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# Numerical simulations of temperature and stress distribution in thermal barrier coatings in the context of differences in input data values – external ceramic layer

## Symulacje numeryczne rozkładu temperatury oraz stanu naprężeń w powłokowych barierach cieplnych w kontekście różnic w wartościach danych wejściowych – warstwa ceramiczna

The article presents the research results on the impact of differences in input data values concerning materials used in thermal barrier coating systems on the results of simulations using the finite element method of temperature distribution and Huber-Mises equivalent stresses. Literature data on basic physical quantities important from the point of view of modelling, i.e. thermal conductivity coefficient, linear expansion coefficient, specific heat, density, Poisson fraction and Young's modulus, were reviewed. It has been shown that the data is characterised by a very wide range of values, which makes the issue of the final simulation results debatable. The study performed a simple statistical analysis of the available data for the 8YSZ compound, using the minimum, maximum, mean, and median values to simulate deadness. It was found that the results of the obtained simulations with the use of these data differ fundamentally from each other.

**Keywords:** FEM, TBC, simulations, input data, reliability of calculations

W artykule przedstawiono wyniki badań nad wpływem różnic w wartościach danych wejściowych dotyczących materiałów używanych w systemach powłokowych barier cieplnych na wyniki symulacji metodą elementów skończonych rozkładu temperatury i naprężeń zastępczych Hubera-Misesa. Dokonano przeglądu danych literaturowych na temat podstawowych wielkości fizycznych istotnych z punktu widzenia modelowania, tj. współczynnika przewodnictwa cieplnego, współczynnika rozszerzalności liniowej, ciepła właściwego, gęstości, ułamka Poissona oraz modułu Younga. Wykazano, że dane charakteryzują się bardzo dużym rozrzutem wartości, co sprawia, że finalne wyniki symulacji są dyskusyjne. W badaniach przeprowadzono prostą analizę statystyczną dostępnych danych dotyczących związku 8YSZ, wykorzystując do symulacji wartości minimalne, maksymalne, średnią i medianę. Stwierdzono, że uzyskane wyniki symulacji z użyciem tych danych różnią się od siebie w sposób zasadniczy.

**Słowa kluczowe:** MES, TBC, symulacje, dane wejściowe, wiarygodność obliczeń

### 1. Introduction

To properly develop a numerical model of any process or phenomenon, input data is necessary in the form of parameters characterising the model's geometry, physical quantities describing the material properties, and boundary conditions, e.g. temperature, pressure, etc. Numerical simulations are beneficial when considering complex interactions of phenomena under high-temperature conditions, such as thermal stresses, creep, sintering, diffusion or oxidation, etc. However, the correct preparation and evaluation of the model using the finite element method are complicated and depend on many variables. One of the most critical, often ignored variables is the input data characterising the physical parameters of the materials under analysis. In particular,

comparing data from various literature sources is essential, translating into their credibility. Data reliability is understood not only as the dispersion of the results of physical quantities but also as the method of their determination and the morphological form of the material to which they refer. What does this mean in practice? Works in the field of numerical modelling are based on material data, the source of which may be the own experiment of the authors of the simulation (which is quite a rare case), as well as may come from literature sources or publicly available databases. However, in the second and third cases, the amount of data and the dispersion of published values of specific parameters is large enough to practically achieve any simulation results, often in line with the expectations of their author. So what is the reality of these simulations?

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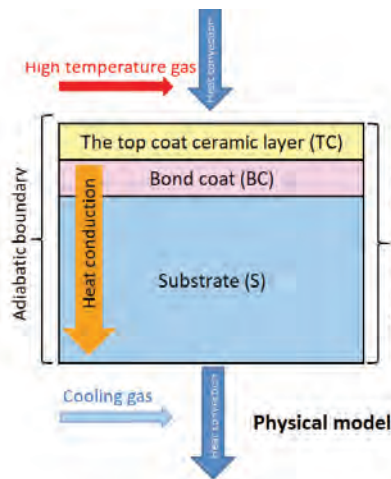


