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Numerical simulations of temperature and stress distribution in thermal barrier coatings in the context of differences in input data values – bond coat and substrate materials

Symulacje numeryczne rozkładu temperatury oraz stanu naprężeń w powłokowych barierach cieplnych w kontekście różnic w wartościach danych wejściowych – warstwa pośrednia i materiał podłoża

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 the finite element method (FEM) simulation of temperature distribution and Huber-Mises equivalent stresses. This article focuses on the material parameters characterizing the intermediate layer and the base material. It was shown that, as in the case of the 8YSZ ceramic layer, the data are characterized by a very wide scatter of values. It was found that the results of the simulations obtained with the use of these data differ significantly from each other, depending on the adopted reference point, i.e. whether minimum, maximum, median or average values were adopted for the simulation. Therefore, considering the total differences in simulations resulting from the scattering of input data for the substrate material, interlayer and ceramic layer, it should be stated that it is possible to obtain virtually any simulation result.

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

Wartykule przedstawiono wyniki badań nad wpływem różnic w wartościach danych wejściowych dotyczących materiałów używanych w systemach powłokowych barier cieplnych na wyniki symulacji metodą elementów skończonych (MES) rozkładu temperatury i naprężeń zastępczych Hubera-Misesa. Skupiono się na parametrach materiałowych charakteryzujących warstwę pośrednią oraz materiał podłoża. Wykazano, że tak jak w przypadku warstwy ceramicznej 8YSZ dane charakteryzują się bardzo szerokim rozrzutem wartości. Stwierdzono, że wyniki symulacji z użyciem tych danych różnią się znacznie od siebie w zależności od przyjętego punktu odniesienia, to znaczy od tego, czy do symulacji przyjęto wartości minimalne, maksymalne, medianę czy średnią. Uwzględniając zatem sumaryczne różnice w symulacjach wynikające z rozrzutu danych wejściowych dla materiału podłoża, międzywarstwy oraz warstwy ceramicznej, należy stwierdzić, że możliwe jest uzyskanie praktycznie dowolnego wyniku symulacji.

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

1. Introduction

The credibility of input data in numerical simulations, e.g. carried out using the finite element method, determines the correctness and reliability of the final results obtained. Introducing incorrect data or data from unreliable and undocumented sources may cause errors in the analyses carried out and threaten the operation of structures, components or other systems operating in specific temperatures, stress and environmental conditions. This problem also concerns shell thermal barriers (TBC), an important element of stationary and non-stationary gas turbines, e.g., aircraft engines [1].

TBC systems are used in gas turbines and their role is to protect the metallic substrate of the combustion chambers or stationary blades from extremely high temperatures. They are extremely effective thermal insulation based on the thermal properties of the materials used for their production (ceramics with ultra-low thermal conductivity) and advanced internal cooling methods [1]. The effectiveness of TBC systems in the operating conditions of gas turbines is determined by their durability, which depends on the operating conditions (high temperature, complex state of stress, aggressive working environment). These factors make TBC systems vulnerable to cracking of the ceramic layer and its detachment [2–4]. Predicting the durability of TBC systems is one of the

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most important aspects of their design. However, as mentioned earlier, the critical factor in the correct simulation calculation process is the correctness of the entered input data. A wide range of material data for the same material (interlayer and substrate) is available in literature sources but with significantly different values, which makes simulations worthless. As mentioned in the article [5], a perfect example is the material data for the basic material used in thermal barriers, i.e. zirconium oxide modified with yttrium oxide (8YSZ: $8\% \text{ Y}_2\text{O}_3 \times \text{ZrO}_2$ in at%). This article, which is a continuation of the analysis from the publication [5], presents the results of research on the influence of the dispersion of input material data on the NiCrAlY interlayer and the nickel-based superalloy used in numerical modelling of temperature distribution and state of stress in thermal barrier coatings. The paper summarizes the data contained in the professional literature in the field of finite element simulation of TBC systems and

