Numerical analysis of thermal stresses in a new design of microtubular stack

1 Introduction

A typical operating temperature of microtubular Solid Oxide Fuel Cells (mSOFCs) is above 650°C, which affects the thermomechanical behaviour of the stack. Therefore, a key issue in the fuel cell improvement and maximizing its efficiency as well as fuel cell endurance is thermal management. The temperature of the mSOFCs is usually controlled by varying the air flow rate supplied to the cathode channels [1]. The average fuel cell temperature can be effectively controlled using this method, but temperature distributions across the stack still will depend on its design. Vijay et al. [2] demonstrated that the fuel cell physical design played an important role in determining the thermal distributions. A new design for the SOFC planar stack included a secondary air channel with flow in the counter direction to that in the cathodic air channel was proposed by [2] for the purpose of effective cooling. The authors found that the new design was capable to reduce the steady state temperature difference across the cell to less than 2 K over a range of voltages, achieving fuel utilization of above 75%. It was noticed that addition of a secondary air stream for cooling led to elimination of the temperature non-uniformity and to a reduction of thermal stresses in the stack. The effect of the uniformity of flow distribution on the performance of a SOFC was analysed also by [3]. The base planar configuration consisted of a cell placed between mesh type flow field at the anode and straight channels at the cathode side. The initial design was modified by changing the flow geometry, also inlet manifolds were modified to reduce heterogeneity in reactant distribution over the active area. About 50% enhancement in performance was observed by introducing better uniformity in the flow distribution. Boigues-Munoz et al. [4] indicated temperature control of the tubular SOFC stack as a major relevance in the overall efficiency of a complete micro-CHP system. High temperature gradients in the tubular fuel cell above 100°C triggered by high current densities or insufficient cooling air stream have to be avoided due to detrimental effects for the cell’s long durability.
Moreover, the high heat-up rates required for SOFC stacks are also responsible for high thermal gradients occurring in the inlet regions of hot gases. In order to avoid high local thermal gradients and prevent high stresses in the stack components Al-Masr et al. [5] simulated the transient heating-up process of a full scale planar SOFC stack. From the predicted temperature distribution it was found that the inlet region of the heating gas was subjected to high thermal loads. It was noticed that after 4180 s of the process the hot spots that appear at the time instant of 2010 s were reduced due to reduction of the mass flow rate of the heating air to its minimum. However, at the end of the heating-up process of 8015 s higher temperature gradients appeared in the gas outlet regions. High temperatures as well as high gradients occurred in the inlet as well as outlet regions. Thus, it was concluded that there is a high probability of existence of considerable thermal stresses in these areas. Similar results were obtained by Mounir et al. [6] for an integrated-planar Solid Oxide Fuel Cell (IP-SOFC). It was found that the IP-SOFC was subjected to moderate thermal stress at the fuel inlet and a high thermal stress at the outlet. In addition, the results showed that the magnitude of the gradient stress was dependent on temperature difference in the anode and electrolyte, as well as on the electrolyte and cathode modulus.

In addition, the temperature distributions of MEA for co-flow and counter-flow cases in planar solid oxide fuel cells were studied by Wang et al. [7]. The average temperature of MEA were 979°C and 996°C in co-flow and counter-flow cases, respectively. The temperature of MEA increased uniformly along the direction of fuel flow and was the highest near the fuel outlet for the co-flow case, while for the counter-flow case the temperature increased rapidly, reached a maximum of 1088°C near the fuel inlet and then gradually dropped. From these two considered flow configurations, the co-flow case had more uniform temperature distribution and smaller temperature gradients from the air inlet to the outlet [7]. Yakabe et al. [8] performed a wide numerical analysis for a planar SOFC with double channels of co-flow or counter-flow pattern. The internal and external steam reforming and the water shift reaction were taken into account in the developed model. Based on the simulated temperature distributions in the electrolyte and interconnector authors calculated stress distributions with the help of finite element program ABAQUS. In the co-flow pattern the drop of the electrolyte temperature was observed due to endothermic steam reforming and an increase of the sheet resistance. For the external reforming the maximum tensile stress was one order of magnitude smaller than those for the internal methane reforming due to lack of the temperature drops coming from the endothermic reaction. Moreover, stress concentration occurred at different areas in comparison to the internal reforming. For the co-flow pattern the maximum tensile stress in the electrolyte was reduced as compared with the counter-flow case [8]. Three flow configuration: cross-flow, co-flow and counter-flow were examined also by Recknagle et al. [9]. For similar fuel utilization and average fuel cell temperature it was found that the co-flow case had the most uniform temperature distribution and the smallest thermal gradients.

Heating up with hot air and in a furnace was considered also by Ki et al. [10], who presented a computational model that allows to investigate transient behavior of a planar SOFC during the start-up process. The study confirmed that different initial heating rates of furnaces as well as different hot air flow rates resulted in different thermal gradients inside the stack. Therefore, heating rates or hot air flow rates have to be controlled depending on the maximum thermal stress or thermal gradient for specific stack design.

The thermal-mechanical deformations and stresses of a joined assembly of a window frame, seal and anode structure were evaluated by a finite element model developed by Weil and Koeppel [11]. The results revealed that the foil seal was able to accommodate a significant degree of thermal mismatch strain between the metallic support structure and the ceramic cell via elastic deformation of the foil and plasticity in the foil to cell braze layer. Yakabe et al. [12] examined experimentally and numerically the residual thermal stresses in the electrolyte of anode supported planar Solid Oxide Fuel Cells. The effect of the sample cut on the residual stress was studied. The simulation results showed that if the cell size was more than 5 mm, the calculated stress was almost independent of the cell size. Moreover, the residual stresses in the electrolyte were calculated for a combination of the anode and electrolyte thickness and it was found that the combination of the thin anode and the thick electrolyte decreased the residual stress in the electrolyte.

