



HEAT TRANSFER ANALYSIS OF THERMAL BARRIER COATINGS ON A METAL SUBSTRATE

Özge ALTUN* ve Y. Erhan BÖKE**

* Eskisehir Osmangazi University, Mechanical Engineering Department, Batımeselik 26480, Eskisehir-Turkey,
Tel.: +90 222 2393750 (3524) ; fax: +90 222 2393613, e-mail: okutlu@ogu.edu.tr.

** Istanbul Technical Univ., Mechanical Engineering Faculty, Gumussuyu 34437, Istanbul-Turkey

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Abstract: Thermal barrier coatings (TBCs) are used in order to protect hot section component parts from high temperature effect, extend the service life of the parts and reduce the maintenance costs in gas turbines. Thermal conductivity of TBCs directly affects the strength temperature of operating parts in hot section. The gas turbines' operating temperatures and efficiency change depending on thermal conductivity of TBCs. For this reason to determine the thermal conductivity of TBCs directly concern the turbine design. In this study, effective thermal conductivity layered structure which is composed of metal substrate and thermal barrier coating has been obtained numerically. Solutions have been performed taking conduction and radiation into consideration for different boundary conditions for TBC which have two different porosity. As a result of analyses, it has been determined that radiation boundary condition solution is 7% lower than the heat conduction solution.

Keywords: Thermal barrier coating, heat transfer, thermal conductivity, numerical analyses.

METAL BİR ANA MALZEME ÜZERİNDEKİ TERMAL BARIYER KAPLAMANIN ISI TRANSFER ANALİZİ

Özet: Termal Bariyer Kaplamalar (TBK) gaz türbinlerinde sıcak kısım parçalarını yüksek sıcaklık etkilerinden korumak, malzemelerin servis ömrünü uzatmak dolayısıyla bakım maliyetlerinin azaltmak amacıyla kullanılmaktadır. TBK'ların ısı iletim katsayısı bu kısımda çalışan parçaların dayanım sıcaklığını doğrudan etkilemektedir. TBK'ların ısı iletim katsayılarına bağlı olarak gaz türbinlerinin çalışma sıcaklıkları ve verimleri değişmektedir. Bu nedenle TBK'ların ısı iletim katsayısının belirlenmesi türbin tasarımını doğrudan ilgilendirmektedir. Bu çalışmada, yüksek sıcaklığa maruz TBK uygulanmış metalden oluşan tabakalı yapının efektif ısı iletim katsayısı nümerik olarak elde edilmiştir. Çözümler, iki farklı gözenekliliğe sahip TBK için farklı sınır şartlarında iletim ve ışınilma ısı geçişi hesaba katılarak yapılmıştır. Analiz sonucunda ışınilma ısı geçişinin hesaba katıldığı çözümlerin, iletim çözümüne nazaran %7 az olduğu tespit edilmiştir.

Anahtar Kelimeler: Termal bariyer kaplamalar, ısı transferi, ısı iletim katsayısı, nümerik analiz.

NOMENCLATURE

c_p	Specific heat [J g ⁻¹ K ⁻¹]
d_v	Pore thickness
\dot{E}_i	Rate of energy transfer into a control volume [W]
\dot{E}_o	Rate of energy transfer out of control volume [W]
k	Thermal conductivity [W m ⁻¹ K ⁻¹]
k_{eff}	Effective thermal conductivity [W m ⁻¹ K ⁻¹]
k_p	Effective thermal conductivity of pore [W m ⁻¹ K ⁻¹]
k_g	Thermal conductivity of gas [W m ⁻¹ K ⁻¹]
k_g^0	Normal conductivity of gas [W m ⁻¹ K ⁻¹]
k_{rad}	Radiative conductivity [W m ⁻¹ K ⁻¹]
n	Refractive index
q''_{rad}	Radiative heat flux

