



NUMERICAL MODELING OF THERMAL CONDUCTIVITY OF AIR-PLASMA- SPRAYED ZIRCONIA WITH DIFFERENT POROSITY LEVELS

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Abstract: The effective thermal conductivity of a porous ceramic coating depends on porosity and the distribution of pores. Due to these aspects, the structure of a ceramic coating plays an important role in the analysis of heat transfer. In this study, using real microstructural images, effective thermal conductivities of air plasma sprayed (APS) zirconia coatings have been calculated via CFD modeling as well as using Maxwell-Eucken and the EMT models. CFD studies were carried out using FLUENT 6.1.22 code. Samples were produced having five different porosities by changing the coating parameters. The porosities of the samples were in the interval of 9% - 31%. Results obtained from analytical and finite volume methods have been compared to experimental thermal conductivity data given in the literature. The numerically calculated effective thermal conductivities are in good agreement with those determined experimentally. This study demonstrates that CFD analysis can be used to predict the effective thermal conductivity of porous ceramic coatings using real digital images. By virtue of this, the model can be used to obtain preliminary values instead of high cost and time-consuming experiments.

Keywords: Thermal conductivity, Porosity, Air plasma spray, Finite volume methods.

FAKLI GÖZENEKLİLİK ORANLARINDAKİ ATMOSFERİK PLAZMA SPRAY ZİRKONYANIN ISI İLETİM KATSAYISININ NÜMERİK MODELLEMESİ

Özet: Gözenekli seramik kaplamanın efektif ısı iletim katsayısı gözeneklilik oranına ve gözeneklerin dağılımına bağlı olarak değişmektedir. Bu nedenle ısı transferi çözümlerinde gerçek mikroyapının kullanılması önemli bir rol oynamaktadır. Bu çalışmada gerçek mikroyapı resimleri kullanılarak atmosferik plazma spray (APS) kaplamanın efektif ısı iletim katsayısı CFD modeli ile literatürde bulunan Maxwell-Eucken ve EMT analitik ifadeleri kullanılarak hesaplanmıştır. CFD modelleri Fluent 6.1.22 kodu kullanılarak yapılmıştır. Numuneler kaplama parametrelerinin değiştirilmesi ile beş farklı gözeneklilikte elde edilmiştir. Numunelerin gözenekliliği 9% - 31% arasında değişmektedir. Analitik ve sonlu hacimler metodundan elde edilen ısı iletim katsayısı değerleri literatürde yer alan deneysel sonuçlar ile karşılaştırılmıştır. Nümerik olarak elde edilen efektif ısı iletim katsayısı değerleri deneysel çalışmalar ile uyum sağlamaktadır. Bu çalışma gözenekli seramik malzemenin efektif ısı iletim katsayısının gerçek mikroyapı resimlerinin kullanılarak elde edilmesinde CFD analizinin kullanılabileceğini göstermektedir. Bu sayede, bu model yüksek maliyetli ve zaman alıcı deneylerden önce ön değer elde etmek amacıyla kullanılabilir.

Anahtar Kelimeler: Isı iletim katsayısı, Gözeneklilik, Atmosferik plazma spray, Sonlu hacimler metodu.

NOMENCLATURE

k	thermal conductivity [W.m ⁻¹ .K ⁻¹]	T	temperature [°C]
k_{eff}	effective thermal conductivity [W.m ⁻¹ .K ⁻¹]	v	volume rate
k_m	solid phase thermal conductivity [W.m ⁻¹ .K ⁻¹]	v_m	solid phase volume rate
k_g	gas phase thermal conductivity [W.m ⁻¹ .K ⁻¹]	v_g	gas phase volume rate
P	porosity %	ΔT	temperature difference between lower and upper surface of coating [°C]
q''	heat flux [W.m ⁻²]		