In most studies mentioned above, either planar or integrated-planar SOFC stacks were considered. Less attention has been given to model the thermal stresses in tubular or microtubular SOFC stacks [13,15]. Nakajo et al. [13] adopted a simplified Weibull analysis to study the evolution of the probability of survival of a tubular SOFC at operating points and load changes. They developed a model for calculating thermal stresses in their tubular cell. The stress fields displayed high tensile stresses in limited areas in the electrolyte at the ends of the fuel cell and significant values in the whole
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The magnitude of the stresses was higher at the fuel and air inlets, where the internal steam-reforming reaction induced a temperature drop.

Cui and Cheng [14] considered also that the stress inside the microtubular SOFC region occurred due to mismatch between the thermal expansion coefficient of the materials of the membrane electrode assembly. The results indicated that the microtubular SOFC can operate safely, but if there is any interfacial defect, or a high tensile stress applied in the electrolyte then a SOFC stack failure arises.

Specific studies were performed by Serincan et al. [15], who investigated the effect of sealant and alumina tube, as well as of the spatial temperature gradient on stress distributions. Two types of analyses were performed: predicting the residual stresses in the standalone SOFC at room temperature and predicting the stresses in an operating SOFC. It was noticed that the effect of the spatial temperature distribution was minimal for typical SOFC operation at mid-range current densities, while near the fuel cell-sealant interface the stress distribution changed significantly.

Moreover, a dynamic model of a single tubular SOFC combining heat, species transport and electrochemical reactions at the steady-state and transient conditions was studied by Xue et al. [16]. The analysis showed non-uniform current and Nernst potential distributions along the longitudinal direction caused by non-uniform fuel and gas partial pressures along the flow direction. The purpose of the present work is to study the thermal stresses in a microtubular SOFC stack based on a developed three-dimensional model that was solved using the commercial software ANSYS Fluent and ANSYS Mechanical. The key feature of the model consists in numerical coupling of the three-dimensional Computational Fluid Dynamics technique, used for an accurate evaluation of the flow and temperature distributions inside the mSOFC stack, with Computational Structural Mechanics Finite Element Method (FEM) analysis that allows to predict thermal stresses. A similar approach was applied by Wei et al. [17], Yakabe et al. [8,12], Nakajo et al. [13], Liu et al. [18] and Peksen [19,20].

Wei et al. [17] estimate thermal stress distributions in a new design of a hexagonal stack consisting of planar anode-supported Solid Oxide Fuel Cells. The results obtained by [17] revealed that the use of Grancrete cell support reduced the maximum principal stress of the planar fuel cell and the calculated maximum von Mises stress was lower that the yield strength of stainless steel. Based on the evidence that it was possible to optimize construction of the planar SOFC stack, a similar approach was developed and is presented in this paper with respect to a microtubular Solid Oxide Fuel Cell stack.

In this paper, a three-dimensional model of a new design of anode-supported microtubular SOFC stack is developed. A parametric analysis has been done to evaluate the effect of some important parameters such as geometric features, fuel cell arrangement in the new mSOFC stack design as well as of material properties and temperature distributions. In addition, a modified air cooling system with longitudinal slots located over the circumference of the dodecagon housing. The applied numerical analysis allowed to study the condition in the new mSOFC stack design without the need to build it saving a significant amount of costs and time.

2 Numerical approach

In this section the numerical approach is presented starting from a description of the coupling of the CFD and FEM analysis, then thermo-mechanical model is explained in more details. Finally, mSOFC stack geometry and numerical mesh as well as boundary conditions are given.

2.1 Thermo-fluid model

For the joint fluid dynamic and heat transfer analysis, performed in the first step of this study, the commercial Computational Fluid Dynamics (CFD) software ANSYS Fluent with additional electrochemistry ANSYS Fuel Cell module were used. The simulations considered mass and heat transfer, fluid flow, species and energy transport at the stack level, while the electrochemical performance in details was analysed at the single fuel cell level. The numerical approach applied in this study for the single fuel cell modelling based on the Membrane Electrode Assembly (MEA) approach, which was presented in references [21,22] will be not discussed here in details. The main idea of the MEA approach was to take into account the fuel channel influence on the processes inside the membrane electrode assembly using a linear concentration distribution at the outer surface of the anode. The single fuel cell model consisted of the conservation equations for mass, momentum, thermal energy and species. These transport equations were coupled with the electrochemical processes through source terms describing the relevant processes in a fuel cell. The electrical sub-model included the ionic/electronic charge transfer equations and the Ohm's law for the ion/
electron transfer in the cell electrolyte. The Butler-Volmer equation was used to describe the reactant concentrations by considering diffusion polarization. During the second step of this study a Computational Structural Mechanics (CSM) analysis based on the Finite Element Method was performed. The calculated temperature distributions were used by the stress solver in the commercial ANSYS Mechanical package to analyze the distribution of thermal stresses on a mSOFC stack including the von Mises stress as well as maximum principal stress in ceramic materials. All these interactions may be summarized schematically in a block diagram presented in Fig. 1.

