta_{ohm} = iR_{ohm} , \quad (11)$$

where, R_{ohm} is the internal voltage on the cell, which can be calculated from the Equation 12:

$$R_{ohm} = \frac{\tau_{anode}}{\sigma_{anode}} + \frac{\tau_{electrolyte}}{\sigma_{electrolyte}} + \frac{\tau_{cathode}}{\sigma_{cathode}} \quad , (12)$$

where, τ and σ thickness and conductivity of each component of the system.

Activation polarization η_{act} occurs due to overcoming chemical reaction activation energy barrier, as at anode and as at cathode. Since the reduction of oxygen at the cathode is much slower than the oxidation of hydrogen at the anode, the activation overvoltage occurs mainly in cathode.

The activation (electrochemical) overvoltage is calculated from the next equation:

$$\eta = E_{c\tau} — E_{вq} , \quad (13)$$

from which $E_{c\tau} = \phi_s — \phi_l$, where, ϕ is the electric potential, and l and s denote the electrolyte and electrode, respectively.

It is assumed that the input potential at the anode is zero, and at the cathode the value is taken as follows:

$$V_{cell} = \Delta\phi_{eq,c} - \Delta\phi_{eq,a} - V_{pol} \quad (14)$$

The concentration polarization η_{conc} is determined by the intensity of fuel electrode diffusion at the electrode/electrolyte interface, due to the transfer of positive charges. To estimate such losses, it is necessary to know the distribution of component concentrations not only in the incoming fuel and air mixture, but also over the thickness of the anode and cathode, respectively. This polarization can cause a rapid cell voltage drop at a high current density.

The equilibrium potential $E_{вq}$, calculated by using the Nernst equation:

$$E_{eq} = E_{eq.ref}(T) - \frac{RT}{nF}\ln\prod_i\left(\frac{p_i}{1atm}\right)^{v_i} \quad , (15)$$

where, T - operating temperature; R - universal gas constant (equal to 8.314 J mol^{-1} K^{-1}); F - Faraday constant (equal to 96485.33°C mol^{-1}); n - number of electrons involved in the process (2 electrons at the anode and 4 electrons at the cathode); 1 atm - standard atmospheric pressure; ν_i - stoichiometric coefficients (positive for half-reaction products (oxidized form), negative for reagents (reduced form)).

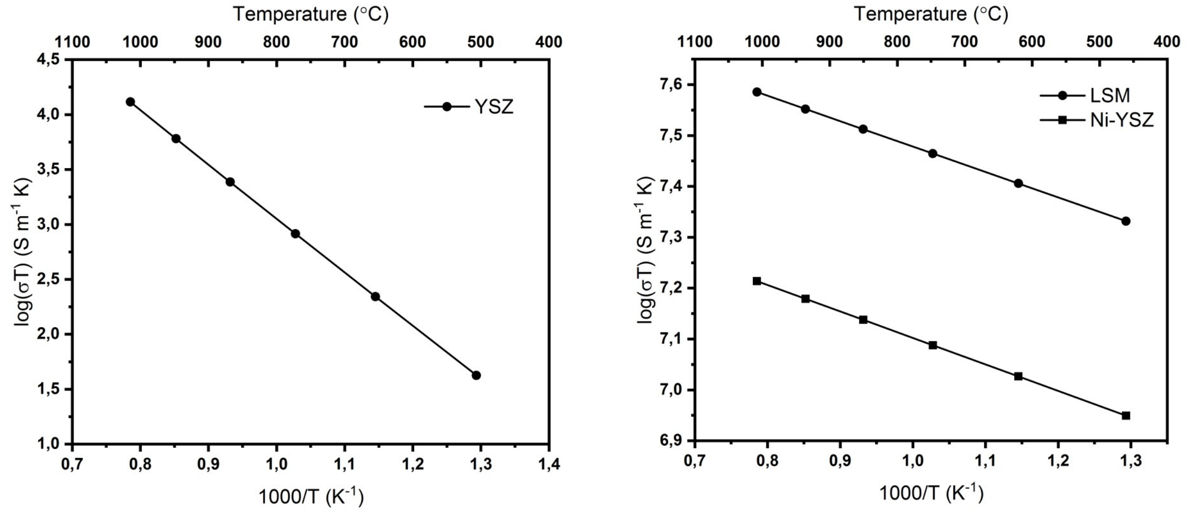
The current density and voltage in a single cell were calculated using the physical parameters, which are listed in Table 2.