INTRODUCTION

Ceramic coatings are engineering materials used in various technological applications and necessary for thermal insulation, thermal corrosion, oxidation, or erosion strength. These types of coatings, such as thermal barrier coatings (TBCs), are applied in gas turbines and diesel engines in order to protect the metallic parts and to increase performance at high temperatures (Teixeira et al., 1999; Demasi-Marcin and Gupta, 1994; Johner and Schweitzer, 1985; Portinha, 2005). TBCs (Herman and Sulit, 2000; Tucker, 1999) can facilitate higher output work in metallic parts by decreasing the exposed heat through low levels of thermal conductivity; they additionally decrease costs by lengthening the lifetime of these parts (Taylor et al., 1999; Brindley and Miller, 1989). Some studies have shown that thermal barrier coatings result in increased thermal efficiency and decreased fuel consumption in diesel engines (Swaminathan and Cheruvu, 1994; Cernuschi et al., 2004). The literature suggests that a large amount of work has been done to obtain the effective thermal conductivity of thermal barrier coatings. Most research dealing with the effective thermal conductivity of TBCs has dealt with materials of 8 to 12% porosity, as determined by experimental (Taylor et al., 1999; Pawlowski and Fauchais, 1992; Zhu et al., 2001), numerical (Alpérine et al., 1997), and analytical methods. In many applications, there are no numerical solutions based on finite element methods for calculating the thermal conductivity of air-plasma-sprayed TBCs with porosity values of 12% or higher using real digital images.

Numerical models are considerably useful in analyzing the effect of microstructure on thermal conductivity and for supporting microstructure designs that can decrease thermal conductivity and exist in theory (Zhu et al., 2001; Alpérine et al., 1997; Jadhav et al., 2006; Bolot et al., 2005; Dorvaux et al., 1997). Jadhav et al. (Jadhav et al., 2006) investigated the thermal conductivity of solution precursor plasma spray (SPPS) and air-plasma-sprayed coatings using (object-oriented) finite element (OFF) models that capture the effect of the real microstructures of TBCs and have found that finite element models were better than analytical models at describing the thermal conductivities.

Bolot et al. (Bolot et al., 2005) studied the computation of heat transfer through a porous structure using a finite-difference-based model. Dorvaux et al. (Dorvaux et al., 1997) investigated the thermal conductivity of porous and micro-cracked ceramic coatings, using a finite difference method applied to digitized images. Dorvaux et al. (Dorvaux et al., 1997) discussed the effect of different types of morphological features on thermal conductivity. In order to describe the effects of the microstructure on heat transfer in greater detail, S. Grandjean, J. Absi, and D.S. Smith (Grandjean et al., 2006) developed a method involving 2D finite element

calculations based on real micrographs of the porous solid. The approach was tested on micrographs of tin oxide samples with pores ranging from 10% to 50%. A reasonable agreement with Rayleigh's model was obtained for pore contents up to 20%.

Baker (Baker, 1997) studied the conductivity of complex porosity or inclusion structures by using the finite element method (FEM). The effects of shape, orientation, and distribution of the dispersed phase on the conductivity were calculated using FEM. With this calculation, the two-dimensional conductivity was obtained, which is considered to be a useful limit of the three-dimensional conductivity.

Golosnoy et al. (Golosnoy et al., 2005) have developed numerical and analytical models for simulating heat flow through plasma-sprayed coatings, allowing the effective thermal conductivity to be predicted as a function of microstructural parameters. The structure was assumed to be composed of lamellar materials (splats) that were separated by (thin) pores, which contained contact areas (bridges). The investigation of the effects of pore geometry on conductive and radiative heat transfer within the TBCs (based on zirconia yttria top coats) over a range of temperatures and gas pressures has shown that the main factor in controlling the conductivity was the inter-splat bridges.

The presented paper concentrates on the aim of developing and evaluating an alternative approach, based on a finite element method, to calculate the thermal conductivity of porous media using real digital images. In this study, in order to investigate the effect of porosity on thermal conductivity, the APS coating method (which produces a nonhomogeneous pore structure and distribution) is preferred. Furthermore, the APS method is the preferred coating type in thermal barrier coatings for reasons of economic and applicability. During coating, by changing the distance between the spray gun and the substrate, structures were obtained with five different porosity values (9.4% - 31%). Microstructural images, which were obtained by the final metallographic analysis of these structures, have been modeled with a finite element method (Fluent 6.1.22) in order to calculate the thermal conductivity. The contact resistance of the coating surface results in a deviation between the numerically calculated effective thermal conductivity which were obtained experimentally; however, the contact surface between the APS coating and the base plate could not be modeled in a CFD analysis. In this analysis, only the thermal conduction in the solid phase and pores was considered. The results have been compared with computed results via analytical expressions which were presented in the literature obtained by experiments, Maxwell-Eucken, and the effective medium theory (EMT). The methodology developed in this study presented results that were compatible with the experimental and analytical results. The numerical

solution method can successfully be applied in determining the effective thermal conductivity of coatings if the theoretical solution has difficulties.