The steady-state laminar fluid flow at Reynolds number equal to 14.1 coupled with heat transfer can be described by the thermo-fluid model consisting of steady-state conservation of mass, momentum and energy equations:

\[ \nabla \cdot ( \rho \vec{u} ) = 0 \]  
\[ \rho \vec{u} \cdot \nabla \vec{u} = - \nabla p + \nabla \cdot \left[ \mu \left( \nabla \vec{u} + \left( \nabla \vec{u} \right)^T \right) \right] - \frac{2}{3} \mu \nabla \cdot \vec{u} \]  
\[ \nabla \cdot \left( \rho c_p T \vec{u} \right) = \nabla \cdot ( \lambda \nabla T ) \]  

where: \( \vec{g} \) is the acceleration due to gravity, \( p \) is the static pressure, \( \rho \) is the density of air, \( \mu \) is the air dynamic viscosity, \( \vec{u} \) is the velocity vector, \( c_p \) is the specific heat capacity, \( T \) is the temperature, \( \lambda \) is the thermal conductivity of the fluid. No-slip boundary conditions for fluid velocity were applied at cell and stack walls. The equations were solved using a pressure-based algorithm.

In the energy balance equation (4) for the k-th surface emission, absorption and reflection of the thermal radiation by solid boundary surfaces of the mSOFC stack and fuel cell tubes were considered:

\[ q_{out,k} = \varepsilon_k \sigma T_k^4 + (1 - \varepsilon_k) q_{in,k} \]  

where: \( q_{in,k} \) is the energy flux incident to a surface from surroundings calculated from Eq. (5):

\[ q_{in,k} = \sum_{j=1}^{N} F_{kj} q_{out,j} \]  

where: \( q_{out,j} \) is the energy flux leaving the j-th surfaces, \( \varepsilon_k \) is the surface emissivity, \( \sigma \) is the Boltzmann constant, \( T_k \) is the temperature of the k-th surface, \( F_{kj} \) is the dimensionless view factor. The Surface to Surface (S2S) radiation model was used in this study with the internal emissivity values of 0.8 for the stack wall and 0.4 for cell tube walls, respectively.

The electrochemical model used in this study was presented in details in reference [21] and based on the ANSYS Fuel Cell module.

### 2.2 Thermo-mechanical model

The thermo-mechanical model has been explained comprehensively in reference [15,23] and the governing equations are summarized below assuming that fuel cell materials, manifolds and housing undergo linear, elastic deformation, when subjected to thermal loads. In this paper similar assumptions were used. However, it should be highlighted that the stack housing constructed of an Inconel X 750 is a metal alloy and will undergo both elastic and plastic deformations. Thus, the assumption...
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In linear deformation the total strain, $\epsilon$, consists of elastic and thermal contributions as follows:

$$\{\epsilon\} = \{\epsilon_{el}\} + \{\epsilon_{th}\}$$  \hspace{1cm} (6)

Strain has three longitudinal and three shear components, $\epsilon_i$ and $\epsilon_{ij}$, respectively. They are expressed in engineering notation as normalized displacement $u_i$ along selected coordinates, $x_j$, where $i \neq j$:

$$\epsilon_i = \frac{\partial u_i}{\partial x_i}$$  \hspace{1cm} (7)

$$\epsilon_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$  \hspace{1cm} (8)

The thermal strain was calculated as:

$$\epsilon_{th} = \alpha \left( T - T_{ref} \right)$$  \hspace{1cm} (9)

where: $\alpha$ is the coefficient of thermal expansion (CTE) of a modeled material, $T$ stands for local temperature obtained from the thermo-fluid model in the first stage of simulation, $T_{ref}$ is the stress free temperature presented in Table 1. The stress free temperature is critical as it affects the magnitude of the thermal stress induced in the material. Therefore, the stress free temperature value was assumed as the sintering temperature of the anode layer with the electrolyte and it was equal to 1473 K, while connection of the anode and electrolyte layers with the cathode layer during the second sintering process was assumed at the sintering temperature of 1323 K. A similar approach in determining the value of the stress free temperature was applied in the numerical considerations carried out by [14,15].

Stress-strain relationship for the linear material was computed as:

$${\sigma} = D{\epsilon}_{el} + {\sigma}_0$$  \hspace{1cm} (10)

where: $\sigma_0$ is the initial stress distribution, which represents the residual stress in the model, $D$ is the elasticity matrix, which for an isotropic material is defined as:

$$D = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu & \nu & 0 & 0 & 0 \\ \nu & 1-\nu & \nu & 0 & 0 & 0 \\ \nu & \nu & 1-\nu & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{(1-2\nu)}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{(1-2\nu)}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{(1-2\nu)}{2} \end{bmatrix}$$  \hspace{1cm} (11)

where: $E$ is the Young’s modulus, $\nu$ is the Poisson’s ratio of the model material.

2.3 mSOFC stack geometry and numerical mesh

The complete mSOFC stack geometry consists of 48 anode-supported fuel cells hexagonally distributed inside the stack as shown in Fig. 2. The outer diameter of the fuel cell tubes was equal to 6.8 mm, the total length of fuel cells was 122 mm, while the active length of the fuel cell was 100.5 mm. Fuel was introduced into the stack through the inlet manifold at the bottom part of the stack presented in Fig. 2b (empty holes in the red surface), while air was supplied to the stack via longitudinal slots located over the circumference of the stack housing as it can be seen in Fig. 2a (blue surfaces). Cold air was radially distributed between fuel cells from the outer part of the mSOFC stack housing towards the outlet air collector with longitudinal slots located in the center of the stack.