The value of the ionic and electronic conductivity of the cell materials were set at temperature range 600–800 °C [24]. For this, an Arrhenius plot, the ratio of σT and 1000/T, was built for each individual SOFC component (8YSZ, LSM and Ni-YSZ) (Figure 2). The Figure 2 clearly displays a straight line of electrical conductivity of the materials. It is also observed that the values of the electrical conductivity of the electrode materials significantly exceed the value of the ionic conductivity of the electrolyte material. It should be noted that the conductivity of both cathode and anode, as well as the electrolyte material were increased within temperature increase.

Table 2

Parameters of SOFC materials used in the modeling

Physical variables	Components of SOFC			Reference
	Cathode LSM	Electrolyte YSZ	Anode NiO-YSZ	
Density, (kg m^{-3})	4375	5160-5757	3030-3310	12, 16
Porosity (units)	0.3-0.4	-	0.3-0.4	2, 3, 12, 14, 15
Thermal conductivity, (W m^{-1} K^{-1})	1.15	1.90-2.7	6.23-11	12, 16
Specific heat capacity, (J kg^{-1} K^{-1})	565	470-658.74	450-595.50	12, 16
Specific surface area, (m^{-1})	2.25×10^6	-	5.57×10^6	4
Permeability, (m^2)	1.76×10^{-9}	-	1.76×10^{-9}	13



a **b**

Figure 2. Arrhenius plot (ratio σT to 1000/T) for each individual SOFC component (a) 8YSZ, (b) LSM and NiO-YSZ.

The conductivities of the pure material (in S cm^{-1} unit) were extrapolated from LSM, YSZ and NiO-YSZ materials information based on the data from Table 3. The Arrhenius graphs on the dependence of temperature conductivity, were compiled to analyze the activation energy and the reaction rate. It should be noted that the pre-exponential factor is most important variable in calculation of the ionic conductivity of materials (Table 3). Moreover, it can be used to study the energy of ion migration within a crystal structure. The Arrhenius equation is described in the following form:

$$\sigma T = A\ exp\left(\frac{E_a}{kT}\right), \tag{16}$$

where A is pre-exponential factor for the reaction, E_a is activation energy of ionic conduction, k is Boltzmann constant, and T is temperature.

Following the expressions presented below, the calculations of the ionic and electronic conductivity of SOFC components were carried out in this research:

$$\sigma_{s,a} = \frac{9.5\times10^7}{T}\exp\left(\frac{-1150}{T}\right) \tag{17}$$

$$\sigma_{s,c} = \frac{4.2\times10^7}{T}\exp\left(\frac{-1200}{T}\right) \tag{18}$$

$$\sigma_{l,el} = 3.34\times10^4\exp\left(\frac{-10300}{T}\right) \tag{19}$$

Table 3

Electronic and ionic conductivity of SOFC components [17, 18, 19]

Components of SOFC	Activation energy, E$_a$ (eV) at 600-800 °C	Pre-exponential factor
LSM	0.0991 (9.56 kJ mol^{-1})	9.50×10^7
YSZ	0.8876 – 0.9804 (85.65 – 94.6 kJ mol^{-1})	3.34×10^4 - 1.64 10^8
NiO/YSZ	0.1034 (9.98 kJ mol^{-1})	4.20×10^7

Results and discussions

In this study, the effect of geometry, temperature, and material properties on the current-voltage and power characteristics of a SOFC are investigated. A comparison of the electrochemical characteristics of three main types of SOFC supported constructions, such as anode-, cathode-, and electrolyte-supported, is performed. It has been established that the use of a NiO/YSZ anode -supporting SOFC structure with a thin electrolyte is promising material in order to provide higher productivity by reducing ohmic losses.