SAMPLE PREPERATION

Samples

Samples were formed of substrates and ceramic coatings. The substrate was 12.7 mm in diameter, 5 mm in thickness, and made of 321 stainless steel. APS coatings were prepared from 92 wt% ZrO₂ and 8 wt% Y₂O₃ solid solution (Metco 240 NS, Sulzer Metco).

Characteristics of Microstructure

Microstructural images of the coatings were obtained by using an optical microscope (Nikon, Epiphot 300) and an electron microscope (Leo, S440). In order to determine the porosity and thickness of the samples sensitively, a Leica Image Analyzer hardware/software system was used. The coating thicknesses and porosity values of the samples are given in Table 1.

Table 1. Sample Properties.

Sample	Coating thickness (μm)	Porosity (%)
8YSZ1	475	9.4
8YSZ2	475	12.4
8YSZ3	475	18
8YSZ4	472	24.8
8YSZ5	470	31.1

EFFECTIVE THERMAL CONDUCTIVITY: NUMERICAL METHOD

For the numerical method, microstructural images of samples with different porosities (obtained by changing the distance of the coating application) were used. Optical images were converted into geometries to be analyzed in a SolidWorks code. For 2D thermal analysis of these geometries, Fluent 6.1.22 code was used. In this study, the calculation of the thermal conductivity of the microstructure was consisted of two steps.

In the first step, the geometry was constituted using the SolidWorks code, and pores of the real structure were constructed (Altun, 2007). Optical microscope images of APS coatings with different porosity values and geometries, processed in SolidWorks code for numerical analysis, are given in Fig. 1. Two zones exist in the microstructural images; gray zone corresponds to ceramic material (8YSZ) and black zone to pores (air).

In the second step, the boundary conditions and the coating and pore domains were defined. The coating was meshed using Gambit code and the mesh element type was triangular in both ceramic and pores. The mesh size was between 39050 – 158905 cell depending on porosity. In the TBC which has porous structure,

heat transfer occurs by conduction in solid areas, and by combination of gas conduction, natural convection and radiative heat transfer in pores. Convection in pores is accepted to be significant if the pores size is larger than 10 μm (Clyne et al., 2006; Stark and Fricke, 1993). In this study the structures which were analyzed have very small pores 10 μm, so heat transfer by natural convection in pores was ignored.

In this study the analysis was performed 100 -1000°C. For 8% YSZ, the contribution of radiative heat transfer to the effective pore conductivity is predicted to become substantial for temperatures above ~ 900°C (Golosnoy et al., 2005). Therefore the effects of the radiation on the thermal conductivity of pores are neglected. Finally, it has been accepted that heat transfer is only by conduction in pores. Air in the pores was taken as inert.

The outer sides of the thermal barrier coating were defined as “wall” boundary type. The pores were defined as “interior”. The temperatures of the lower and upper sides (T_{lower} , T_{upper}) were assumed to be constant. Adiabatic boundary condition was applied to the left and right sides (Fig.2).

In order to investigate the effect of the pore structure on the temperature distribution, microstructural images were divided into 50 sections in Gambit code, and the porosity and temperature changes were analyzed for each region (Altun and Boke, 2008). The boundary conditions were shown on an image of a divided microstructure with the porosity of 9.4% (Fig. 2). The temperature difference between the upper and lower surface was taken as 10°C, and CFD analysis was carried out at average temperatures ranging between 100°C and 1000°C with 100°C interval. The heat flux (q'') through the lower and upper surfaces of the coating was taken as convergence criteria and the solution converged for the heat flux residual below 1×10^{-5} .

Because the structure of the porous media and the pore distribution were not homogenous and regular, the CFD method was found to be more appropriate for calculating the temperature distribution. The real distribution of the pores was random, and the shapes of the pores differed from each other. In order to determine the effect of the pore distribution, the porous media were not converted to a regular structure. The porous structure causes the formation of the two dimensioned temperature distribution even the solution appears one dimensional. The length and the depth of the control zone were 0.475 mm and 0.126 mm respectively. Being given the adiabatic boundary condition based on the considered control zone that is a small part of a coating in the infinite length. The porosity of each surface in the depth dimension is close to each other. Besides this, the shape and the arrangement of the pores have a similar character. The porosity and the shape of the pores have significance on the thermal conductivity of TBSs. The each considered surface has similar temperature profile.