P	Pressure [atm]
T	Temperature [°C]
T_u	Upper Surface Temperature [°C]
T_l	Lower Surface Temperature [°C]
δ	Penetration depth
σ	Stefan-Boltzman constant
ϵ	Extinction coefficient

INTRODUCTION

Thermal conductivity of a porous media is important in various engineering fields. As a matter of fact, in many industrial applications, materials are selected primarily by considering their mechanical and thermal properties. In aerospace, power generation and automotive

industries, porous ceramic thermal barriers are widely used for manufacturing the most advanced components (Cernuschi et al., 2004). However knowing the thermal properties of the thermal barrier coatings (TBCs) is important in these applications.

TBCs have been widely used in hot-section metal components of gas turbines either to increase the inlet temperature with a consequent improvement to the efficiency or to reduce the requirements for the cooling air (Swadzba et al., 2007). For this reason to investigate the effect of microstructural defect distribution on the heat transfer is very important for the design of plasma-sprayed TBCs for which the thermophysical properties are important depending on the usage area.

In previous studies (Jadhav et al., 2006; Bakker 1997) only the heat transfer by conduction at the coating domain were analyzed. Temperature distribution in the substrate on which the coating had been applied was not taken into consideration.

The development and increased capacity of computers with their associated software packages over the last 30 years open up an alternative approach. Finite element analysis software can now calculate temperature and heat flux distributions for complex heterogeneous materials in steady state or transient conditions (Kulkarni et al., 2003; Laschet et al., 2001). Numerous models were developed for the simulation of the heat flow through various types of porous coatings and TBCs.

Bolot et al. (2005) have quantified the contribution of pores and cracks in the decrease of the effective thermal conductivity of TBCs. A finite difference based model was used for the computation of heat transfer through a porous structure. In order to describe the effects of the microstructure on heat transfer in greater detail, Grandjean et al. (2006) have developed a method involving 2D finite element calculations based on real micrographs of the porous solid. The approach was tested on micrographs of thin oxide samples with pores ranging from 10% to 50%. Up to 20% of pore volume fraction, good agreement was obtained between the numerical simulations and predictions by the analytical expressions of Maxwell-Eucken and Landauer. In fact, at this porosity level, the best agreement was achieved by the Rayleigh expression, which also physically corresponds to a two-dimensional approach.

Golosnoy et al. (2005) have simulated the heat flow through plasma-sprayed coatings in order to derive the effective thermal conductivity as a function of microstructural parameters by numerical and analytical models. The structure was assumed to be composed of lamellar materials (splats), separated by (thin) pores, which contained contact areas (bridges). The effects of pore geometry on conductive and radiative heat transfer within the coating have been investigated over a range of temperatures and gas pressures. It has been determined that the main factor controlling the

conductivity was the intersplat bridge area. This study was oriented towards TBCs, based on zirconia-yttria top coats.

Bakker (1997) has studied the conductivity of complex porous or inclusion structures by using finite element method (FEM). From these computations, the two dimensional conductivity was obtained, that represents a useful lower limit of the real 3-D thermal conductivity. As an example, the influence of the microstructure of irradiated UO_2 on the conductivity has been calculated.

In the present study, numerical model is developed for the prediction of the thermal conductivity of a layered structure, which is intended to be representative for plasma-sprayed coatings. The starting point is a micrograph of coating. Models consist of a hot gas domain, the coating with its real microstructure, and a steel substrate. Heat transfer analysis has been carried out by radiation heat transfer between gas and coating and by conduction between coating and substrate. The results of numerical model performed with FLUENT and have been compared with numerical and experimental results found in literature. It was seen that numerical heat transfer analysis results including substrate are compatible with experimental results.

GEOMETRY, MESH STRUCTURES AND BOUNDARY CONDITIONS

In this study, radiation analysis which contains gas, coating and metal domains has been carried out in greater detail. The results with radiation solution were compared to results without radiation solution which cover only coating domain. In the radiation analysis solution, together with real microstructural image, the metal which represents the substrate and the gas domain in which the coating was exposed to high temperature were modeled. Heat transfer analyses have been carried out by radiation between gas domain and coating, and by conduction between the coating domain and the metal substrate for 9.4% and 24.8% porosity.