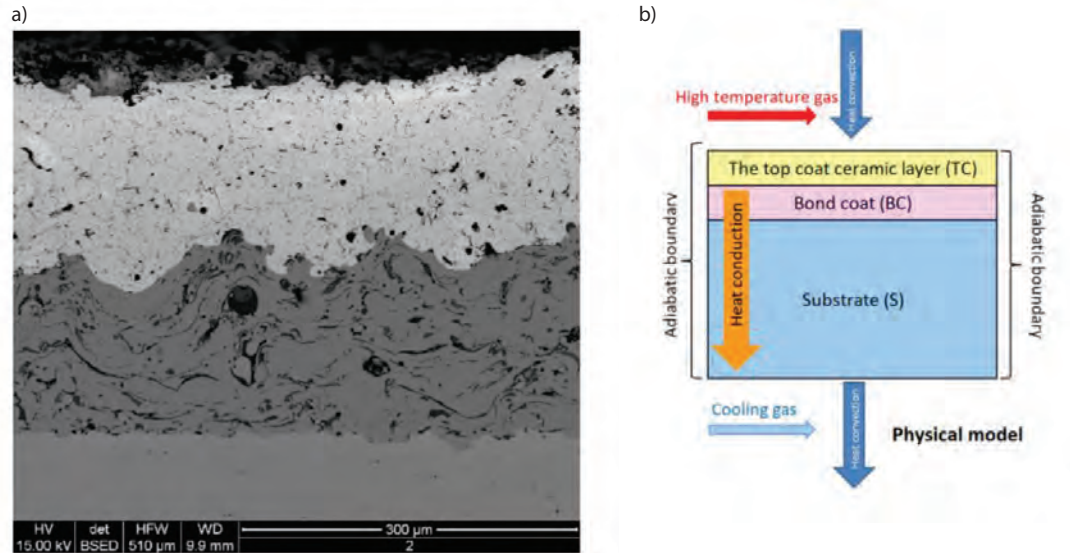


Fig. 1. Physical model of the TBC system: a) actual microstructure, b) schematic structure of the model with ceramic coating
Rys. 1. Model fizyczny systemu TBC: a) mikrostruktura, b) schemat modelu z powłoką ceramiczną

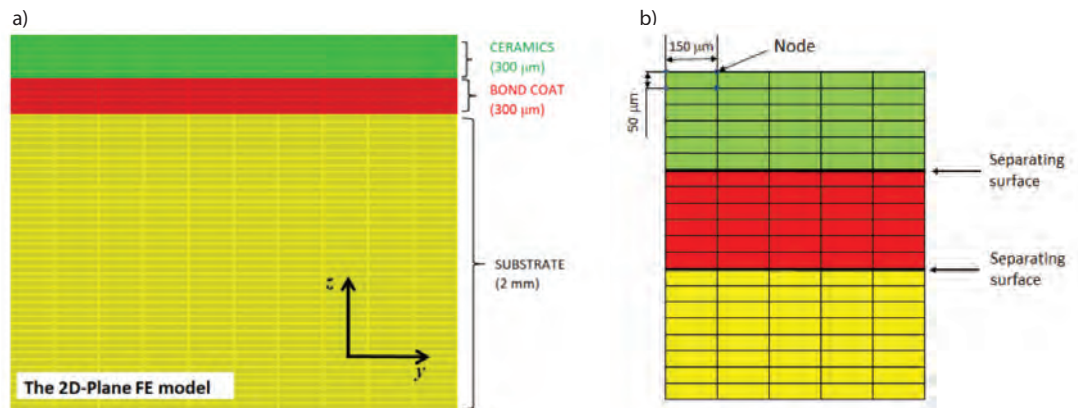


Fig. 2. Discrete model of the TBC system: a) fragment of the finite element mesh of the model, b) ceramic coating with a typical finite element mesh