Fig. 1. Physical model of the TBC system

Rys. 1. Model fizyczny systemu TBC

An ideal example of those above is complex thermo-mechanical interactions in an aggressive oxidizing/corrosive environment in thermal barrier coatings (TBC). TBC systems are used in aero engines and stationary gas turbines to protect the metallic substrate of combustion chambers or stationary blades from extremely high temperatures. Combustion chambers and stationary blades are made of nickel-based superalloys whose melting point is lower than the flue gas temperature. Therefore, it is necessary not only to cool these elements internally but also to use TBC systems, whose leading role is to reduce the surface temperature. This is due to using a ceramic insulating layer with a very low thermal conductivity coefficient. Consequently, a strong temperature gradient of at least 100°C should be expected [1]. The physical model of the considered TBC system is shown in Fig. 1.

The effectiveness of TBC systems in operating conditions is determined by their durability, which depends on the operating conditions. In operating conditions, these systems are exposed to high temperatures and corrosive environments, which generate unfavourable stress conditions, leading to the cracking of the ceramic layer and its detachment [2–4]. Predicting the durability of TBC systems is one of the most critical aspects of their design and involves the use of finite element method (FEM) simulation methods. FEM simulations of sheath thermal barriers have been used for about 45 years [5]. Thanks to them, the mechanisms of stress generation in sheath thermal barriers subjected to external stresses and without these stresses have been well recognised [6].

However, as mentioned earlier, the critical factor in the correct simulation calculation process is the correctness of the entered input data. Meanwhile, in the literature sources, there is a wide range of physical data on the same material, but with significantly different values, which makes simulations basically worthless. An excellent example is the data on the primary material used in thermal barrier coatings, i.e., zirconium oxide modified with yttrium oxide (8YSZ: 8%  $Y_2O_3-ZrO_2$  in at%). Not only that, in many cases, it is not specified which oxide composition the available data refer to ( $Y_2O_3$  content), and there is also no information on whether the described layer, sinter or 8YSZ single crystal is described. As a result, we have available very different data with a wide spread of results [7–35]. Therefore, there is a need to indicate this problem as very important from the point of view of the correctness of the obtained simulation results and the secondary assessment of the durability of TBC systems, i.e. de facto safety of operation of aviation and stationary gas turbines.

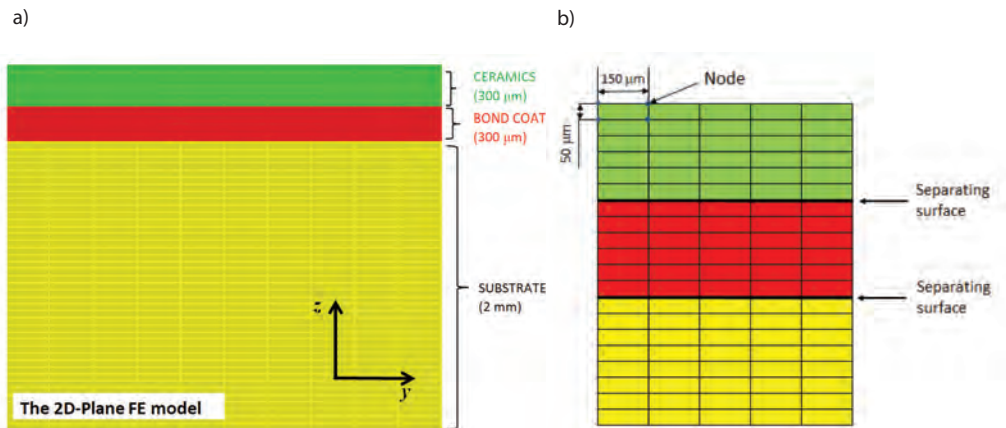


Fig. 2. Discrete model of the TBC system: a) fragment of the finite element mesh of the model, b) ceramic coating with a typical finite element mesh

Rys. 2. Model dyskretny systemu TBC: a) fragment siatki elementów skończonych modelu, b) powłoka ceramiczna z typową siatką elementów skończonych

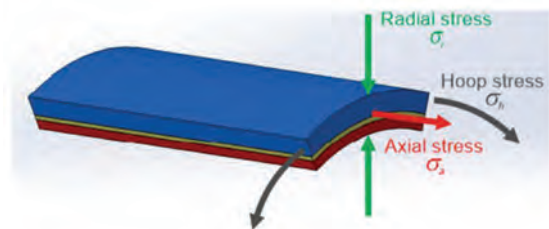


Fig. 3. Axis-symmetric character of stresses in the adopted physical model of the TBC system

Rys. 3. Osiowo-symetryczny charakter naprężeń w przyjętym modelu fizycznym systemu TBC

The article presents the research results on the influence of the dispersion of input material data available in the literature, used in numerical modelling of temperature distribution and state of stress in thermal barriers. The paper summarises the data in the professional literature on the finite element simulation of TBC systems. For this article, only the minimum and maximum values and the standard deviation of the results are presented.

