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# FINITE VOLUME INVESTIGATION OF 8Y-PSZ/NiCrAlY AS THERMAL BARRIER COATING OVER AlSi ALLOY

**A. K. SAINI**

Department of Mechanical Engineering, Panjab University SSG Regional Centre, Hoshiarpur, Punjab, India

## ABSTRACT

Zirconia ($ZrO_2$) has attracted the worldwide researchers working in the field of development of thermal barrier coatings due to its excellent properties. In the present investigation, finite volume methodology based technique was employed to observe the effectiveness of yttria (8% by wt.) partially stabilized zirconia (8Y-PSZ) as thermal barrier coating applied over a substrate material of AlSi (12% by wt.) using an intermediate bond coat of NiCrAlY. The results showed that the coating was highly effective in reducing the heat penetration into the substrate which could be analyzed as an enhancement in thermal efficiencies of the high temperature operating engineering systems or as a decrease in the cooling load of the system for the same efficiency level.

**KEYWORDS:** Finite Volume Modeling (FVM), Thermal Barrier Coating (TBC), Thermal Behavior, Yttria Partially Stabilized Zirconia

## INTRODUCTION

Thermal barrier coatings (TBCs) are the coatings of materials of low thermal conductivity suitable to be applied to the engineering components experiencing high temperatures in their working conditions such as top surface of piston of internal combustion engines or blades of particularly leading stages of gas turbines. Application of TBC results into an appreciable reduction in the heat loss through the substrate from within the working medium. Transformation of the lost heat to useful energy can be used as increased useful work in expansion stroke of IC engines and/or decreased heat content moving to the exhaust or cooling system [1]. Similarly, significant rise in the turbine entry temperature (TET) of gas turbine systems is possible to be achieved with the deposition of TBCs [2-3].

Finite volume modeling (FVM) of a problem is based upon its control volume formulation, which means that the whole domain under study is discretized into multi sub domains, known as control volumes (CVs) with each such control volume surrounding a grid point. FVM approach considers integration of the governing equation over each control volume to get its discretized form. The present investigation deals with the application of same technique to quantize the effect of a well established thermal barrier coating, zirconia, partially stabilized with yttria (8% by wt.).Taking into consideration the explicit stability constraint, a fully implicit FVM based theoretical numerical model was framed for the thermal analysis and was solved in MATLAB 7.10.0 (R2010a) for 8Y-PSZ/NiCrAlY TBC structure over AlSi (12 wt. %) substrate for different Y-PSZ thicknesses and different operating temperature conditions.

## METHODOLOGY

### Mathematical Modeling of Physical Phenomenon

In the high temperature engineering components, a part of the heat from hot environment primarily through convection through the exposed surface gets conducted within the solid part which essentially is to be taken away from the substrate with the help of some coolant. For the present work, only 1-D transient analysis was considered to avoid complexity and cumbersomeness of the problem and its solution. Thus, the governing equation used here is,

$$\rho c \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) \quad (1)$$

where, 'T' is temperature (in K) and is a function of a space coordinate (x) and a time coordinate (t), 'ρ' is density of the material in $kg/m^3$, 'c' is specific heat of the material in J/kgK and 'k' is thermal conductivity of the material (considered isotropic) in W/mK.

Also, $\left(k \frac{\partial T}{\partial x}\right) = (-q)$ i.e. heat flux (1.1)

**Boundary Conditions**

For the present numerical modeling, boundary heat flux was specified through convection heat film coefficient and surrounding fluid temperature conditions, for both the surfaces across which heat transfer through conduction takes place. Lateral surfaces were considered to be insulated. The surface boundary conditions were defined by temperature of hot environment in Kelvin ($T_{fg}$), convection heat transfer coefficient for hot environment in $W/m^2K$ ($h_{fg}$), temperature of coolant in Kelvin ($T_{fc}$) and convection heat transfer coefficient for coolant in $W/m^2K$ ($h_{fc}$).

**Discretization Equations Formation**

For the 1-D analysis of heat conduction from one surface to another when the both the surfaces are subjected to different convection conditions, three different types of equations would be required in finally discretized form. One type of equation will be applicable to the external grid point on hot environment exposed surface, second type of equation will be applicable for all the inside grid points and the third type of equation will be applicable to another external grid point on the surface exposed to the coolant. Figure 1 shows a typical one-dimensional control volume grid structure as used in the analysis.