The main contribution to power losses is made by the resistance of electrochemical reactions taking place on the cathode, as well as the ohmic resistance of the electrolyte. Therefore, the efficiency of a solid oxide fuel cell is determined, first of all, by its total internal resistance. In previous studies [21], the thickness of each element with one of the supporting elements has a strong impact on many processes occurring in SOFC. So, for example, SOFCs with an electrolyte-supporting structure have ohmic losses in the electrolyte layer. Therefore, SOFCs are so tied to the thickness of the electrolyte substrate [23]. In SOFCs with a cathode-supporting structure, the cathode electrode is a problem because oxygen diffusion is suppressed due to the thickness of the cathode layer. Also, a thin anode layer leads to overvoltage and the process of delamination. However, these effects do not affect SOFC characteristics as much as ohmic losses [21] (details of studies of electrolyte-supporting and cathode-supporting design are presented in “Supporting information”).

A specific optimal geometry is inherent to each SOFC element, along with the choice of electrochemical and physical parameters for the materials involved. These selections are made considering the temperature-dependent behavior of the materials. Modeling details and a list of input parameters are given in “Supporting information”. To simplify the model, the following assumptions were made: i) all gases behave as ideal gases; ii) the fuel cell operates under steady state condition; iii) water is only in the vapour phase; iv) flow is laminar.

The output power density was calculated from Ohm's law by Equation 20.

$$P_{density} = I_{density} \times V_{cell}, \quad (20)$$

and output power of SOFC can be calculated by Equation 21.

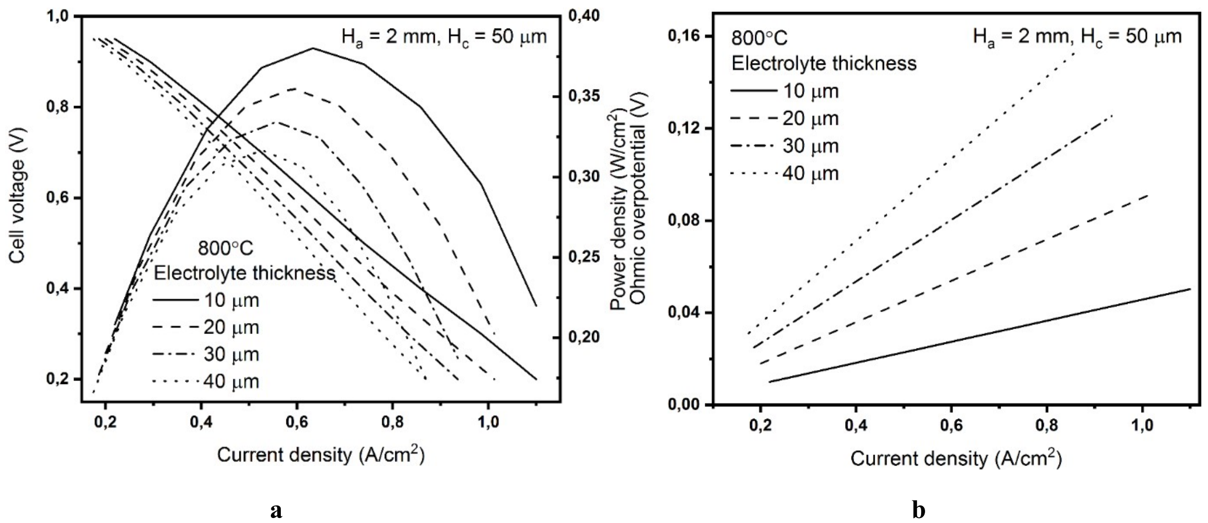
$$P = P_{density} \times S_{active} \quad (21)$$

Effect of support layer thickness at anode-supported SOFC

Based on the theoretical and experimental results of works [1-3], the selection of the optimal thickness of the SOFC supported element was made.

The effect of electrolyte and cathode thickness on polarization losses. Analysis of the obtained electrochemical characteristics

Figure 3 shows the results of calculations for the ohmic losses of the anode-supporting SOFC for various electrolyte thicknesses. The thickness of the electrolyte varied from 10 to 40 µm, with the anode thickness H_a=2 mm and the cathode thickness H_c=50 µm at the same operating temperature of 800°C. The influence of the electrolyte thickness on the current-voltage and power characteristics were studied (Figure 3a).



a **b**

Figure 3. Effect of electrolyte thickness on (a) current-voltage and current-power characteristics, (b) ohmic overpotential at the 800 °C.