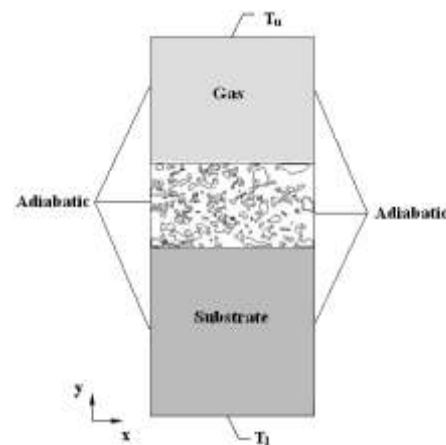


Figure 1. The border regions formed in The Gambit program belonging to the microstructure image with porosity for radiation analysis 24.8%.

Schematic illustration of the problem and coordinate system has been given in Figure 1. While modeling the gas domain, the practical applications of TBCs such as hot section components of gas turbines have been taken into the consideration. The effective thermal conductivity of a porous ceramic coating depends on porosity and the distribution of pores (Altun and Boke, 2008b). Therefore, using the real microstructure of the coating plays an important role in heat transfer analysis. The procedure for obtaining real microstructures of coating which has been used in modeling is explained below.

Microstructure: Samples which were used in microstructure analysis were made of 321 stainless steel substrate and Air Plasma Sprayed (APS) TBC. Samples were disc shaped and diameters were equal 12.7 mm. The APS coating has been prepared by 8% yttria stabilized zirconia (92wt% ZrO_2 and 8wt% Y_2O_3) using Metco 240 NS. The porosity difference of the samples has been obtained by increasing the coating application distance via moving away equipment torch from the samples.

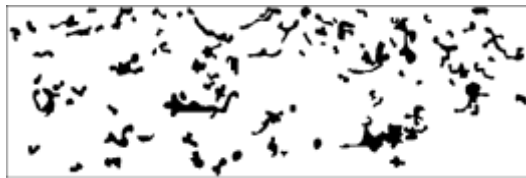


(a)



(b)

Figure 2. (a) Micrograph of a 9.4%. (b) Micrograph of a 24.8%



(a)



(b)

Figure 3. A Binary image used in heat transfer analysis (a) porosity of 9.4%. (b) porosity of 24.8%

The control volume mesh becomes more dense in the TBC region. For different porosity of network structure, cell number and the number of node points change as well (Table 2).

Table 1. The cell number of geometry

Domain Name	Cells
Gas	32927
Coating	27691
Pores	16278
Metal	50320

In the third stage of the analysis, definition of material properties, boundary conditions and thermal analyses were carried out using Fluent 6.1.22 (Fluent, 2002) code. The left and right boundaries are taken as adiabatic. The upper surface of the geometry is

Figure 2 shows a micrograph of a typical coating cross section of samples after been polished using routine metallographic techniques. The average porosity of these samples determined sensitively by Leica Image Analyzer hardware/a software system. The porosity of the samples has been determined as 9.4% and 24.8%.

The real image has been digitalized at the first stage of the analysis. The SolidWorks (SolidWorks, 1998) CAD program has been used for this process. In this process, micrographs have been opened as the Sketch Picture in the SolidWorks program.

Then the SolidWorks model has been formed to geometry for analysis. The SolidWorks model relevant with microstructure for numerical analysis is given in Figure 3.

In the second stage of the analysis, obtained geometry has been enmeshed by using the mesh generator program of Gambit, and the boundary types were defined. The mesh element type was triangular in all geometry. The mesh sizes for each domain are given in Table 1.

maintained at temperature T_u which is greater than the lower surface temperature T_l (Fig.1).