The mesh generated for the fluid-thermal model consisted of approximately 712 thousand tetrahedral computational cells with a maximum aspect ratio of 15.8. A double precision pressure-based (segregated) solver was used. Due to a low averaged Reynolds number a laminar flow was assumed. The model equations (1)–(5) were solved using the ANSYS Fluent 14.0 code. The momentum, species and energy equations were discretized by second-order upwind schemes, while pressure based on the standard scheme. Convergence criteria were set for the residuals of continuity and velocities below $10^{-5}$, while those for species and energy equations were below $10^{-7}$. The computations were performed on a four 6-node Windows cluster.

For the thermal-mechanical model a separate geometry and 3D mesh were created in the ANSYS Workbench Design Modeler and ANSYS Meshing softwares, respectively. The employed geometry contained beyond the mSOFC stack also two manifolds, dodecagon housing, internal cylindrical collector of exhaust air as well as internal and external support rings. The manifolds were located on both sides of the stack, one at the fuel inlet and other
at the fuel outlet. Both manifolds provided sealing for fuel flow through the mSOFC stack. The same materials were defined for sealants and manifolds. A stack housing based on a dodecagon enclosure. Fig. 3 shows the design of hexagonal mSOFC stack with manifolds and exhaust air collector. The computational mesh consists of 1.15 million of numerical cells and was built using the commercial software ANSYS 15.0 Workbench Meshing. Numerical grids were generated to optimize computation time. The mesh size created for the FEM calculations was finer in comparison to the mesh used at the CFD modelling level. The mSOFC stack geometry used in the CFD simulations was simpler, while in the FEM approach additional elements such as solid parts of the stack housing, manifolds, sealants were included in the computational domain. The CFD calculations were performed only for the domain occupied by the cathode gas, while the FEM calculations were carried out also in the solid parts of the stack and therefore the number of computational cells had to be higher. Due to different densities of the computational grids the temperature distributions were averaged during transfer from the CFD code into the FEM tool. The impact of the mesh density was not taken into account in the present study. In order to evaluate the thermo-mechanical behavior of the mSOFC components the FEM simulations were carried out using the ANSYS Mechanical 15.0 code.

2.4 Material properties

For numerical simulations, the mechanical properties of the mSOFC layer materials used in this study are given in Table 1. It was assumed that the considered anode supported microtubular SOFC stack includes nickel yttria stabilized zirconia (Ni-YSZ) anodes, yttria stabilized zirconia (YSZ) electrolytes and lanthanum strontium cobalt ferrite (LSCF) cathodes.

The following assumptions were used in simulations:
- stress free temperatures were used for anodes and electrolytes, while for cathodes the same values were adopted as in [15],
- the operating temperature was equal to 750°C.

Basic physical parameters for the other components of the hexagonal mSOFC stack are listed in Table 2.

Literature values of the Young’s modulus and tensile strength as a function of temperature for selected parts (Macor machinable glass ceramic, Hastelloy X and Inconel X 750) of the mSOFC stack are presented in Figs. 4 and 5, respectively. Changes in the value of the Young’s modulus with temperature were defined in the properties of materials entered the ANSYS Mechanical Static Structural software, whereas constant values of the tensile strength were applied in the FEM simulations.
2.5 Boundary conditions

The coupling of the thermo-fluid analysis with the thermo-mechanical approach was in one-way manner, which means that it was assumed temperature field affects the stress distribution, while the reverse effect was not taken into account in this study. In the first step the thermo-fluid model was solved for the mSOFC stack with the air as a computational domain, then the predicted temperature distribution was applied into the thermo-mechanical model. It should be mentioned that the impact of the electrochemical processes occurring at the single cell level was included in the numerical consideration only by defining the local value of heat flux along the electrochemically active surface of the mSOFC tubes, which was estimated in the simulations presented in details [21,22]. The proposed approach greatly simplified the complexity of the calculations and reduced the computational time. Therefore, the simulation analysis

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**Table 1**: Mechanical properties of mSOFC layer materials.

| Property                | mSOFC material                  |
|-------------------------|---------------------------------|
|                         | Anode (Ni-YSZ)                | Electrolyte (YSZ) | Cathode (LSCF) |
| CTE $10^{-6}$, K$^{-1}$ | 12.2 [14]                      | 10.3             | 13 [15]        |
|                         |                                 |                  |                |
| E, GPa                  | 57 [13]                        | 215 at 298 K     | 185 at 1073 K  |
|                         |                                 | [23,24]          | 161 [15]       |
| ν                       | 0.28 [13]                      | 0.32/0.313 [13] | 0.32 [15]      |
| ρ, kg m$^{-3}$          | 4500 [25]                      | 6050 [24]        | 6820 [15]      |
| λ, W mK$^{-1}$          | 1.86 [13]                      | 2.2 [24]         | 1.31 [25]      |
| C$_p$, J kg$^{-1}$ K$^{-1}$ | 500 [25]                  | 600 [25]        | 470 [25]       |
| Tensile yield strength, MPa | 115 [23]                      | 332/256 [13]     | 155 [26]       |
| Compressive strength, MPa | 100                          | 1000 [23]       | 100 [23]       |
| Stress free temperature, K | 1473 [23]                    | 1473 [23]       | 1323 [15]      |