Ohmic losses of the electrolyte and cathodic polarization resistance are two important issues that hinder the SOFC from lowering its operation temperature from the traditional 1000 °C to an intermediate range of 500–800 °C. The ohmic losses can be decreased by the reduction of the thickness of the conventional yttria-stabilized zirconia (YSZ) electrolyte and/or the use of materials with faster ionic transport over YSZ.

The ohmic polarization on the current density dependance was studied. Figure 3b shows a linear relationship between current density and ohmic polarization. Ohmic losses increase with the raise in the thickness of the electrolyte. They reach up to 0.16 V at a current density of 0.85 A/cm^2.

Indeed, a decrease in the thickness of the electrolyte leads to a lower internal resistance of the cell and high power characteristics [20]. Figure 3a displays that the shape of all power curves has the same character when the thickness of the electrolyte changes. The power characteristics increase from 0.31 to 0.38 W / cm2 with a decrease in the thickness of the electrolyte from 40 to 10 microns. The maximum output power density is achieved with an electrolyte thickness of 10 microns, which is 0.38 W/cm^2 at a current density of 0.62 A/cm^2.

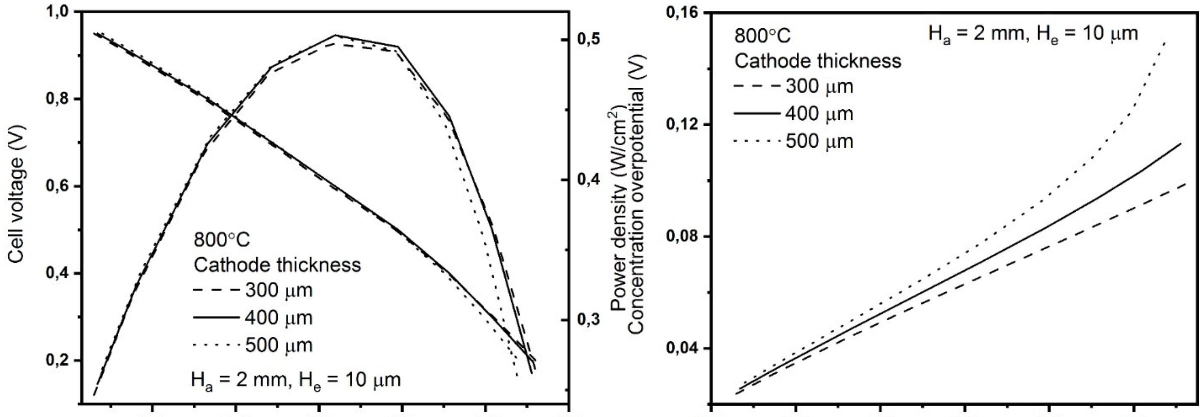
The decrease in the equivalent resistivity of SOFC is apparently due to an increase in the surface area through which oxygen ions are goes into the electrolyte. In the case of a porous cathode, this area is limited by the points of contact of the cathode granules with the electrolyte. In the case of a thin-film dense cathode, this area is the entire surface of the electrolyte covered by the cathode.

In studying the effect of the thickness of the cathode of the SOFC anode-supporting structure on the electrochemical characteristics and in order to achieve the most optimal geometry with the best performance, a number of observations was made. The cathode thickness was varied from 300 to 500 μm at a fixed anode thickness of H_a=2 mm and an electrolyte thickness of H_e=10 μm, at an operating temperature of 800°C. However, it should be noted that there were no obvious changes in the power characteristics with a change in the cathode thickness (Figure 4). The largest value of the output power density was 0.5 W/cm^2 at a current density of 0.85 A/cm^2. Changing the thickness of the cathode does not affect the increase or decrease in ohmic losses. However, while studying the concentration losses, the dependence of the concentration polarization on the current density showed that the largest concentration losses are observed at a cathode thickness of 300 μm (1.5 V at a current density of 1.2 A/cm^2), and the smallest losses are observed at 500 μm (0.9 V at a density current 1.3 A/cm^2). However, at a cathode thickness of 400 μm, minimal concentration losses (0.11 V at a current density of 1.3 A/cm^2) and the best power characteristics are also observed (Figure 4 a, b).