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

Table 1. Set of material data used in FEM simulations

Tabela 1. Zestaw danych materiałowych użytych w symulacjach MES

Material	Properties	Values of material properties						
		min.	max.	st. dev.	average	median	kurtosis	skewness
8YSZ – top ceramic coat	λ [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]	8.20×10^{-6}	12.20×10^{-6}	0.92×10^{-6}	9.52×10^{-6}	9.68×10^{-6}	3.43×10^{-6}	1.14×10^{-6}
	E [GPa]	17.5	210.0	60.7	74.7	48.0	1.69	1.66
	ν	0.10	0.26	0.06	0.19	0.20	-1.63	-0.36
	ρ [kg/m ³]	5.40	6.04	0.27	5.76	5.60	3.58	-1.85
MeCrAlY (Me = Ni, Co) – bond coat	λ [W/mK]	4.30	25.00	8.16	11.6	11.2	2.23	1.41
	c_p [J/kgK]	0.40	0.501	0.06	0.5	0.5	-	-1.73
	CTE [1/K]	11.60×10^{-6}	15.50×10^{-6}	1.50×10^{-6}	13.6×10^{-6}	13.3×10^{-6}	-1.89×10^{-6}	0.07×10^{-6}
	E [GPa]	137.90	225.00	25.47	188.3	200.0	0.30	-0.89
	ν	0.27	0.32	0.01	0.3	0.3	4.00	-1.25
	ρ [kg/m ³]	7.32	7.80	0.34	7.6	7.6	-	-
Ni-based superalloys – substrate	λ [W/mK]	7.00	90.00	35.73	38.25	12.53	-2.02	0.69
	c_p [J/kgK]	0.41	0.48	0.03	0.44	0.45	-1.17	-0.32
	CTE [1/K]	9.67×10^{-6}	16.40×10^{-6}	1.78×10^{-6}	12.91×10^{-6}	13.10×10^{-6}	0.22×10^{-6}	-0.09×10^{-6}
	E [GPa]	15.00	220.00	52.97	177.29	200.50	5.69	-2.23
	ν	0.25	0.32	0.02	0.30	0.30	0.99	-1.35
	ρ [kg/m ³]	7.9	8.9	3.97	8.42	8.23	-2.44	0.18

Source: the author, based on [3, 5–7, 9, 10–65].

Źródło: opracowanie własne na podstawie [3, 5–7, 9, 10–65].

concerning material data. For the purposes of this article, only the minimum and maximum values and the standard deviation of the results, as well as the mean and median values, are presented.

2. Experiment procedure

TBC numerical models allow you to simulate the behaviour of systems, such as thermal barriers when operating under real conditions, which helps in the analysis and optimization of the system. Discrete models are particularly useful because they allow individual layers of finite elements to be evenly distributed, translating into more accurate results. An important aspect of the analysis of TBC models is the consideration of the thermo-mechanical properties of materials (such as coefficients of thermal expansion, strength, modulus of elasticity, etc.), thermal and mechanical interactions between the layers, and evaluation of the behaviour of the TBC under operating conditions.

The procedure for finite element modelling with the main steps is presented below:

1. Definition of the model's geometry: an axisymmetric two-dimensional model.
2. Division of geometry into finite elements (discretization of elements that form the whole model).
3. Determining the boundary conditions that correspond to the real conditions of the model operation. Temperature load assignment.
4. Determination of material properties: Young's modulus, Poisson's ratio, thermal expansion coefficient, thermal conductivity, etc.
5. Formulation of equations: based on physical and mathematical equations, such as equilibrium equations, heat equations, etc., appropriate equations were formulated describing the behaviour of the material and its response to defined boundary conditions.
6. Performing a numerical analysis by solving a system of equations for all finite elements in the model. The result of the calculations will be the distribution of temperature, stresses and strains in the entire model.

Based on the real picture of the microstructure of TBC systems, a discrete model of thermal barriers was developed, shown in Fig. 1. The geometric model includes three layers: a base made of IN 625 nickel superalloy with a thickness of 2 mm, 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: $8\text{Y}_2\text{O}_3 \times \text{ZrO}_2$ 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 2D discrete 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. In the analysed problem, 2D axisymmetric, four-node elements were adopted.

The following assumptions were taken into account for the analysis of the temperature field and stress state at high temperatures:

- 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 the analysis of elastic deformations. Two variants of the calculation procedure were adopted in the numerical analysis. In the first one, the following assumptions were made: the material properties of the ceramic layer were taken as their median, the physical properties of the base material were taken based on the IN 625 alloy manufacturer's data [6]. The interlayer was characterized by the following values of material properties: minimum value, maximum value, average value and corresponding to the median. In the second variant, the median values of material parameters for ceramics and the interlayer were assumed as the output parameters. In contrast, the properties of the substrate material (IN 625) were assumed in the form of values corresponding to minimum, maximum, average and median. The first stage of the research was to conduct a numerical analysis of the temperature field. The conditions of heat transfer on the outer surfaces of the body were determined by applying the boundary conditions of the first kind. The solution to the problem consisted in determining the temperature distribution based on the considered body's given initial and boundary conditions and material properties. In the analysed model, a temperature load was assumed. The temperature of 1500°C was set on the surface of the insulating ceramic layer of the TBC system, while the temperature of 800°C was assumed on the outer surface of the nickel superalloy. The next research stage was to determine the distribution of equivalent stresses following the Huber-Mises hypothesis for all variants of the assumptions of material values. The material data set in Table 1 was used for the FEM analysis. It includes the maximum and minimum values of the parameters (derived from literature data) as well as the mean value and the median (and other statistical parameters) determined for the purposes of this article. To illustrate the dispersion of the data, the standard deviation for each parameter was also introduced.