**Table 2**: Mechanical properties of mSOFC stack materials used in the FEM simulations [27-29].

| Property                | mSOFC material                  |
|-------------------------|---------------------------------|
|                         | Manifolds and seals             | Housing & air distributor | Housing & air distributor |
|                         | Macor machinable glass ceramic | Hastelloy X              | Inconel X 750               |
| CTE $10^{-6}$, K$^{-1}$ | 12.3                            | 15.6                       | 9.3                         |
| E, GPa                  | 66.9*/40.5*                     | 205/153*                  | 213.7/127.5*                |
| ν                       | 0.29                            | 0.32*                      | 0.29                        |
| ρ, kg m$^{-3}$          | 2520                            | 8220                       | 8280                        |
| λ, W mK$^{-1}$          | 1.46*/1.25*                     | 9.1/27.2*                 | 12.0/23.6*                  |
| C$_p$, J kg$^{-1}$ K$^{-1}$ | 790*                       | 486/699*                   | 431/716*                    |
| Ultimate tensile strength, MPa | 94*/41*                       | 767/310*                   | 758.4/261.3*                |
| Tensile yield strength, MPa | -                             | 379/194*                   | 320.6/189.6*                |
| Compressive strength, MPa | 345 (to 900)                 | -                          | 1175.5*                     |

where symbols used in Table 2 can be explained as follows: CTE – coefficient of thermal expansion, * - at 25°C, ± - at 800°C, * - sheet at 25°C/871°C, ± - at 21°C/816°C, ± – at 704°C.

**Figure 4**: Young's modulus as a function of temperature for selected elements of the mSOFC stack [27-29].

**Figure 5**: Tensile strength as a function of temperature for selected elements of the mSOFC stack [27-29].
presented in this study was carried out using two separate sets of assumptions:

1. for thermo-fluid model at the stack level:
   - local heat flux values along the electrochemically active surface of the mSOFC tubes were defined in order to take into account heat transfer, hydrodynamic and thermo-electrochemical processes occurring at the Membrane Electrode Assembly (MEA) in single fuel cells. Details can be found in paper [21],
   - air was distributed through slots in external housing of the hexagonal mSOFC stack with the mean velocity of 2.0 m s$^{-1}$, as a starting point, and at the inlet temperature equal to 700°C,
   - pure air was assumed as the working medium and it was treated as ideal gas,
   - the computational domain was the cathode air volume of the mSOFC stack,
   - radiative heat transfer was taken into account via non-participating media by the surface-to-surface model,
   - the stack walls were defined as stationary walls with zero heat losses, i.e. adiabatic,
   - the active part of the fuel cell tubes was defined as stationary wall with 2424.6 W m$^{-2}$ heat flux and emissivity of 0.4,
   - the inert part of the fuel cell tubes was also assumed adiabatic.

2. for thermo-mechanical model:
   - the effect of gravity was neglected,
   - structural constraints with one degree of freedom were used in the axial direction at the right outer surface of the stack housing as presented in Fig. 6.
   - the reference temperature for the operating conditions was equal to 25°C, while the reference temperatures of 1200°C and 1050°C were assumed respectively for the first stage of sintering the anode-electrolyte layers and the second stage sintering the anode-electrolyte layers with the cathode layer,
   - the only load in the model was working temperature of fuel cells obtained in the first stage CFD simulations and then implemented into the ANSYS Mechanical software,
   - constant temperature of 750°C was assumed for supporting structure of the mSOFC stack, because only fuel cell temperature distributions were transferred from the CFD into the FEM calculations.

3 Simulation results

3.1 CFD results

Validation of the CFD prediction at the single cell level modelling has been done by comparison of the V–I curve with the experimental data [25] under the same operating conditions. The fuel cell was tested at 700°C and 60% of pure hydrogen fuel utilization was assumed.

It can be concluded from Fig. 7 that agreement between the predicted CFD V–I curve for microtubular SOFC with the experimental data [25] was good.

Figs. 8 and 9 show the velocity and pressure distributions inside the mSOFC stack. Temperature distributions predicted by CFD in the stack are presented in Fig. 10. As expected, temperatures across the horizontal surfaces are slightly higher near the axis of the mSOFC stack, where the exhaust air leaves the stack as well as in the areas located close to the second and third rows of fuel cells due to weaker cooling. This effect is particularly well for the middle and lower horizontal surfaces, where
the wall fuel cell temperature reached 1030 K. However, analysis of the simulated distribution of local temperature within the mSOFC stack showed that most of the microtubular fuel cells were cooled very well at the inlet air velocity of 2.0 m s\(^{-1}\).

In order to predict the thermomechanical stress the calculated temperature fields from the CFD simulation were implemented into the FEM model as illustrated in Fig. 11. The imported thermal distributions may slightly vary due to the interpolation from the CFD domain with a lower number of computational cells than in the FEM. Nevertheless, in general the temperature fields reflect well the operating conditions in the mSOFC stack.

### 3.2 FEM results

The stress distributions were calculated based on the von Mises theory, thus the results show the von Mises stress distribution as well as the total axial, tangential and radial stresses distribution of the mSOFC stack with supporting structure under thermal load.
The axial stresses during mSOFC operation and the total axial stresses in the stack were analyzed along the mid-thickness lines, respectively of the anode, electrolyte and cathode for three cell types: an external fuel cell ("cross-section I") and an internal fuel cell marked "cross-section II". These cross-sections were labeled in Fig. 12 at the right side.

Cross-section I was subjected to the strongest cooling conditions in the stack, while cross-section II denoted fuel cells located close to the axis of the stack with the weakest cooling.