Table 2. Node points and cell number belonging to network structure on a different pores for constant temperature analysis.

Porosity	Cells	Faces	Nodes
% 9.4	83245	125307	42062
% 24.8	127216	191346	64130

Thermal conductivity of the steel substrate and dense yttria-stabilized zirconia is necessary at the stage of identification of the material properties. Thermal conductivity of steel substrate has been measured by the laser-flash method, which is able to accurately measure thermal conductivity at high temperatures (Altun and Boke, 2008a). Thermal conductivity values of dense

yttria-stabilized zirconia which are used in modeling were taken from literature (Schlichting et al., 2001) (Figure 4).

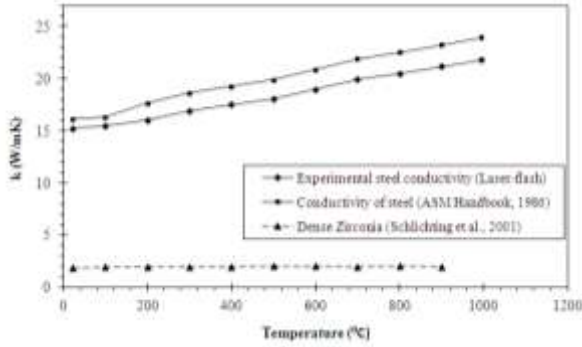


Figure 4. Thermal conductivity of 321 stainless steel and dense zirconia.

In order to perform a heat conduction analysis in the coating medium, effective thermal conductivity of TBC is needed. 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 pore size is larger than $10 \mu\text{m}$ (Clyne et al., 2006; Stark and Fricke 1993). In this study the structures which were analyzed have very small pores $10 \mu\text{m}$, so heat transfer by natural convection in pores was ignored. Under steady-state with no energy generation conditions, conservation of energy for pores,

$$\dot{E}_i - \dot{E}_o = 0 \quad (1)$$

$$\frac{\partial q''_{cond}}{\partial x} - \frac{\partial q''_{rad}}{\partial x} = 0 \quad (2)$$

For gas phase conduction in pores,

$$q''_{con} = k_g \frac{\partial T}{\partial x} \quad (3)$$

The steady-state conservation of energy for one-dimensional heat transfer in the pores yields the partial differential equation in Eq.(4)

$$\frac{\partial}{\partial x} \left(k_g \frac{\partial T}{\partial x} \right) - \frac{\partial q''_{rad}}{\partial x} = 0 \quad (4)$$

The terms in brackets on the left hand side represent the conduction and the other term represents the radiation. Thermal conductivity of the gas (k_g) can be estimated using a simple analytical expression (Jadhav et al., 2006)

$$k_g = \frac{k_g^0}{1 + \frac{BT}{d_v P}} \quad (5)$$

where k_g^0 is the normal conductivity of the gas at the temperature concerned, d_v is the pore thickness, P is the pressure, T is the temperature, and B is a constant ($2.5 \times$

$10^{-5} \text{ Pa m K}^{-1}$) for air. k_g^0 values for air were taken from literature (Incropera and Dewitt, 1996). Thermal conductivity of the gas in the pores is affected significantly by the temperature and pore thickness. Moreover, because of the relatively high (Fox and Clyne, 1998) gas permeability of the TBCs, thermal conductivity is also affected by pressure (Eq.5).