3. Results

As in the case of the YSZ-type material [5], the first stage of the research was the analysis of source data characterizing the basic physical parameters of the materials used in the simulations. This part discusses the data on the interlayer and substrate materials – NiCrAlY-type alloys and nickel-based superalloys.

Data on the material properties of the NiCrAlY interlayer show a large dispersion, especially in thermal conductivity and, to some extent, Young's modulus. The remaining parameters show a small dispersion of results, which is also expressed by statistical parameters. Due to the relatively small amount of data, we failed in all cases of kurtosis and skewness.

The situation is slightly different in the case of the base material in the form of a nickel superalloy. The spread of data in this case is comparable to the material dedicated to the insulating layer, i.e. YSZ. This applies to the thermal conductivity value, coefficient of thermal expansion and Young's modulus.

The analysis of the source data in the case of the ceramic material 8YSZ [5] indicated the reason for the differences in the data values characterizing the physical properties of the materials used in FEM simulations. There are differences in the morphology and form of material processing. On the other hand, in the case of NiCrAlY-type superalloys, there are quite limited morphological differences. The main data concerned the NiCrAlY material in thermally sprayed coatings. Hence, the scatter of results is smaller than in the case of ceramic material

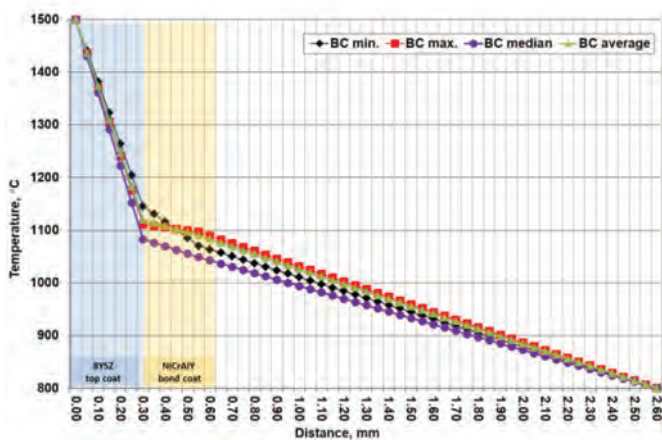
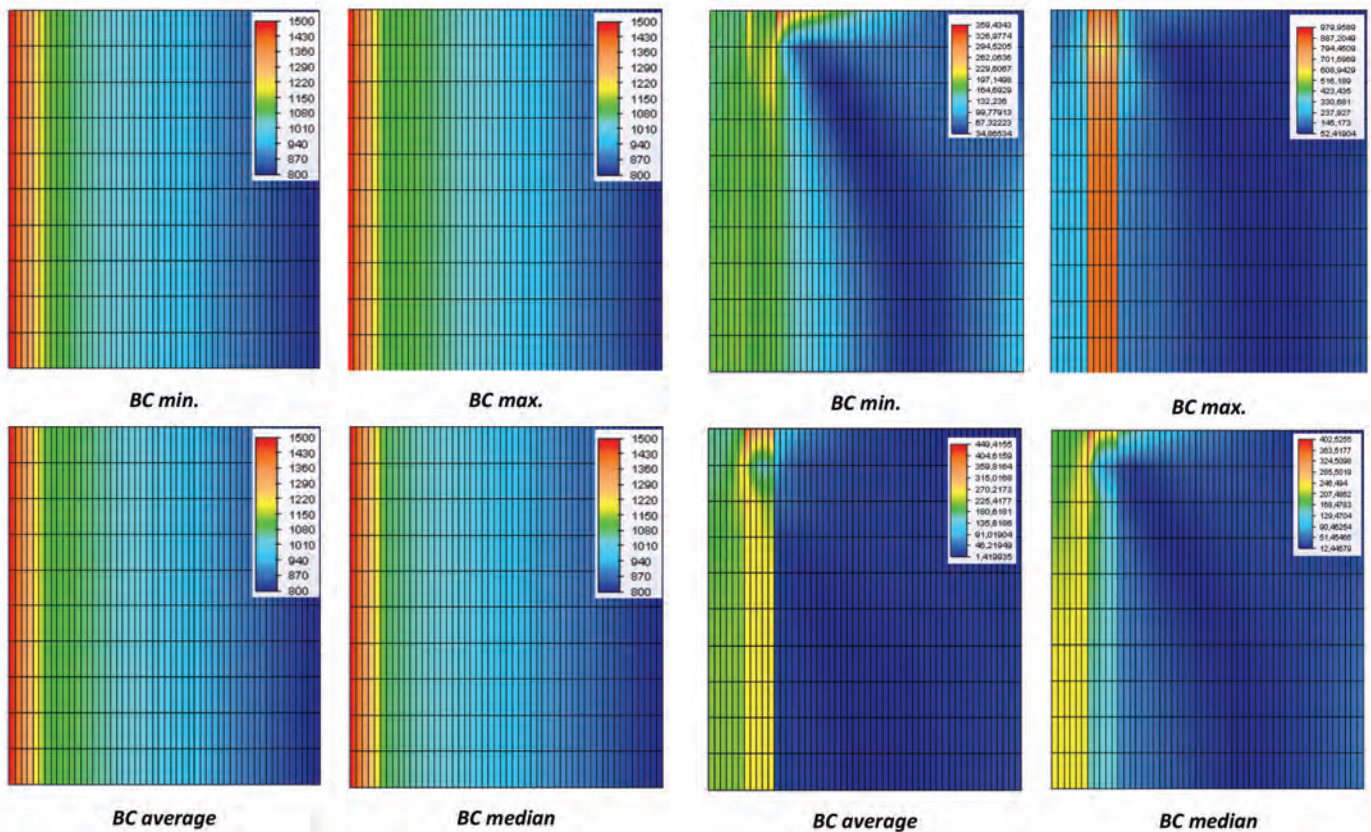