As the inlet temperature is increased, the electrochemical reaction is enhanced, and thus the position of the maximum current density is shifted towards the region where hydrogen concentration is higher. The main reason for the performance deterioration is an increase in the internal resistance of the cell due to a decrease in the ionic conductivity of the electrolyte material. Therefore, it is necessary to use the materials with higher ionic conductivity or to reduce the thickness of the electrolyte to move to the intermediate temperature range.

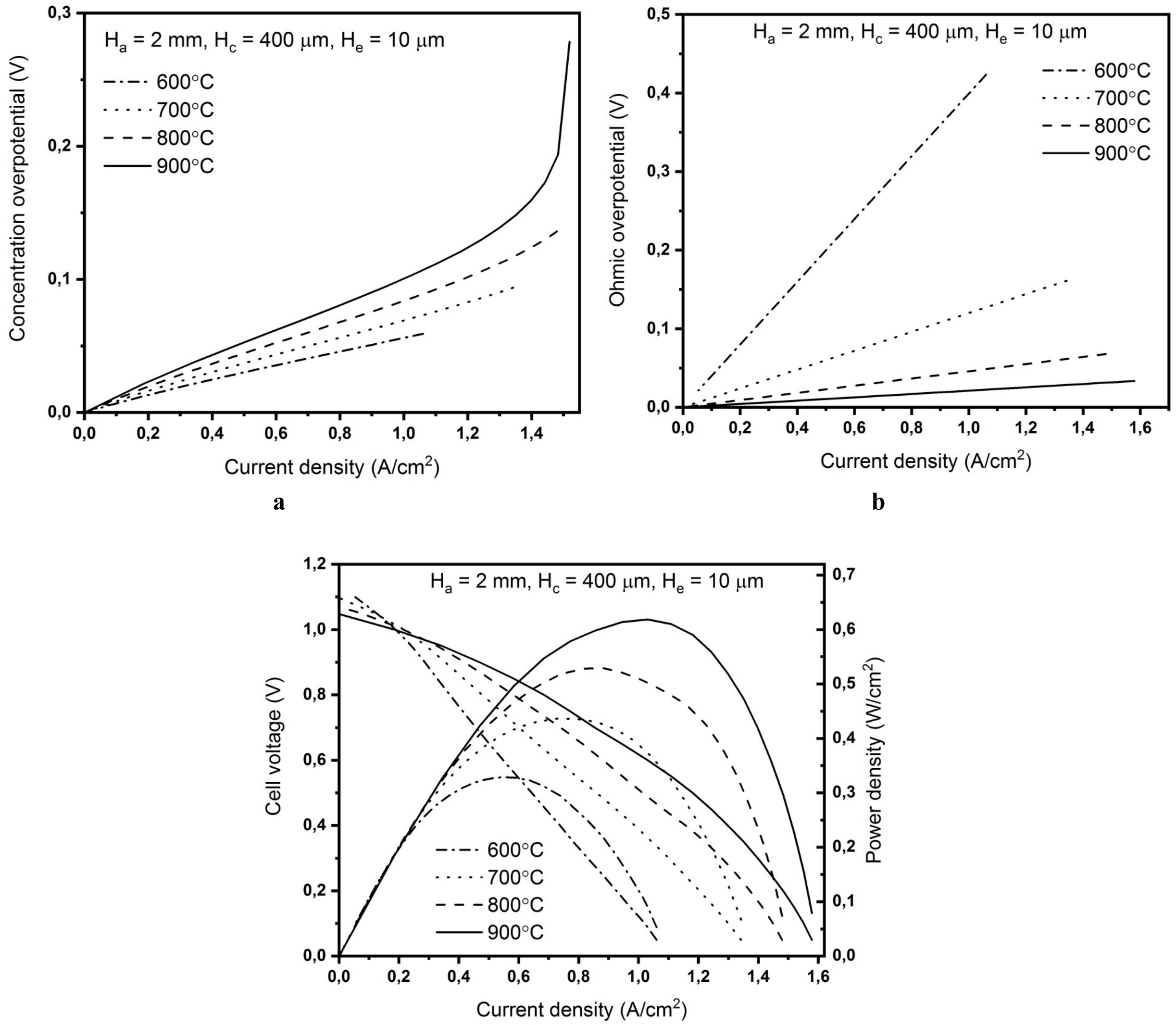
Effect of electrode's porosity.