## 2. Experiment procedure

In the work, a discrete model of coating thermal barriers was developed, which is shown in Fig. 2a and 2b. The geometrical model includes three layers: a base made of a 2 mm thick IN 625 nickel superalloy, an intermediate layer (interlayer) made of Amdry 962 alloy (Ni–22Cr–10Al–1Y in at%) with a thickness of 300 μm and an insulating ceramic coating of the Metco 204NS type (8YSZ: 8%  $Y_2O_3-ZrO_2$  in at%) also with a thickness of 300 μm. In the case of simple geometric elements used in the model, as shown in Fig. 2a, the discrete 2D model allows for the even distribution of individual layers of finite elements. Each layer corresponds to the corresponding material, i.e. the substrate, the interlayer and the ceramic layer. The number of rows of individual finite elements allows for any control of the thickness of each layer of the analysed TBC system. Figure 2b shows the analysed TBC system's discrete internal structure and geometry. Due to simplifying the calculation procedure, an axisymmetric character of the assumed stresses was proposed (Fig. 3).

The Algor program was used for the numerical simulation. The following assumptions were used:

**Table 1. Material data set used in FEM simulations: 8YSZ****Tabela 1. Zestaw danych materiałowych użytych w symulacjach MES: 8YSZ**

Properties	8YSZ						
	min.	max.	SD $\sigma$	average	median	kurtosis	skewness
$\lambda$ [W/mK]	0.90	2.17	0.46	1.49	1.10	-1.97	0.40
$c_p$ [J/kgK]	0.405	0.656	0.085	0.502	0.500	2.62	1.25
CTE [1/K]	$8.20 \times 10^{-6}$	$12.20 \times 10^{-6}$	$0.92 \times 10^{-6}$	$9.52 \times 10^{-6}$	$9.68 \times 10^{-6}$	$3.43 \times 10^{-6}$	$1.14 \times 10^{-6}$
$E$ [GPa]	17.5	210.0	60.7	74.7	48.0	1.69	1.66
$\nu$	0.10	0.26	0.06	0.19	0.20	-1.63	-0.36
$\rho$ [kg/m <sup>3</sup> ]	5.40	6.04	0.27	5.76	5.60	3.58	-1.85

Source: : the author, based on [7–35].

Źródło: opracowanie własne na podstawie [7–35].

- axisymmetric two-dimensional model (Fig. 3),
- description of the geometry of the TBC system model (Fig. 2a),
- model discretisation (Fig. 2b),
- selection of physical properties of materials used in the model (Tables 1, 2),
- determination of the calculation procedure,
- simulation implementation,
- analysis of the results obtained.

Considering the complexity of calculation procedures, the method of task minimisation was applied by using axisymmetric calculation models (this assumption reduces the number of necessary calculations). In the analysed problem, 2D axisymmetric, four-node elements were adopted. The task is solved with contact and friction. Boundary conditions were set: the displacement of the lower surface of the model in the direction of the z-axis was received. The following assumptions were taken into account for the analysis of the TBC temperature field in high-temperature conditions:

- all layers are homogeneous and isotropic;
- the left and right sides of the model are treated as adiabatic boundaries, where there is no heat exchange with the environment;
- the temperature near the ceramic layer was assumed to be 1500°C (flue gas temperature), while the surface temperature was 800°C (cooling air temperature).