Fig. 3. The results of the simulation of temperature distribution for different values (minimum, maximum, median, average) of physical parameters of materials – bond coat

Rys. 3. Wyniki symulacji rozkładu temperatury dla różnych wartości (minimum, maksimum, mediany, średnie) parametrów fizycznych materiałów – międzywarstwa

8YSZ. The situation is different in the case of the base material where the literature data often lacks information on the type of superalloy used. There are also simulations in which pure nickel was introduced as the base material, the thermal conductivity of which is many times greater than the thermal conductivity of any nickel superalloy. Hence, significantly greater differences in the simulation results are considered from the point of view of the input data for the substrate material compared to the analogous results for the interlayer.

Figures 3–6 show the temperature and stress distribution simulation results. Obtained based on the data contained in Table 1,

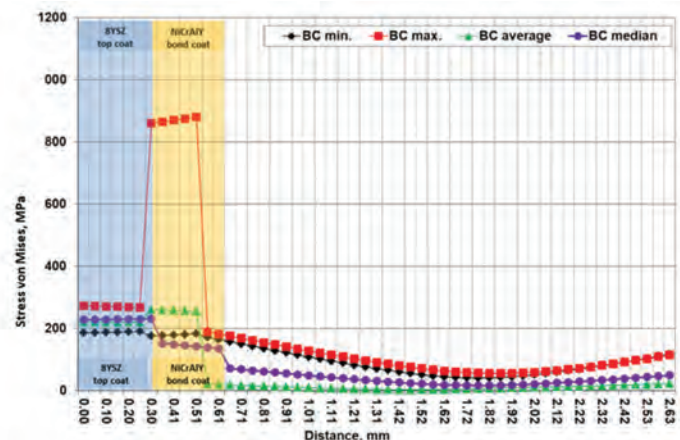
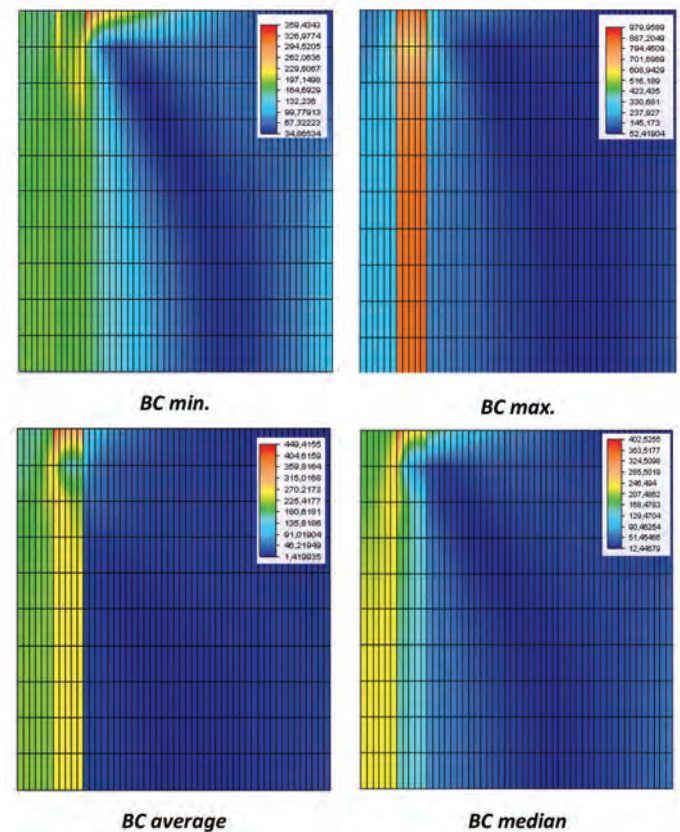


Fig. 4. Results of simulation of von Mises stress distribution for different values of physical parameters of materials: for a constant temperature of 1200°C – bond coat

Rys. 4. Wyniki symulacji rozkładu naprężeń według hipotezy Hubera-Misesa dla różnych wartości parametrów fizycznych materiałów: dla stałej temperatury 1200°C – międzywarstwa

i.e. minimum values, maximum, median and average of the basic parameters characterizing the physical properties of materials necessary in the FEM modelling process.

Similarly to the YSZ [5], the analyses showed that introducing extreme values results in obtaining simulation results significantly different in temperature distribution. Considering the effect of the interlayer, it should be noted that if minimum values are entered, the temperature on the surface of the interlayer differs by as much as approx. 25°C compared to the maximum values and 65°C to the median. Considering the influence of the substrate material these differences are much greater and