To create a highly efficient electrochemical device, various SOFC parameters are optimized, including the porosity of the electrode material. Electrode's porosity is an important microstructural parameter because it affects both the gas



a b

Figure 4. Effect of cathode layer thickness on (a) current-voltage and current-power characteristics, (b) concentration losses.



a

b

c

Figure 5. Effect of temperature on (a) concentration losses, (b) ohmic overpotential, (c) current-voltage and current-power characteristics of anode-supported SOFC.

transport and the charge transport properties. Increasing the electrode's porosity will improve gas diffusivity. Studies on the effect of porosity on the current-voltage and power characteristics prove that the current density and the output power density increase with the raise in porosity. For example, at a porosity of 30%, the maximum output power is 0.5 W/cm^2 at a current density of 0.83 A/cm^2, and at an electrode material porosity of 45%, the maximum output power density is 0.58 W/cm^2 at a current density of 1.1 A/cm^2 (Figure 6). These results helped us to create a numerical model close to reality based on the parameters of experimental literature data. We settled on more realistic parameters with a porosity of 30% (close to the practical electrode's porosity).

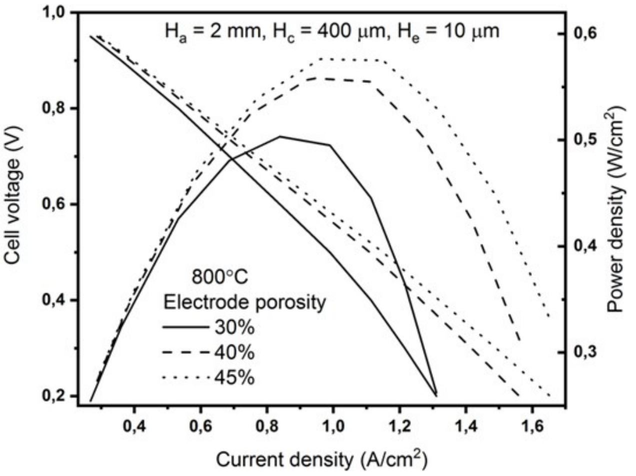


Figure 6. Effect of electrode's porosity on current-voltage and current-power characteristics of anode-supported SOFC.

During the study, an analysis of polarization was carried out on the concentration and ohmic losses with a change in the porosity of the electrode material. It was found that the change in the electrode's porosity in the range of 0.3-0.45 does not significantly effect on the concentration and ohmic losses.

Parametric optimization analysis

Table 4

Comparative characteristics of SOFC with the main types of supported element at an operating temperature of 900 °C.

Type of supported element	Thickness of SOFC main components, mm			Maximum output power density at 900 °C, W cm^{-2}
	Anode	Electrolyte	Cathode	
Anode-supported	2	0.01	0.4	0.585
Cathode-supported	0.15	0.002	0.5	0.54
Electrolyte-supported	0.04	0.15	0.08	0.325

Comparative analysis of investigated types of supported constructions of planar SOFC under different operating parameters is presented in Table 4 and operating temperatures of 600 °C and 800 °C in Figures 7 and 8.

The results demonstrate the fact that when the temperature decreases from 900 °C to 600 °C, the characteristics of SOFC based on the traditional materials (NiO/YSZ – YSZ – LSM) drop off dramatically. The electrochemical characterization of the single SOFC demonstrated in Figures 7 and 8 shows that when the temperature drops from 900 °C to 600 °C, the output power density of all the presented types of constructions drops by 2 times.