Depending on the temperature, in gas medium and porous solid materials, radiative heat transfer has important roles. If radiation penetration depth is higher than thickness of the lamella, there is scattering in the pores (Lee and Kingery, 1960). The radiation in the pores can be considered as a diffusion process, and the radiation heat flux, q''_{rad} , can be reduced to (Zhao et al., 2009):

$$q''_{rad} = -k_{rad} \frac{\partial T}{\partial x} \quad (6)$$

In order to determine the radiative contribution to the effective thermal conductivity of pores, the below analytical expression (Golosnoy et al., 2005) can be used,

$$k_{rad} \approx \frac{16n^2}{3\epsilon} \sigma T^3 \quad (7)$$

where n is the refractive index, ϵ is an extinction coefficient and σ is the Stefan-Boltzman constant. The extinction coefficient ϵ is equal to sum of scattering (β) and absorption (κ) coefficients. Scattering tends to dominate for zirconia materials, for this reason the extinction coefficient is equal to scattering coefficients. In using this formulation, uniform radiation scattering is assumed, and any wavelength dependence or boundary effects are neglected. It is common to express the behavior in terms of a penetration depth, given by

$$\delta = \frac{1}{\epsilon} \quad (8)$$

In this study, as a result of literature survey (Golosnoy et al., 2005) the penetration depth value was taken approximately as $10 \mu\text{m}$ and refractive index value as approximately 2.2. Radiative conductivity values obtained from Eq. 7 are given in Fig. 5.

The pores' effective thermal conductivity, k_p , is defined as,

$$k_p = k_g + k_{rad} \quad (9)$$

The first term in Eq. (6) represents the thermal conductivity of gas conduction and the last term represents radiative conductivity.

Fig. 5 shows effective thermal conductivity of pores for conduction and radiation contribution ($k_p = k_g + k_{rad}$). In this figure, temperature-dependent thermal conductivity values of air have been taken from literature (Incropera and Dewitt, 1996), and radiative contribution to the effective thermal conductivities of pores have been obtained from Eq. 7. When calculating the thermal conductivity of gas in pores which have different

thicknesses, the pressure values have been taken as 1 atm and 20 atm, and pore thickness has been taken as 2 μm , and k_g values obtained from Eq. 2.

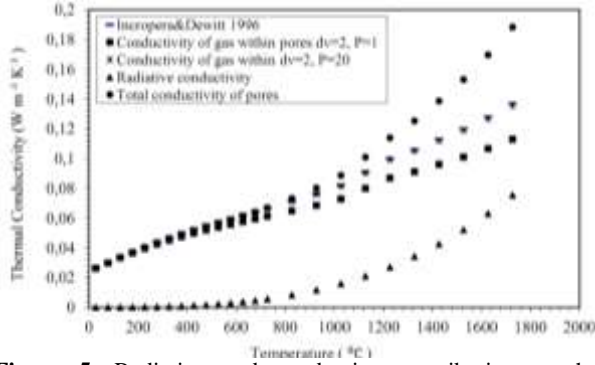


Figure 5. Radiative and conductive contribution to the effective thermal conductivity of pores.

In Fig. 5, it has been observed that radiation contribution to the effective thermal conductivity of pores is influential above 900 °C. Between 900 °C and 1000 °C, conductivity value is about 0.01 W / mK. In this study the analyses were performed between 100°C-1000°C. For 8% yttria stabilized zirconia (8 YSZ), the contribution of radiative heat transfer to the effective pore conductivity is predicted to become substantial for temperatures above $\sim 900^\circ\text{C}$. Therefore the effects of the radiation on the thermal conductivity of pores are neglected. Finally, it has been assumed that heat transfer takes place only by conduction in pores. Air in the pores was taken as inert.

In the coating interface which contacts with gas domain, heat transfer by radiation has been taken into account, so Emissivity value of the coating material is taken as 0.5 (Slifka et al., 1998) and the Discrete Ordinates (DO) radiation model has been chosen. The discrete ordinates radiation model solves the radiative transfer equation for a finite number of discrete solid angles, each associated with a vector direction fixed in the global Cartesian system. This model has been used in a wide thick optical space and it can analyze the problem from surface to surface and allow radiation analysis in semi permeable mediums.