Figs. 13–16 present obtained profiles of the von Mises stress and axial/tangential/radial stress components in an operating microtubular SOFC stack with supporting structure along the horizontal centerlines of each layer for the chosen two cross-sections I to II.

The results presented in Figs. 13 and 14 reveal that the operating stress along the fuel cell tube is more uniform for the cross-section I, where the cooling air flow was better, while the von Mises stress is more uniform for both cross-sections.
Irregular distributions at the ends of the fuel cell, which can be noticed in Figs. 13–16 result from the contact points between the fuel cells with manifolds. Due to a smaller difference in the CTE value between the manifold and the anode than the manifold and the cathode, the irregularity is less apparent at the length of 0 mm. A greater disturbance can be noticed for the second fuel cell end due to greater anode thickness and stronger impact on other layers. Moreover, the highest operating stresses were noticed in the electrolyte layer and the smallest in...
the anode close to -50 MPa (compressive) as well as in the cathode of around -250 MPa (compressive). In addition, from Fig. 15 that the highest operating tangential stress of the mSOFC stack was recognised in the electrolyte layer (tensile), the smallest one in the anode, close to 0 MPA, and compressive stress in the cathode layer slightly more than -100 MPa. The operating radial stresses are negligible for all MEA layers.

The simulation results indicate also that the highest absolute value of axial stress the external cell row. Moreover, high values of the axial stresses were also noticed for the lower part of the internal fuel cells. In contrast, the lowest axial stress values were found in the upper part of the fuel cells located in the middle part of the hexagonal design of the mSOFC stack. It should be noticed that in most fuel cell layers the absolute values of the axial stress are smaller on the fuel cell side, where the cooling air flows across with two exceptions of the electrolyte and anode located in the external row of the mSOFC stack. In addition, the axial stress profiles obtained for anode, electrolyte and cathode are characterized by non-linear trends along their length. Their temperature distribution is non-uniform, therefore the tension in one fuel cell at two different positions can vary up to about 100 MPa. The total axial stress values in the assembly along the vertical centerlines of anode, electrolyte and cathode layer at the half length of the tube for three fuel cells: internal, middle and external cells are assembled in Table 3. It should be noted that the cathode stress for the external fuel cells was quite high (92 and 98 MPa) and close to the maximum level, because the compressive strength of cathode has been reported to be about 100 MPa.

Figs. 17−19 show profiles of the total stresses in the assembly containing the hexagonal mSOFC stack design, sealants, manifolds and housing with air cooling flow from the external side to the middle part of the stack.

The total stresses were the lowest for anode layers with compressive value of -34 MPa in the upper part of the internal fuel cell and up to -54 MPa in the upper part of the outer fuel cell. However, the calculated compressive

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**Figure 15:** Distribution of operating tangential stress of the mSOFC stack with supporting structure along the horizontal centerlines of each layer: (a) cross-section I, (b) cross-section II.

**Figure 16:** Distribution of operating radial stress of the mSOFC stack with supporting structure along the horizontal centerlines of each layer: (a) cross-section I, (b) cross-section II.
stresses in electrolytes were the highest of -494 MPa at the top part of the external fuel cell and the lowest of -418 MPa at the top part of the internal fuel cell. Yet for the cathode the axial compressive stresses were -98 MPa at the bottom part of the external fuel cell and -44 MPa in the upper part of the internal fuel cells, respectively. Such high values obtained in the simulations stem from large differences in the coefficient of thermal expansion between the fuel cell, sealants and manifolds. There is some probability that such high values are also due to linear, elastic deformation assumed in this study, while the non-linear approach would perhaps reduce their extent. In addition,
with the adopted stack design the use of sealing material could not be avoided. The stress distribution was analysed by taking into account also the residual stresses resulting from manufacturing processes, hence it was possible to understand the operating conditions and anticipate the probabilities of failure. It should be underlined that three different FEM simulations were carried out in this study. Firstly, thermal analysis of the anode and electrolyte sintering process was done, then sintering process of the joined anode – electrolyte layers with the cathode layer was analysed and finally estimation of the operating temperature impact on the fuel cell was considered. Therefore, the reference temperature was varied at different stages as it was mentioned in the thermo-mechanical model assumptions. High values of the total compressive stresses were simulated in the electrolyte layer, while its radial stresses were negligible. Tangential stresses were more homogeneous than the axial stresses for both the external and internal fuel cells presented respectively as cross-sections I and II. The highest axial stresses were almost two times higher than the peripheral one.

The total compressive and tangential tensile stresses were also computed in the cathode layer (Figs. 17–19). Again the radial stresses were negligible, while the biggest, almost two times higher than the circumferential was the total axial stress in the cathode layer.

For the anode layer a similar to the electrolyte behaviour was recognized. The only exception was development of insignificant total tensile tangential stresses predicted for the inner row of the fuel cells (cross-section II). In addition, almost completely negligible impact had the radial and tangential strain. The largest were the total axial stresses in the anode layer. It follows from Figs. 17–19 only the external cells marked as the cross-section I showed better homogeneity of the total stress along the fuel cell length compared to the internal fuel cells marked as the cross-section II.

The highest overall axial stress can be observed in the electrolyte layer (compressive stress of -500 MPa), the smallest one in the anode layer (close to -50 MPa of compressive stress) and the compressive stress in the cathode layer at the order of magnitude of -100 MPa.