CFD simulations were performed using a temperature based steady-state segregated implicit solver. A second-

order upwind scheme was selected for the energy equations.

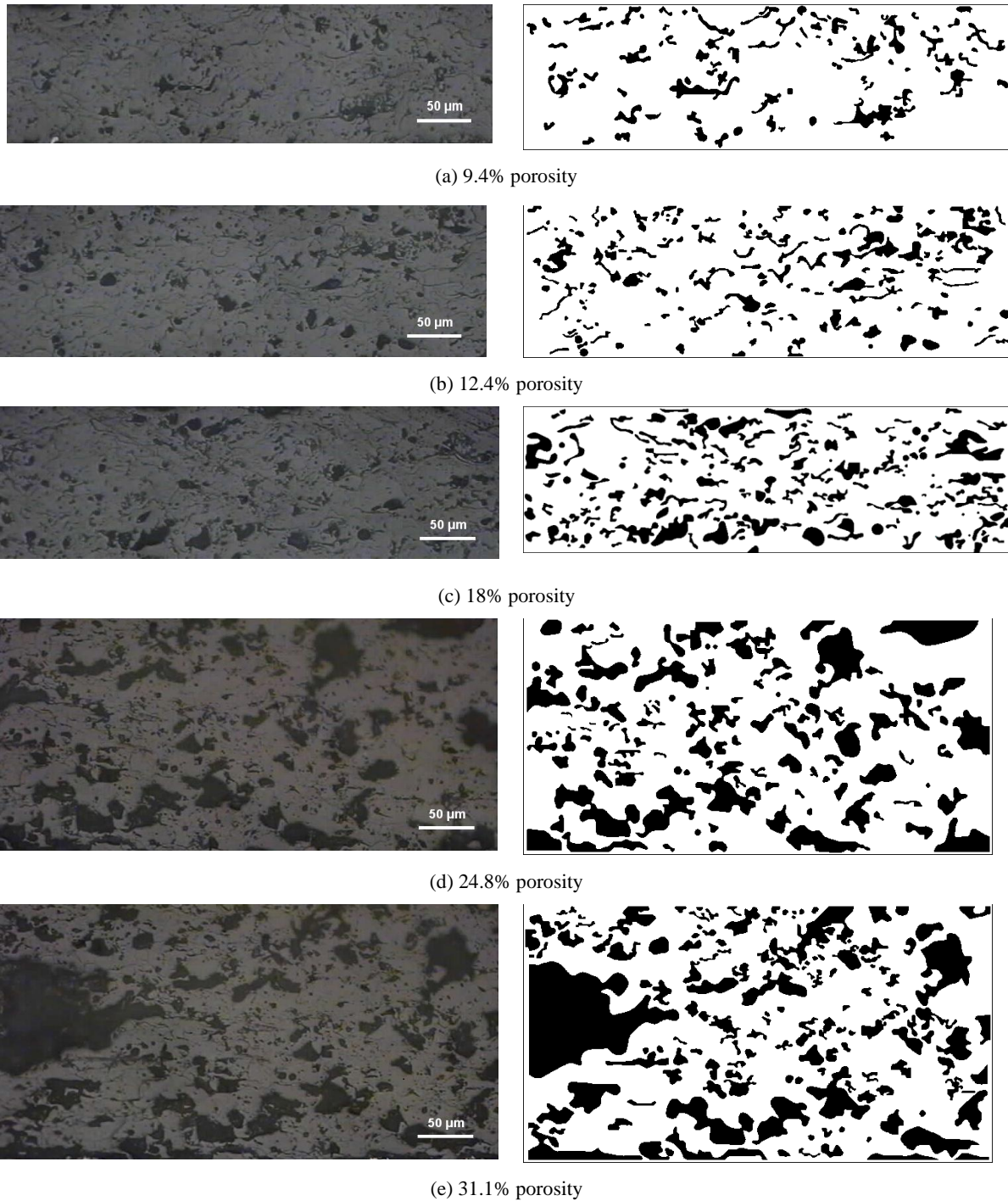


Figure 1. Optical microscope images and SolidWorks versions of microstructures analyzed with CFD code.