The tests include an analysis in the field of elastic deformations. The first stage of the research was to conduct a numerical analysis of the temperature field. The conditions of heat exchange on the external surfaces of the body were determined by setting the boundary conditions. They can be determined for heat conduction in solids in various ways. In the analysed model, boundary conditions of the first kind, the so-called Dirichlet conditions, are defined by the temperature distribution on the body's surface at any time. The solution to the problem when considering temperature fields in solids was formulated as a simple task of determining the temperature distribution from the given initial and boundary conditions and the material properties of the considered body. The temperature load was assumed on the surfaces of the model respectively. The temperature of 1500°C was set on the surface of the TBC ceramic layer, while the temperature of 800°C was assumed on the outer surface of the nickel superalloy.

The second stage of evaluating the state of effort of elements covered with TBC ceramic coatings subjected to thermal loads was to conduct numerical calculations determining the stress level. In this case, the calculation basis is a numerical calculation model used in thermal

**Table 2. Material data set used in FEM simulations: NiCrAlY, IN 625****Tabela 2. Zestaw danych materiałowych użytych w symulacjach MES: NiCrAlY, IN 625**

Properties	NiCrAlY – bond coat		IN 625 – substrate	
		[10]		[35]
$\lambda$ [W/mK]	4.3	[10]	9.8	[35]
$c_p$ [J/kgK]	0.501	[10]	0.410	[35]
CTE [1/K]	$11.60 \times 10^{-6}$	[10]	$12.80 \times 10^{-6}$	[35]
$E$ [GPa]	225	[10]	204.8	[35]
$\nu$	0.3	[10]	0.31	[35]
$\rho$ [kg/m <sup>3</sup> ]	7.32	[10]	8.44	[35]

Source: the author, based on [7–35].

Źródło: opracowanie własne na podstawie [7–35].