The material of the substrate is 321 stainless steel and the TBC is composed of 8 YSZ. Polynomial expressions have been derived for thermal conductivity and specific heat values of both substrate and TBC at investigated temperature range:

321 Stainless steel thermal conductivity (W/mK):

$$k = -116.681 + 1.0974T - 0.0037T^2 + 6.49 \times 10^{-6}T^3 - 6.262 \times 10^{-9}T^4 + 3.118 \times 10^{-12}T^5 - 6.351 \times 10^{-16}T^6 \quad (10)$$

Dense 8YSZ thermal conductivity (W/mK):

$$k = 1.1397 + 0.0015T - 5 \times 10^{-6}T^2 + 8 \times 10^{-9}T^3 - 7 \times 10^{-12}T^4 + 2 \times 10^{-15}T^5 + 5 \times 10^{-19}T^6 \quad (11)$$

Air thermal conductivity (W/mK):

$$k = -0.00219 + 0.00014T - 3.53 \times 10^{-7}T^2 + 1.142 \times 10^{-9}T^3 - 2.137 \times 10^{-12}T^4 + 2.149 \times 10^{-15}T^5 - 1.097 \times 10^{-18}T^6 + 2.242 \times 10^{-22}T^7 \quad (12)$$

321 Stainless steel specific heat (J/kg K):

$$C_p = 500 \text{ J/kg K} \quad (13)$$

8YSZ specific heat (J/kg K):

$$C_p = 0.6516 - 0.0027T + 1.2357 \times 10^{-5}T^2 - 2.4294 \times 10^{-8}T^3 + 2.56 \times 10^{-11}T^4 - 1.5041 \times 10^{-14}T^5 + 4.6457 \times 10^{-18}T^6 - 5.8813 \times 10^{-22}T^7 \quad (14)$$

Air specific heat (J/kg K):

$$C_p = 1.066 - 0.00041T + 6.7327 \times 10^{-7}T^2 + 5.935 \times 10^{-10}T^3 - 1.5782 \times 10^{-12}T^4 + 1.032 \times 10^{-15}T^5 - 2.283 \times 10^{-19}T^6 \quad (15)$$

In the thermal analysis, total heat flux passing through coating-gas and metal sub surfaces was checked and the analysis continued to be done until the difference between two values reached 1×10^{-5} W.

RESULTS AND DISCUSSION

In this study, in accordance with the usage purpose of TBCs, gas domain, coating and metal domain were modeled together for average temperatures between 100°C and 1000°C. Analyses results for porosity 9.4% have been given in Fig. 6 (a). Pores have been observed to resist heat transfer along the heat flow direction. In general, the arrangement of the pores affected the temperature distribution in the microstructure.

Temperature distribution obtained from radiation analysis occurred in gas, coating and metal substrate has been given in Fig. 6 (b), for porosity 24.8% at 1000 °C.

The pores have built up resistance to heat transfer, and cold regions were thicker on the surfaces where the pores are more. Moreover, pores perpendicular to the heat transfer direction have a bigger effect on temperature distribution than the pores parallel to heat transfer.