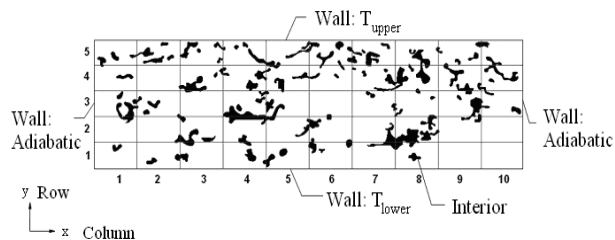


Figure 2. Divided microstructure with 9.4% porosity and boundary conditions.

EFFECTIVE THERMAL CONDUCTIVITY: ANALYTICAL EXPRESSIONS

The prediction of the effective thermal conductivity of heterogeneous or composite materials is an area of interest in heat transfer applications, and there are many expressions in the literature for the modeling of effective thermal conductivity (Wang et al., 2006).

Thermal characteristics of TBCs vary depending on the coating technique and process parameters used. These factors are affected by the shape and orientation direction of the pores in the TBCs. In the literature, the distribution of porosity is classified as symmetric or asymmetric, depending on the distribution of pores (Nait-Ali B et al., 2006). The porosity distribution of APS coatings is asymmetric, and Maxwell-Eucken and EMT expressions are used in analysis, which were derived for the asymmetric model.

The first expressions derived for the asymmetric model were proposed by Landauer (Landauer, 1952) and Rayleigh (Rayleigh, 1892). The Maxwell-Eucken model assumes a dispersion of small spheres within a continuous matrix of a different component, with the spheres being far enough apart such that the total distortions due to the temperature distribution around each sphere do not interfere with neighboring temperature distributions (Wang et al., 2006). The effective thermal conductivity k_{eff} of the Maxwell-Eucken model is;

$$k_{eff} = \frac{k_m v_m + k_g v_g \frac{3k_m}{2k_m + k_g}}{v_m + v_g \frac{3k_m}{2k_m + k_g}} \quad (1)$$

Here, k_m and k_g are the thermal conductivities of the solid matrix and of the gas found in the pores, respectively, v_m and v_g are the volume rates of these phases, and k_{eff} is the effective thermal conductivity.

However, in the effective medium theory (EMT) given in Eq. (6), it is accepted that the pores are randomly dispersed within the matrix at the same time (Wang et al., 2006; Landauer, 1952).

$$0 = v_m \frac{k_m - k_{eff}}{k_m - 2k_{eff}} + v_g \frac{k_g - k_{eff}}{k_g + 2k_{eff}} \quad (2)$$

RESULTS

Numerical analysis was carried out for the average temperatures between 100°C and 1000°C. The temperature difference between the upper and lower surface was chosen as 10°C. In Fig. 3, temperature contours in a microstructure with 9.4% porosity are given for the average temperature of 1000°C. The temperature of the coating decreased as the porosity increased in the microstructure. It was observed that the pores decreased the heat transfer along the heat flow direction. The shape and orientation direction of the pores in the TBC affected the thermal conductivity. The pores aligned perpendicular to the heat flow decreased the heat transfer more than the pores aligned parallel to the heat flow. Overall, the arrangement of the pores affected the temperature distribution in the microstructure.

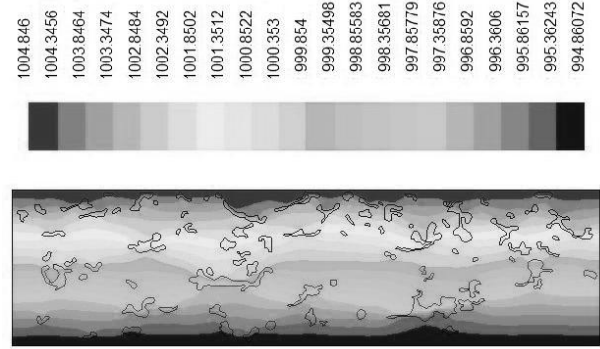


Figure 3. Numerically calculated temperature distribution in a microstructure with 9.4% porosity for an average temperature of 1000°C.

In CFD analysis, the thermal conductivity of dense 8 YSZ was taken both constant and as a function of temperature. The constant thermal conductivity of dense 8 YSZ is 2 W/mK (Zhu et al., 2001). The temperature dependence of the thermal conductivity of dense 8 YSZ is given in the literature (Schlichting et al., 2001).