From Fig. 18 it can be seen also that the greatest total circumferential strain of the electrolyte layer with the compressive stress of -300 MPa was obtained, while the smallest one in the anode close to 0 MPa and stretching stress slightly more than 50 MPa for the cathode layer. Total radial stress is again negligible for all MEA layers.

| Region of centerline | Axial stresses, MPa |
|----------------------|---------------------|
| cathode electrolyte anode |
| Top part of the external fuel cell | -92 | -494 | -54 |
| Bottom part of the external fuel cell | -98 | -480 | -53 |
| Top part of the middle fuel cell | -49 | -431 | -37 |
| Bottom part of the middle fuel cell | -63 | -434.6 | -39.5 |
| Top part of the internal fuel cell | -44 | -418 | -34 |
| Bottom part of the internal fuel cell | -81 | -457 | -45 |

The contour maps of operating maximum and minimum principal stresses of the assembly with supporting structure were presented in Figs. 27–28, and show global system behavior in relation to its reference for the entire structure of the fuel cell stack.

The maximum operating principal stresses presented in Fig. 27 in the direction of elongation showed a tendency to accumulation of the stresses in the corners resulting in high stresses in the housing from -114 to 687 MPa. The
values compared to the stresses in the fuel cell stack equal to -71 to 500 MPa indicated the need of changing the structure from the dodecagon into the cylindrical.

A similar situation can be recognised in Fig. 28 for the minimum principal stresses in the main direction. In the mSOFC stack the operating minimum principal
stresses were in the range from -487 to 24 MPa, while in the housing the corresponding values were from -733 to 163 MPa. However, the most part of the housing was exposed to stress of the order of -92 to 35 MPa. Critical negative stress values were registered in the areas of contact of the dodecagon housing with the manifolds.

Finally, to evaluate the thermo-mechanical resistance of the mSOFC stack with supporting structure, distribution of von Mises stress was shown in Fig. 29. Hence, the regions with high values of the von Mises stress need attention and be analyzed in more detail.

As shown in Fig. 29 the maximum operating von Mises stress was equal to 464 MPa. Special attention should be paid to the stress in the housing, where its value was up to 747 MPa. However, the majority of the housing is exposed to the stress up to 184 MPa. The accumulation of the von Mises stress can be visible in the corners of the supporting structure, which confirms the need to change the structure of the dodecagon into the cylindrical. Furthermore, a noticeable increase in the stress values can be observed in the contact areas of the supporting structure due to the CTE differences between the manifolds and the air distributor as well as between the manifolds and the external stack housing.

As shown in Figs. 27–29 the greatest stresses arise on the housing corners. Several limitations of this specific housing shape appeared during the analysis and a more effective shape for the housing can be considered, e.g. circular. However, it has to be mentioned that in most housing regions the stresses were less than 110 MPa with one exception of contact points with manifolds and the air distributor due to large number of cut-outs in the material, where the value of 170 MPa was noticed. Nevertheless, these values are still lower than the breaking point of the housing materials at the operating temperatures.

4 Conclusions

Three dimensional coupled CFD and FEM simulations of the new design of the mSOFC stack with supporting dodecagon structure were performed and their capabilities
Numerical analysis of thermal stresses in a new design of microtubular stack were examined. The influence of the hexagonal mSOFC stack configuration and dodecagon housing as well as temperature distributions determining the stress distributions in the assembly with supporting structure were estimated. Both the compressive and tensile stresses were noticed in the structure. The highest total stress was noticed in the electrolyte and it was the compression stress. Tensile stress was defined only in the cathode and was lower than 100 MPa. The areas of the highest values were determined as those requiring special attention. The need to develop a more accurate temperature transfer protocol from the CFD to FEM tools was deduced since various computational domains were used in the flow solver and in the stress solver. Moreover, the performed FEM simulations based on the assumption of linear, elastic deformation, which was a considerable simplification regarding the stack housing constructed of the metal alloy. Therefore, the non-linear elastoplastic deformation should be considered in the further simulations.

A significant advantage of the present study is that the obtained stress distributions provide helpful guidance in the optimization of the new hexagonal mSOFC stack design with the dodecagon supporting structure.

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References

[1] Fardadi M., Mueller F., Jabbari F., Feedback control of solid oxide fuel cell spatial temperature variation, J. Power Sources, 2010, 195, 13, 4222-4233. DOI: 10.1016/j.jpowsour.2012.09.004.
[2] Vijay P., Hosseini S., Tade M. O., A novel concept for improved thermal management of the planar SOFC, Chem. Eng. Research & Design, 2013, 91, 560-572. DOI: 10.1016/j.cherd.2012.09.004.
[3] Dey T., Singdeo D., Basu R. N., Bose M., Ghosh P. C., Improvement in solid oxide fuel cell performance through design modifications: an approach based on root cause analysis, Int. J. Hydrogen Energy, 2014, 39, 17258-17266. DOI: 10.1016/j.ijhydene.2014.08.025.
[4] Boigues-Munoz C., Santori G., McPhail S., Polonara F., Thermochemical model and experimental validation of a tubular SOFC cell comprised in a 1 kWel stack design for CCHP applications, Int. J. Hydrogen Energy, 2014, 39, 21714-21723. DOI: 10.1016/j.ijhydene.2014.09.021.
[5] Al-Masri, Peksen M., Blum L., Stolten D., A 3D CFD model for predicting the temperature distribution in a full scale APU SOFC short stack under transient operating conditions, Applied Energy, 2014, 135, 539-547. DOI:10.1016/j.apenergy.2014.08.052.
[6] Mourir H., Belaiche M., El Marjani A., El Gharad A., Thermal stress and probability of survival investigation in a multi-bundle integrated planar solid oxide fuel cells IP-SOFC (integrated planar solid oxide fuel cell), Energy, 2014, 66, 378-386. DOI: 10.1016/j.energy.2014.01.017.
[7] Wang G., Yang Y., Zhang H., Xia W., 3D model of thermos-fluid and electrochemical for planar SOFC, J. Power Sources, 2007, 167, 398-405. DOI: 10.1016/j.jpowsour.2007.02.019.
[8] Yakabe H., Ogwara T., Hishinuma M., Yasuda I., 3D model calculation for planar SOFC, J. Power Sources, 2001, 102, 144-154. DOI: 10.1016/S0378-7753(01)00792-3.