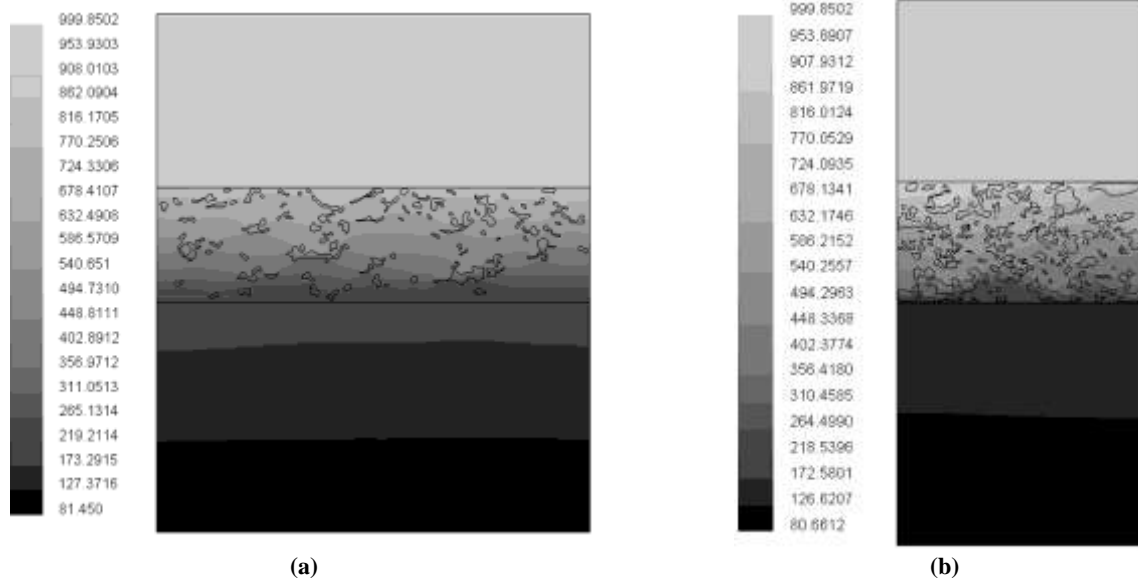


Figure 6. Temperature distribution from the heat transfer analysis for radiation analysis at 1000 °C belonging to microstructure images (a) with 9.4% porosity, (b) with 24.8% porosity

When the gas temperature is 1000 °C, temperature which the metal is exposed to, falls significantly due to coating, so metal substrate is not affected from high temperatures too much because of TBC. Besides, depending on the porosity ratio of the coating, temperature distributions change in the metal part. The more the porosity increase, the less the metal temperature gets. The temperature of the metal substrate decreases where the porosity increases in the microstructure.

For the change of the effective thermal conductivity of the TBC depending on the temperature, the results taken from without radiation analysis, which includes only coating domain and with radiation analysis, are shown Fig. 7 and compared with experimental results found in literature (Ravichandran et al., 1999). Emissivity value was taken as 0.5 in heat transfer analysis for the TBC in the radiation analysis. In this analysis, TBC reflects some of the energy coming on it, and transfers less energy to the metal than without radiation analysis. For this reason, effective thermal conductivity values have been obtained lower in with radiation analysis than in without radiation analysis.

The difference of the effective thermal conductivity values between two models is 0.6% for porosity % 9.4. The reason for the difference is because radiation has been taken into account on the coating surface and depending on that some of the energy on the coating surface has been reflected. Moreover, when numerical modeling results are compared to the experimental results in the literature, it is determined that they are close to each other within 8%. These results show the accuracy of designed modeling, and they may be used before doing high cost experiments for obtaining preliminary values.

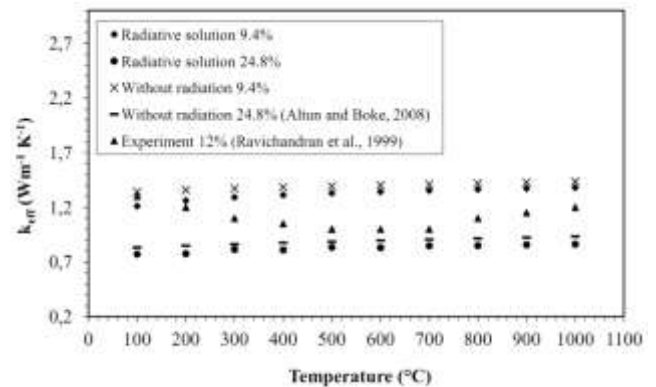


Figure 7. The comparison of with and without radiation analysis

When the difference between without radiation analysis and with radiation analysis is examined, in the solutions in which porosity is low, depending on the density of ceramic material, radiation boundary conditions play a dominant role. Therefore, the without radiation solutions which dealt with only the coating domain give different results than the radiation analysis for lower porosity.