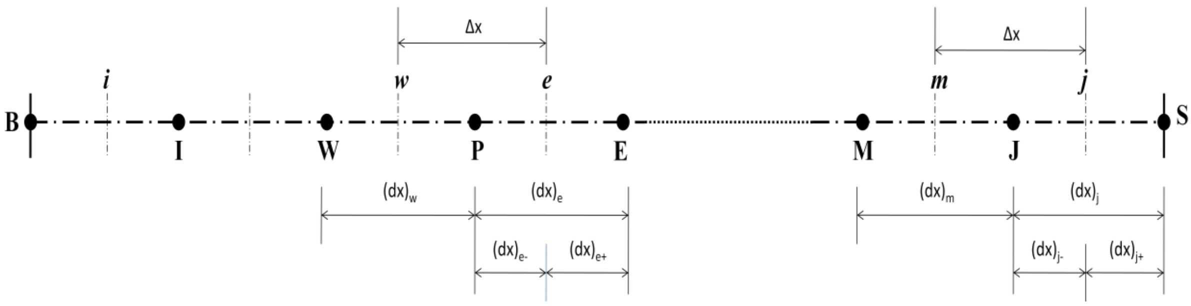


**Figure 1: One Dimensional Control Volume Grid Structure**

For any general grid point 'P', there is one surrounding CV of length 'Δx' bounded by faces 'w' and 'e' in the left and right of 'P', respectively. $(dx)_w$ is distance between 'P' and its left neighbor grid point 'W', while $(dx)_e$ is distance between 'P' and its right neighbor grid point 'E'. Further, distances of an interface 'e' from its left neighbor node 'P' and right neighbor node 'E' are represented as $(dx)_{e-}$ and $(dx)_{e+}$ respectively.

Considering point 'B' as the point exposed to hot environment and integrating Eq. (1) over half CV from 'B' to 'i' and taking time step 'Δt', Eq. (1) was fully implicitly solved taking into account $q_B$ equal to $h_{fg}$ ($T_{fg}$ - $T_B$) as per convection boundary condition and $q_i$ equal to $k_i$ ($T_B$ - $T_I$) / $(dx)_i$ as per Fourier's law of heat conduction. The new equation obtained was,

$$a_B T_B^1 = h_{fg} T_{fg} + a_I T_I^1 + a_B^0 \quad (2)$$

where,

$$a_I = k_i / (dx)_i \quad (2.1)$$

$$a_B^0 = \rho\, c\, \Delta x / (2\, \Delta t) \quad (2.2)$$

$$a_B = a_B^0 + h_{fg} + a_I \quad (2.3)$$

The superscripts '0' and '1'were used to represent respectively the current value at time 't' and the next value after a time step '$\Delta t$'.

Integrating Eq. (1) over CV around any general point 'P' within the solid part from 'w' to 'e' and taking time step '$\Delta t$', fully implicit solution resulted into following equation,

$$a_P\, T_P^1 = a_E\, T_E^1 + a_W\, T_W^1 + a_P^0\, T_P^0 \quad (3)$$

where,

$$a_E = k_e / (dx)_e \quad (3.1)$$

$$a_W = k_w / (dx)_w \quad (3.2)$$

$$a_P^0 = \rho\, c\, \Delta x / \Delta t \quad (3.3)$$

$$a_P = a_P^0 + a_E + a_W \quad (3.4)$$

Similarly, a node 'S' was considered to be exposed to coolant conditions and Eq. (1) was integrated over half CV from 'j' to 'S' with time step '$\Delta t$' and taking into account $q_S$ equal to $h_{fc}$ ($T_S$ - $T_{fc}$) as convection boundary condition and $q_j$ equal to $k_j$ ($T_J$ - $T_S$) / $(dx)_j$ as per Fourier's law of heat conduction. Fully implicit solution resulted into following equation,

$$a_S\, T_S^1 = h_{fc}\, T_{fc} + a_J\, T_J^1 + a_S^0\, T_S^0 \quad (4)$$

where,

$$a_J = k_j / (dx)_j \quad (4.1)$$

$$a_S^0 = \rho\, c\, \Delta x / (2\, \Delta t) \quad (4.2)$$

$$a_S = a_S^0 + h_{fc} + a_J \quad (4.3)$$

**Interface Values Treatment**

Since an interface is a common face to two control volumes, in case both the CVs are from different materials as in composites, the interface value of a particular property was calculated assuming that there was a linear variation of the quantity between the grid points such that,