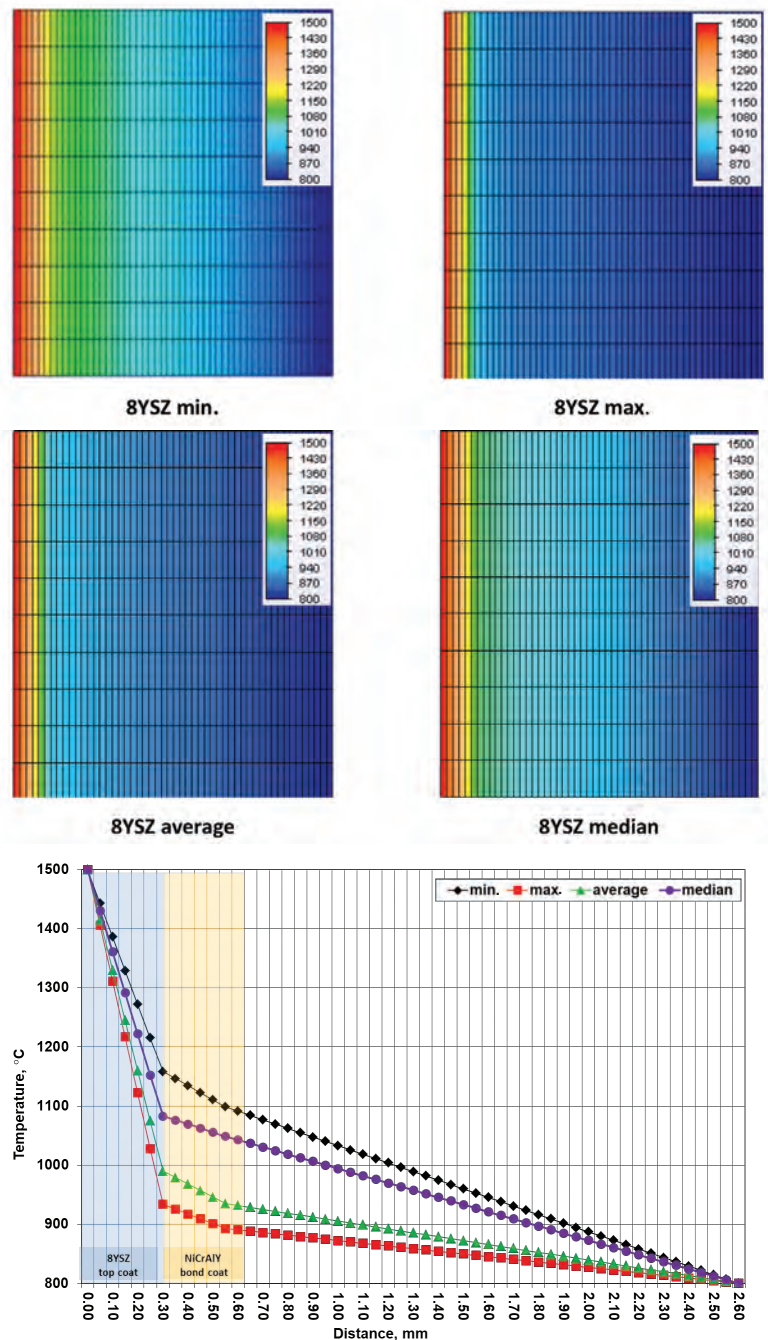


Fig. 4. The results of the simulation of the temperature distribution for different values (minimum, maximum, median, average) of physical parameters of materials

Rys. 4. Wyniki symulacji rozkładu temperatury dla różnych wartości (minimum, maksimum, mediany, średnie) parametrów fizycznych materiałów

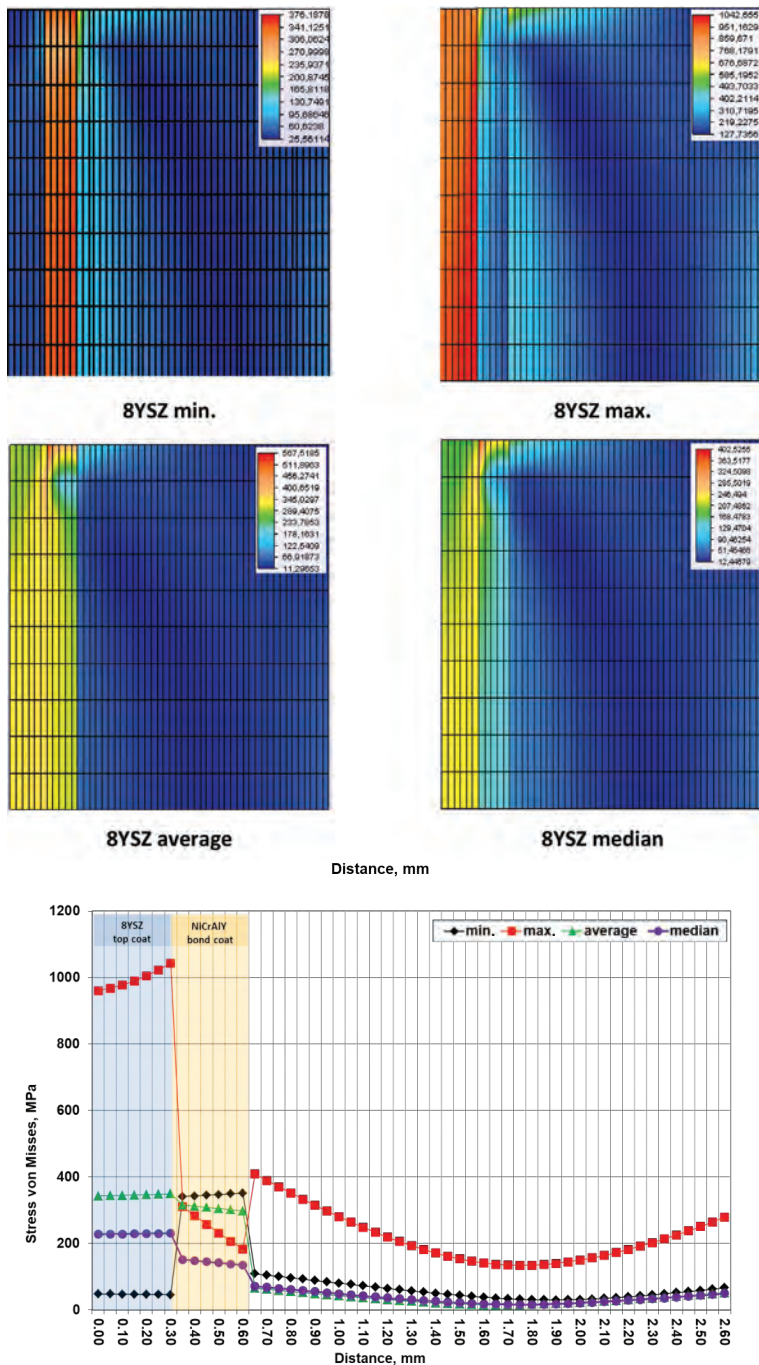


Fig. 5. Simulation results of von Mises stress distribution for various values (minimum, maximum, median, average) of physical parameters of materials – for a constant temperature of 1200°C