Experimental results in literature (An and Han, 2006; Filla, 1997; Brandt et al., 1986; Zhu et al., 2001; Slifka et al, 1998) with different porosity, experimental methods and coating, substrate thickness are given in Table 3. It is observed that there are differences between the thermal conductivities of TBCs which have same chemical composition (8 YSZ) and which have been applied by same coating method (Plasma Sprayed) in the Table 3. It is difficult to obtain the thermal conductivity of TBC by experimentally. This difficulty is causing from very thin coating thickness, more surface roughness, and transparent property of zirconium oxide at high temperatures.

Table 3. Comparison of the effective thermal conductivities of 8YSZ air plasma sprayed coating obtained from experiments and heat transfer analyses.

Experimental Study	Coating Thickness (mm)	Substrate Thickness (mm) and materials	Porosity	Measurement method	Measurement Temperature (°C)	Thermal conductivity (W/m.K)
An and Han (2006)	0.4±1.2	15.075±11.875 AISI 304	12%	Their experimental setup	200-1000	0.25
Filla (1997)	1±3	5 SS410	-	Guarded hot plate	127-800	1.31
Slifka (2000)	1±3	- SS410	-	Infrared microscope measurement	127-527	0.58
Brandt et al. (1986)	0.97	-	10%	Laser-Flash	300-1300	1.15
Brandt et al. (1986)	0.97	-	14%	Laser-Flash	300-1300	1.0
Zhu et al. (2001)	0.254-0.4	-	10%	Laser-Flash	1316	1.0±1.4
Slifka et al. (1998)	1±3	SS410	16.5%	Guarded hot plate	127-527	0.62
Numerical Study	Coating Thickness (mm)	Substrate Thickness (mm) and materials	Porosity	Numerical Solution	Measurement Temperature (°C)	Thermal conductivity (W/m.K)
Altun and Boke	0.475	321 stainless steel	9.4%	With radiation analysis	100-1000	1.36
Altun and Boke	0.472	321 stainless steel	24.8%	With radiation analysis	100-1000	0.85

For this reason, there are differences between thermal conductivity values which have been obtained different experimental methods. Also the effective thermal conductivity values obtained from with radiation analysis are given in Table 3. There is an average 10% difference between the results obtained from experiments and the with radiation analyses. The reason why the results obtained from the experiment in effective thermal conductivity values are being lower than that obtained from the numerical analysis, is that the spaces between zirconium oxide plunge which became solid accumulating in the shape of leaves on each other is not seen in microstructure images.

CONCLUSIONS

It is important to know the thermal properties of TBCs which are used in high technologic applications such as aerospace and gas turbine industries. In this study, it has been aimed to carry out a model suitable to the working conditions of TBCs and determining the thermal conductivity. In accordance with this purpose, coating, metal substrate to which coating is applied and hot gas domain to which coating is exposed are modeled together to get more sensitive modeling. Using this model provided in this study, the obtained numerical analyses results are in good agreement with experimental results found in literature. Before doing practical applications, proper determination of the thermal properties of TBCs which are applied to special alloyed and expensive parts provides both time and cost savings. As a result of this, it may be more easy to obtain the most suitable TBC application for our needs with less trials.

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Ozge Altun, Dr is an Assistant Professor in the Mechanical Engineering Department at the Eskişehir Osmangazi University in Eskişehir. She received her PhD from the same university in 2007. Her main scientific interests include heat transfer in porous media, numerical modeling ceramic coatings, especially thermal barrier coatings and experimental thermal conductivity measurements. As an author she has published 14 papers in refereed conferences and journals.



Y. Erhan Böke Dr is an Associated Professor at the Department of Mechanical Engineering, Division of Thermodynamics and Thermal Technologies, Istanbul Technical University, Istanbul, Turkey. He received his PhD in Thermal Technologies, from Istanbul Technical University, Turkey in 1993. His areas of interest are thermal technologies, combustion, CFD modeling. He participated in many scientific conferences. As co-author or an author he has published 45 papers in refereed conferences and journals.