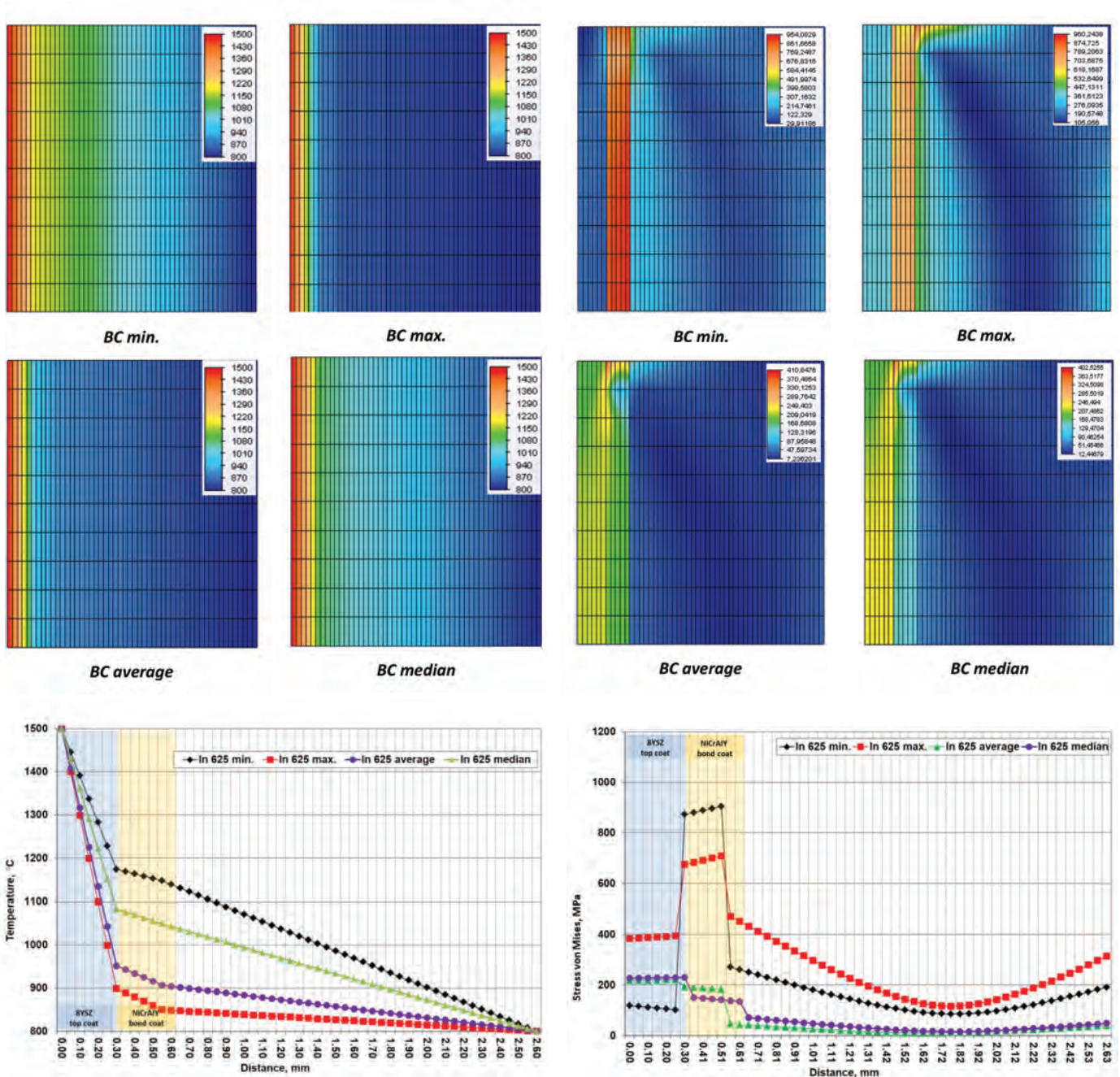


Fig. 5. The results of the simulation of the temperature distribution for different values (minimum, maximum, median, average) of the physical parameters of the materials – the substrate

Rys. 5. Wyniki symulacji rozkładu temperatury dla różnych wartości (minimum, maksimum, mediany, średnie) parametrów fizycznych materiałów – podłoże

amount to approx. 275°C for the minimum and maximum extreme values.

In the case of the bond coat, it is difficult to talk about a trend when entering the minimum, maximum, mean or median values, which is quite an unusual observation. On the other hand, in the case of the substrate material, for the median, the temperature on the surface of the interlayer is close to that obtained for the minimum value and the average value to the maximum value.

In the case of reduced stresses (for the interlayer), the strongest gradient effect was obtained for maximum values. In the remaining cases, the differences in stress at the separation boundaries

Fig. 6. Results of simulation of von Mises stress distribution for different values of physical parameters of materials: for a constant temperature of 1200°C – substrate

Rys. 6. Wyniki symulacji rozkładu naprężeń zastępczych według hipotezy Hubera-Misesa dla różnych wartości parametrów fizycznych materiałów: dla stałej temperatury 1200°C – podłoże

of individual sublayers are very similar. When considering the variant concerning the base material, the most favourable stress distribution can be observed after introducing the median or the average as input parameters for the FEM simulation.

4. Conclusions

The analyses carried out in the form of FEM simulations, regarding the interlayer’s influence on the distribution of temperature and stresses showed that significant differences are observed in the case of reduced von Mises stresses (for the

maximum and minimum values). In the case of temperature distribution, the differences are relatively small. However, an unusual relationship is visible when the median or mean value is entered. In this case, the temperature distribution is not located between the maximum and minimum values. This suggests that other factors besides thermal conductivity also affect the temperature distribution.

In the case of simulations based on data on the physical properties of the base material (nickel superalloys), a large scatter of input data causes significant differences in the results of simulations of temperature distribution and reduced stresses. In the context of the scattering of input data, the observed differences in simulation results are obvious.

These data also show that the most favourable substrate material, from the point of view of temperature distribution, is a nickel superalloy with the highest possible thermal conductivity value. The most favourable state of stress was observed for the mean and median values of the introduced physical properties of the base material.

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