The effect of the thermal conductivity of dense 8 YSZ on the effective thermal conductivity of the coating of the porosity 9.4% is shown in Fig. 4 as a function of temperature. The maximum deviation in the thermal conductivity of the coating as the thermal conductivity of the dense 8 YSZ was assumed to be constant and temperature dependent was 4% for temperatures less than 400°C. In this study, the thermal conductivity of dense ceramic material was taken as a function of temperature to create an accurate model.

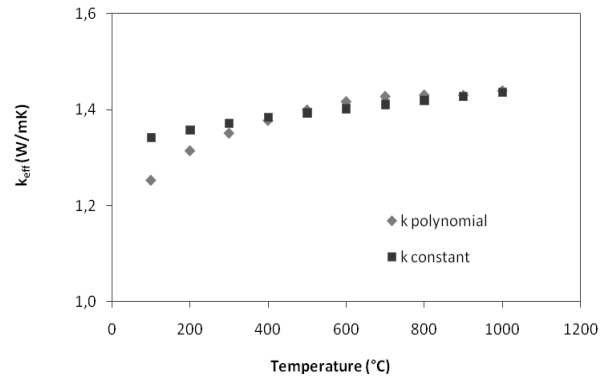


Figure 4. Predicted effective thermal conductivity for coating with 9.4% porosity, taking thermal conductivity of dense 8 YSZ as constant and temperature dependent.

Experiments take time and can bring some mistakes because of the test conditions which cannot be under control. Modeling of the microstructure using the optical microscope image takes shorter time and it is possible to adapt of various boundary conditions easily. But model results should be validated using the experimental study which is carried by shelf or given in literature. This comparison is given in Figure 5. After this validation the cases for the other porosities were run.

The effective thermal conductivity of a coating with 12.4% porosity was calculated to be between 1.12 - 1.31 W/mK for the temperature range of 100-1000°C (Fig. 5). In the literature, the experimentally defined effective thermal conductivity has been given as 1–1.4 W/mK for a coating with 12% porosity (Pawlowski and Fauchais, 1992; Ravichandran and An, 1999). The maximum deviation between the experimental and the calculated effective thermal conductivity was 8%.

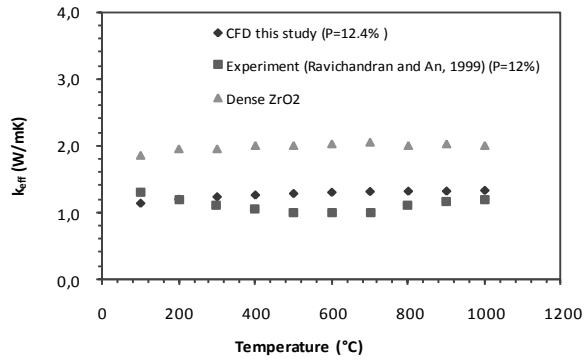


Figure 5. Comparison of experimentally and numerically determined thermal conductivities of a coating with 12.4% porosity.

The effective thermal conductivities of coatings with various porosities for 800°C determined by means of a CFD method, the Maxwell-Eucken and Effective Medium Theory (EMT) model are given in Fig. 6. The difference between the effective thermal conductivities of the coating determined by analytical methods and the numerical method increased with increasing porosity. The maximum difference was observed for the Maxwell-Eucken method and the numerical solution. The deviation between these methods was 15% for porosities in the range of 9.4% to 18%. The maximum difference between the predicted and analytically calculated effective thermal conductivity was 35% for the porosity of 31.1%. Although the effective thermal conductivity of the EMT method was less than that obtained with the Maxwell-Eucken model, the difference was 15% for the minimum porosity and 35% for the maximum porosity, as compared with the predicted ones. The Maxwell-Eucken model assumed a dispersion of small spherical or small cylindrical pores within a continuous matrix. Analytical methods have accepted that pores are homogenous and distributed in an orderly pattern throughout the coating. However, the real pore geometry and distribution modeled at the numerical study, and the porous media were not converted to a regular structure. Due to the difference in pore structure taken into account by the analytical methods, more accurate results were obtained by the numerical method.

It was observed that the results of the CFD analysis were in good agreement with the measured thermal conductivities (Fig 5). The numerical analysis was more accurate than the analytical calculation. The contact resistance on the coating surface resulted in a deviation

between the numerically calculated effective thermal conductivity and experimental results. The contact surface between the APS coating and the base plate could not be modeled in the CFD analysis.