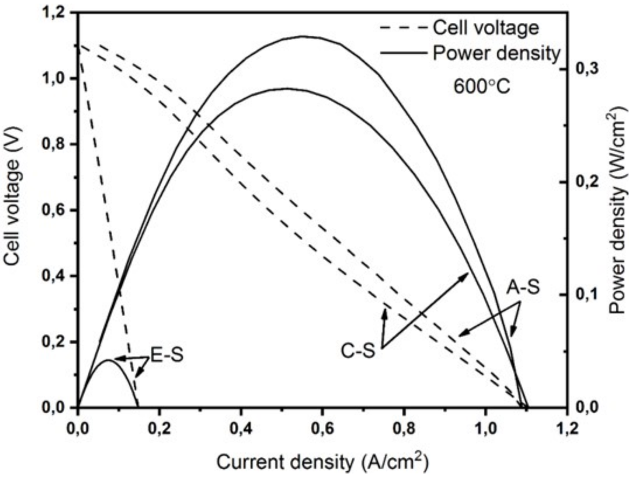


Figure 7. Comparative analysis of the effect of type construction (anode-, cathode-, electrolyte-supported) on I-V and power characteristics at an operating temperature of 600°C.

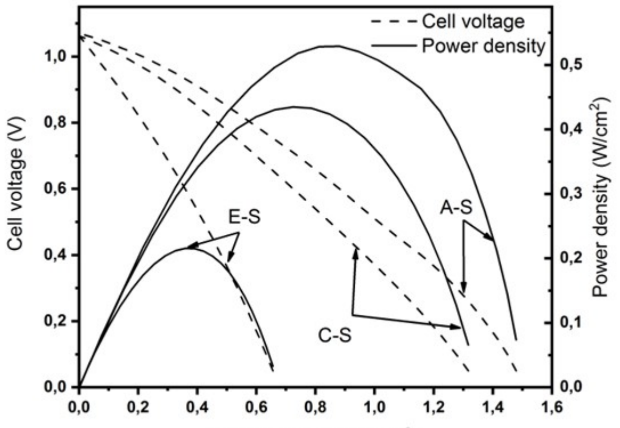


Figure 8. Comparative analysis of the effect of type construction (anode-, cathode-, electrolyte-supported) on I-V and power characteristics at an operating temperature of 800 °C.

Conclusions

Thus, a 3D model was developed to predict the performance of the SOFC. Detailed comparisons between types of construction, such as anode-, cathode-, and electrolyte-supported, are made to illustrate the role of the cell design on the SOFC's performance.

We studied the performance of the fuel cell components in different values of concentration and ohmic polarizations along its gas channels; temperature; porosity and geometry under optimal boundary conditions. The obtained results allow us to analyse qualitatively and quantitatively and design fuel cells with optimal characteristics. This is especially important for the fabrication of IT-SOFCs, and they are useful to consist of thin-film layers of electrolyte and electrodes. Currently, the highest performance is achieved in SOFCs with a supporting anode, in which the thickness of one of the electrodes is much larger than the thickness of the other two layers of the electrode-electrolyte structure. In cells of this type, the mass transfer in the reference electrode significantly affects the power and efficiency of the cell as a whole. However, it should be noted that the electrolyte thickness also depends on the electrolyte material.

Numerical analyses have shown that the highest output power density is observed in the SOFC anode-supporting structure at an operating temperature of 900 °C and reaches a value of 0.585 W cm^{-2} at a current density of 1 A cm^{-2}. In the cathode-supported SOFC at an operating temperature of 900 °C, the output maximum power density reaches 0.54 W/cm^{2} at current density of 0.9 A/cm^{2}. In the electrolyte-supporting SOFC structure at an operating temperature of 900 °C, the maximum output power density is 0.325 W cm^{-2} at a current density of 0.58 A cm^{-2}. In future studies, authors intend to extend this study by performing a time-dependent analysis and thus define a dynamic model for SOFC performance.