$$k_e = [(dx)_e^+ / (dx)_e]\, k_P + [(dx)_e^- / (dx)_e]\, k_E \quad (5.1)$$

$$\rho_e = [(dx)_e^+ / (dx)_e]\, \rho_P + [(dx)_e^- / (dx)_e]\, \rho_E \quad (5.2)$$

$$c_e = [(dx)_e^+ / (dx)_e]\, c_P + [(dx)_e^- / (dx)_e]\, c_E \quad (5.3)$$

**Model Application to a TBC System**

For the present analysis, a TBC system was considered having a substrate of AlSi (12% by wt. Si) overcoated with a top coat (TC) of 8Y-PSZ using an intermediate bond coat (BC) of NiCrAlY. Figure 2 shows one dimensional control volume set up for such a TBC system comprising 0.300 mm thick TC layer over 0.150 mm thick layer of NiCrAlY and a 5.0 mm thick substrate.

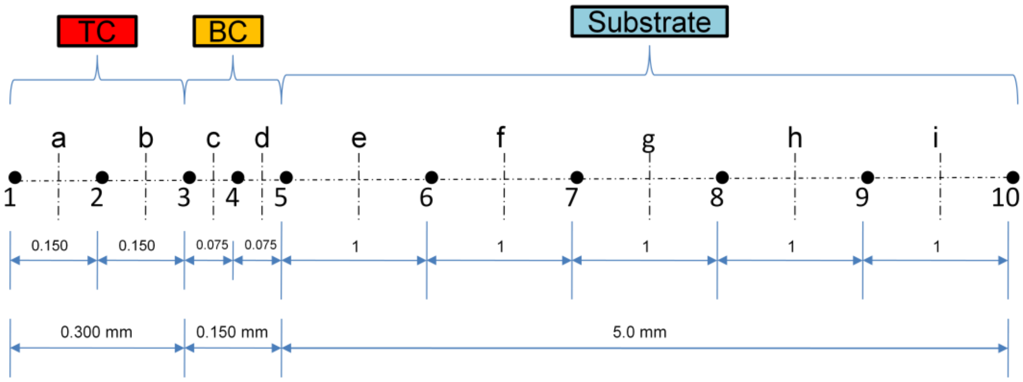


**Figure 2: One dimensional Grid Set Up for a TBC Coated Substrate**

The 0.300 mm thick ceramic coating was divided into two sub regions, each of 0.150 mm thickness. Similarly, bond coat layer was subdivided into two equally spaced regions, each of thickness 0.075 mm. Further, 5.0 mm thick substrate was divided into five sub regions, each 1.0 mm thick region. The thickness of coating layer being very less as compared to that of substrate, such a non-uniformly spaced grid was considered. Node-1 being on the ceramic layer was therefore surface node exposed to the high temperature conditions and node-10 was surface node exposed to the coolant conditions.

Now, it follows that Eq. (2) is applicable to node-1. Eq. (3) is applicable to all internal grid points from node-2 to node-9 and Eq. (4) can be applied to node-10. This generates a set of 10 equations in fully implicit form. Similarly, an uncoated AlSi (12% by wt.) substrate of 5 mm thickness was considered with its grid structure of 6 equally spaced nodes as shown in Figure 3.

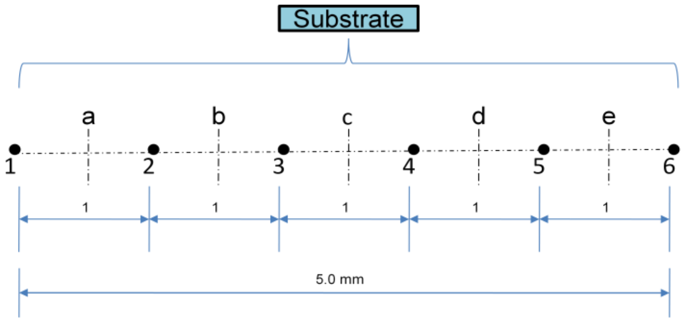


**Figure: 3 One Dimensional Grid Set Up for an Uncoated Substrate**

Node-1 was considered to be exposed to high temperature conditions while node-6 was coolant exposed such that Eq. (2) is applicable to node-1, Eq. (3) is applicable to all internal grid points from node-2 to node-5 and Eq. (4) can be applied to node-6. This generates a set of 6 equations in fully implicit form.