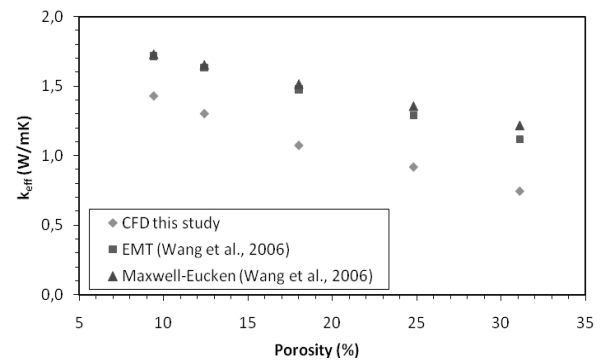


Figure 6. Numerically and analytically defined thermal conductivity at 800°C.

The effective thermal conductivities of a coating with 12.4% porosity obtained using the Maxwell-Eucken and EMT methods were compared with the experimental values given in the literature (Ravichandran and An, 1999), as shown in Fig. 7. Although the results obtained from the Maxwell-Eucken and EMT analytical expressions were similar, there was a large deviation between results from the analytical methods and the experimentally defined thermal conductivity. In both analytical methods, only the volumetric ratio and thermal conductivities of the pores were considered, but pore sizes and shapes were neglected.

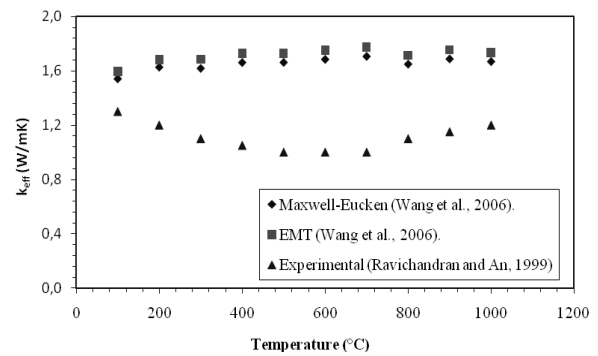


Figure 7. Comparison of experimentally and analytically defined thermal conductivity of a coating with 12.4% porosity.

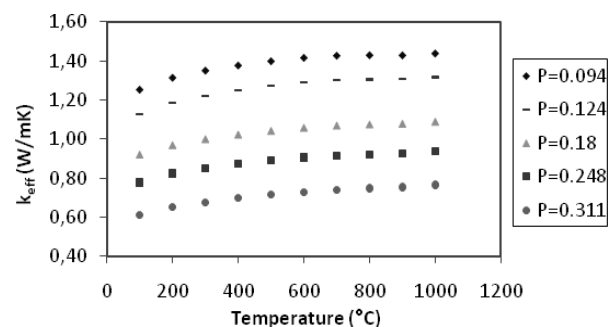


Figure 8. Effective thermal conductivities of coatings with different porosities.

The effective thermal conductivities of APS coatings with different porosities defined by numerical analysis are given in Fig. 8 for the average temperature range of 100 - 1000°C. The effective thermal conductivity decreased with increasing porosity and increased with increasing average temperature.

CONCLUSIONS

Knowing the thermal properties of the TBCs exposed to high temperatures plays an important role at developing these coatings. TBCs have different thermal characteristics depending on the coating technique, porosity, pore shapes and the thickness of coating. As already known, TBC applications are very expensive and high technologic applications used especially in gas turbines, aerospace industry etc. Also different fields need different TBC properties. Knowing the thermal characteristics and behaviors of these coatings is important to define the efficiency of gas turbines and estimate service life of the components. The main aim of this study is to obtain predicted effective thermal conductivity of the coating using numerical method instead of employing expensive applications and spending time.

In this study the effective thermal conductivities of APS coatings with different porosities were defined by means of numerical analysis, using real microstructural images of the coating. A comparison of the numerically obtained thermal conductivities with the experimentally and analytically obtained values showed that the numerical analysis is more accurate method for determining the thermal conductivity of TBCs. This numerical analysis could successfully be applied to TBCs, and, in particular, this model could be generalized and applied to numerical modeling of TBCs with different porosity characteristics (EB PVD, HVOF). In order to increase the accuracy and sensitivity of numerical model, the thermal conductivity of dense ceramic material (ZrO₂) and fluid in pores should be determined more accurately and microstructural images should be converted into geometries more carefully.

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