Rys. 5. Wyniki symulacji rozkładu naprężeń von Misesa dla różnych wartości (minimum, maksimum, mediany, średniej) parametrów fizycznych materiałów – w stałej temperaturze 1200°C

calculations along with information on the temperature value in each geometric point of the object. This is a necessary condition for the definition of boundary conditions in the strength analysis. The effort of TBC models loaded with a constant temperature field was also assessed. A constraint on the freedom of the models was given. It was assumed that the cross-sections of the developed models do not move in the direction of the z-axis. Knowing the axisymmetric temperature field in the analysed models, the state of stress occurring in them was determined.

The material data set in Tables 1 and 2 was used for the FEM analysis. It includes the maximum and minimum values of the param-

eters (derived from literature data) and the average value determined for this article. To illustrate the dispersion of the data, the standard deviation for each parameter was also introduced.

### 3. Results and discussion

The first stage of the research was analysing source data characterising the basic physical parameters of the materials used in the simulations. In practice, only the data concerning the ceramic material in the form of the 8YSZ compound were discussed. These data are presented in Tables 1, 2 and, at first glance, indicate a large dispersion of practically each parameter. The statistical evaluation was based on determining the extreme values, i.e. the maximum and minimum, and the value characterising the mean value, the median and the spread expressed by kurtosis and skewness.

These data clearly show that the thermal conductivity and the Poisson fraction are characterised by a large dispersion concerning the average value with a shift of the distribution curve to the right (thermal conductivity) and the left (Poisson fraction). In other cases, kurtosis indicates a relatively intense concentration of individual values around the mean, suggesting a smaller data scatter. However, the extreme values show very large differences, e.g., in Young’s modulus (*E*).

The analysis of the source data also indicates that the differences in the values of the data characterising the physical properties of the materials used in FEM simulations are caused by differences in the morphology and form of material processing. In many cases, data was also provided without providing the technological history of the material. This makes the FEM numerical simulation process unreliable, at least until the introduction of uniform and unambiguous information about the source of material data, considering the morphological form of these materials.

Figure 4 presents the results of the temperature distribution simulation, obtained based on the data in Tables 1 and 2, i.e. the minimum, maximum, median and average values of the basic parameters characterising the physical properties of materials necessary in the FEM modelling process.

The obtained simulations clearly show that the introduction of extreme values results in obtaining simulation results significantly different in temperature distribution. If minimum values are entered, the temperature on the surface of the interlayer differs by as much as approx. 225°C, which is a colossal difference. Entering the average value allows us to obtain results close to the maximum. In contrast, in the case of the median, the results are similar to those obtained when entering the values of the minimum physical parameters of materials.

Similar differences can be observed in the simulation of the distribution of equivalent stresses, determined according to the Huber-Mises hypothesis for a constant temperature of 1200°C (Fig. 5) and for the variable temperature variant according to Fig. 4 (Fig. 6). The analysis of these simulations allows for a very wide range of interpretations, the credibility of which, however, is quite a matter of convention.

### 4. Conclusions

The correctness of input data in finite element simulations is a decisive factor for the final results’ credibility. Therefore, it is