[9] Reckangle K. P., Williford R. E., Chick L. A., Rector D. R., M. A., Khaleel M. A., Three-dimensional thermos-fluid electrochemical modeling of planar SOFC stacks, J. Power Sources, 2003, 113, 109-114. II: S0378-7753(02)00487-1.

[10] Ki J., Kim D., Computational model to predict thermal dynamics of planar solid oxide fuel cell stack during start-up process, J. Power Sources, 2010, 195, 3186-3200. DOI: 10.1016/j.jpowsour.2009.11.129.

[11] Well K. S., Koeppel B. J., Comparative finite element analysis of the stress-strain states in three different bonded solid oxide fuel cell seal designs, J. Power Sources, 2008, 180, 343-353. DOI: 10.1016/j.jpowsour.2008.01.093.

[12] Yakabe H., Baba Y., Sakurai T., Yoshitaka Y., Evaluation of the residual stress for anode-supported SOFCs, J. Power Sources, 2004, 135, 9-16. DOI: 10.1016/j.jpowsour.2003.11.049.

[13] Nakajo A., Stillier C., Harkegard G., Bolland O., Modeling of thermal stresses and probability of survival of tubular SOFC, J. Power Sources, 2006, 158, 287-294. DOI: 10.1016/j.jpowsour.2005.09.004.

[14] Cui D., Cheng M., Thermal stress modeling of anode supported micro-tubular solid oxide fuel cell, J. Power Sources, 2009, 192, 400-407. DOI: 10.1016/j.jpowsour.2009.03.046.

[15] Serincan M. F., Pasaogullari U., Sammes N. M., Thermal stresses in an operating micro-tubular solid oxide fuel cell, J. Power Sources, 2010, 195, 4905-4914. DOI: 10.1016/j.jpowsour.2009.12.108.

[16] Xue X., Tang J., Sammes N., Du Y., Dynamic modeling of single tubular SOFC combining heat/mass transfer and electrochemical reaction effects, J. Power Sources, 2005, 142, 211-222. DOI: 10.1016/j.jpowsour.2004.11.023.

[17] Wei S. S., Wang T. H., Wu J. S., Numerical modeling of interconnect flow channel design and thermal stress analysis of a planar anode supported solid oxide fuel cell stack, Energy, 2014, 69, 553-561. DOI: 10.1016/j.energy.2014.03.052.

[18] Liu L., Kim G. Y., Chandra A., Modeling of thermal stresses and lifetime prediction of planar solid oxide fuel cell under thermal cycling conditions, J. Power Sources, 2010, 195, 2310-2318. DOI: 10.1016/j.jpowsour.2009.10.064.

[19] Peksen M., 3D thermomechanical behaviour of solid oxide fuel cells operating in different environments, Int. J. Hydrogen Energy, 2013, 38, 13408-13418. DOI: 10.1016/j.ijhydene.2013.07.112.

[20] Peksen M., A coupled 3D thermofluid-thermomechanical analysis of a planar type production scale SOFC stack, Int. J. Hydrogen Energy, 2011, 36, 11914-11928. DOI: 10.1016/j.ijhydene.2011.06.045.

[21] Pianko-Oprych P., Kasilova E., Jaworski Z., Proceedings of 11th European SOFC and SOE Forum 2014, (1-4 July 2014, Lucerne, Switzerland), 2014, A1322, 1-10.

[22] Pianko-Oprych P., Cell, Stack and System Modelling, Solid Oxide Fuel Cell, Lambert Academic Publishing, 2014, ISBN 978-3-659-62295-3.

[23] Li J., Lin Z., Effects of electrode composition on the electrochemical performance and mechanical property of micro-tubular solid oxide fuel cell, Intern. J. Hydrogen Energy, 2012, 37, 12925-12940. DOI: 10.1016/j.ijhydene.2012.05.075.

[24] Anderman Industrial Ceramics Ltd. Zirconia Yttria Stabilised, brochure, (2014).

[25] SUAV data, internal project report, 2014.

[26] Delette G., Laurencin J., Usseglio-Virett F., Villanova J., Bleuet P., Lay-Grindler E., Le Bihan T., Thermo-elastic properties of SOFC/SOEC electrode materials determined from three-dimensional microstructural reconstructions, Intern. Journal of Hydrogen Energy, 2013, 38, 12379-12391. DOI: 10.1016/j.ijhydene.2013.07.027.

[27] Corning MACOR Machinable Glass Ceramic 01, 02, brochure, 2014.

[28] Haynes International Hastelloy X Alloy, brochure, 2014.

[29] Inconel Special Metals Alloy X 750, brochure, 2014.