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REFERENCES

1. Wang K., et al. A review on solid oxide fuel cell models. *International journal of hydrogen energy*, 2011. 36/12, 7212-7228.
2. Kakac S., Pramuanjaroenkij A., Zhou X.Y. A review of numerical modeling of solid oxide fuel cells. *International journal of hydrogen energy,* 2007. 32/7, 761-786.
3. Andersson M., Yuan J., Sundén B. Review on modeling development for multiscale chemical reactions coupled transport phenomena in solid oxide fuel cells. *Applied Energy*, 2010. 87/5, 1461-1476.
4. Chan S., Khor K., Xia Z. A complete polarization model of a solid oxide fuel cell and its sensitivity to the change of cell component thickness. *Journal of power sources*, 2001, 93/1-2, 130-140.
5. Patcharavorachot Y., Arpornwichanop A., Chuachuensuk A. Electrochemical study of a planar solid oxide fuel cell: Role of support structures. *Journal of Power Sources*, 2008, 177/2, 254-261.
6. Bessler, W.G., et al., Model anodes and anode models for understanding the mechanism of hydrogen oxidation in solid oxide fuel cells. *Physical Chemistry Chemical Physics*, 2010, 12/42, 13888-13903.
7. Bessler W.G., Gewies S. Vogler M.A new framework for physically based modeling of solid oxide fuel cells. *Electrochimica Acta*, 2007, 53/4, 1782-1800.
8. Hajimolana S.A., et al. Mathematical modeling of solid oxide fuel cells: A review. *Renewable and Sustainable Energy Reviews,* 2011, 15/4, 1893-1917.
9. Huang C., Shy S., Lee C. On flow uniformity in various interconnects and its influence to cell performance of planar SOFC. *Journal of Power Sources*, 2008, 183/1, 205-213.
10. Khazaee I., Rava A. Numerical simulation of the performance of solid oxide fuel cell with different flow channel geometries. *Energy*, 2017, 119, 235-244.
11. Aguiar P., Adjiman C., Brandon N.P. Anode-supported intermediate temperature direct internal reforming solid oxide fuel cell. I: model-based steady-state performance. *Journal of power sources*, 2004, 138/1-2, 120-136.
12. Sui Z.-J., et al. Effect of preparation method and particle size on LaMnO3 performance in butane oxidation. Catalysis Communications, 2011, 12/15, 1437-1441.
13. Peksen M., et al. Numerical modelling and experimental validation of a planar type pre-reformer in SOFC technology. *International journal of hydrogen energy*, 2009, 34/15, 6425-6436.
14. Yuan J., et al. Analysis of parameter effects on chemical reaction coupled transport phenomena in SOFC anodes. *Heat and Mass Transfer*, 2009, 45/4, 471-484.
15. Andersson, M., et al. Modeling validation and simulation of an anode supported SOFC including mass and heat transport, fluid flow and chemical reactions. in International Conference on Fuel Cell Science, Engineering and Technology, 2011.
16. Tseronis K., Kookos I., Theodoropoulos C. Modelling mass transport in solid oxide fuel cell anodes: a case for a multidimensional dusty gas-based model. *Chemical Engineering Science*, 2008, 63/23, 5626-5638.
17. Joy P., Date S. On the low-temperature anomaly in the AC susceptibility of La0. 9Ca0. 1MnO$_3$. *Journal of magnetism and magnetic materials*, 2000, 220/2-3, 106-114.
18. Shi J., Xue X. CFD analysis of a symmetrical planar SOFC with heterogeneous electrode properties. *Electrochimica Acta*, 2010, 55/18, 5263-5273.
19. Ni M., LeungM.K., LeungD.Y. Micro-scale modelling of solid oxide fuel cells with micro-structurally graded electrodes. *Journal of Power Sources*, 2007, 168/2, 369-378.
20. Kuzmin A., et al., Chemical solution deposition and characterization of the La1-xSrxScO3-α thin films on La1-xSrxMnO3-α substrate. *International Journal of Hydrogen Energy*, 2018, 43/41, 19206-19212.
21. Ilbas M., Kumuk B. Numerical modelling of a cathode-supported solid oxide fuel cell (SOFC) in comparison with an electrolyte-supported model. *Journal of the Energy Institute*, 2019, 92/3, 682-692.
22. Comsol, V., 3.5, Comsol AB, Stockholm, Sweden.
23. Milewski J., Miller A. Influences of the type and thickness of electrolyte on solid oxide fuel cell hybrid system performance. *J. Fuel Cell Sci. Technol.* 2006, 3/4, 396-402. DOI: 10.1115/1.2349519
24. Yamamoto O. Solid oxide fuel cells: fundamental aspects and prospects. *Electrochimica Acta,* 2000, 45/15-16, 2423-2435.