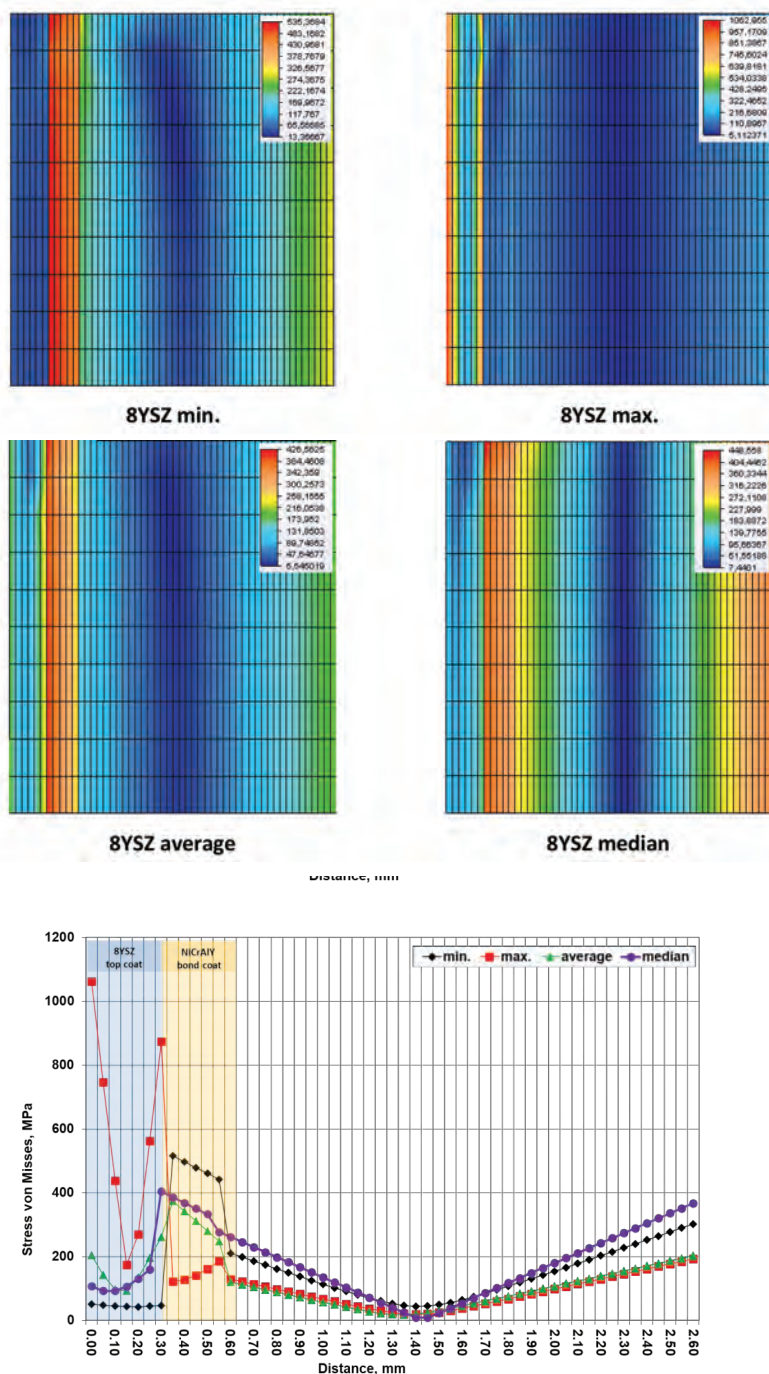


Fig. 6. Simulation results of the von Mises stress distribution for different values (minimum, maximum, median, average) of the physical parameters of materials – for the temperature distribution as in Fig. 4

Rys. 6. Wyniki symulacji rozkładu naprężeń według hipotezy Hubera-Misesa dla różnych wartości (minimum, maksimum, mediany, średniej) parametrów fizycznych materiałów – rozkład temperatury jak na rys. 4

essential to verify the sources of material data, not only by reviewing the latest publications containing them but also by searching for primary sources, sometimes from 40 years ago.

Another element that should be considered is the dispersion of data present in the literature. The best tool to assess this effect is simple statistical parameters such as mean, median, kurtosis and skewness. They will make it possible to define the range of values to which we can assign the material data used and determine their reliability.

The ill-considered use of material data, without even superficial analysis, makes the value of such simulations debatable.

It is, therefore, necessary to introduce a kind of analytical model of the microstructure, which will be based on clearly defined data describing the system in terms of the morphological form of the material, its technological history and parameters describing the microstructure. In the case of coating thermal barriers, this must be information on processing 8YSZ compounds (sinter, APS sprayed coating, general, spherical and horizontal porosity, crack density, thickness and width of strands, etc.).

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