The iterative solution approach for multi simultaneous equations was handled in MATLAB 7.10.0 (R2010a) by selecting a time step value of 0.025s and initial temperature at all the grid points as 300 K. The typical values of thermal convection conditions selected were $T_{fg}$ as 923 K, $h_{fg}$ as 800 W/m$^2$K, $T_{fc}$ as 300 K and $h_{fc}$ as 1392 W/m$^2$K [4-5]. Further, values of thermal properties of top coat, bond coat and substrate were considered as per Table 1 [6-7].

**Table 1: Typical Values of Properties of Materials Used as Top Coat, Bond Coat and Substrate**

| Material | Thermal Conductivity, k (W/mK) | Density, ρ (kg/m$^3$) | Specific Heat, c (J/kgK) |
|---|---|---|---|
| 8Y-PSZ | 1.05 | 5650 | 483 |
| NiCrAlY | 95 | 8210 | 468 |
| AlSi (12 wt. %) | 150 | 2660 | 977 |

Keeping thickness of intermediate bond coat of NiCrAlY constant as 150 microns, the model was solved for varying top coat thickness of 150, 300, 600, 900, 1200 and 1500 microns. As compared to an uncoated substrate, the lowering down of the temperatures within the substrate was thus observed for different thicknesses of 8Y-PSZ at constant bond coat thickness. Further, a typical 300/150 model (0.300 mm 8Y-PSZ and 0.150 mm NiCrAlY) was solved for a range of operating temperatures from 400 K to 1800 K to observe the behavior of same coating at different operating temperatures of working medium.

## RESULTS AND DISCUSSIONS

Figure 4 shows the variation in top substrate temperature for different coating thicknesses as the time of exposure to thermal loading conditions increases.

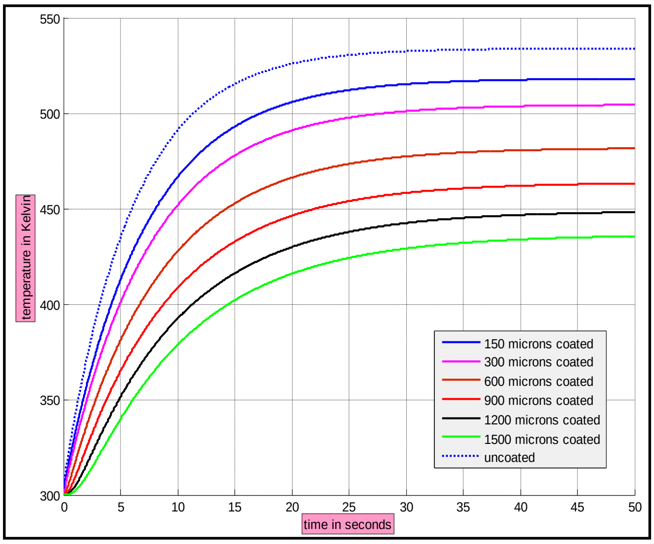


**Figure 4: Effect of Top Coat 8Y-PSZ Layer Thickness on Top Substrate Transient Temperature**

It is very clear from the above figure that the temperature at the surface of substrate is more in case, it is uncoated as compared to the TBC coated cases. In other words, thermal barrier coating over the substrate causes sufficient reduction in the top substrate temperature, and therefore, lowers the temperatures within the substrate also. Further, as the top ceramic Y-PSZ layer thickness increases, more reductions in the substrate temperatures are observed.

This clearly indicates that deposition of 8Y-PSZ coating over the substrate has the considerable potential to increase its life by reducing heat penetration into it. This suggests the use of TBC either as the decrease of cooling load of the system or increase of working temperature for same substrate temperatures.

Same conclusions can be drawn by observing the results in Figure 5, where the temperatures of top ceramic surface are plotted against time of exposure for different coating thicknesses. The figure shows that the coated substrate experiences increase in temperature at the top surface of coating.

Further, increase in top layer thickness results into increase in the top surface temperature. This increase in temperature at the top surface of coating also supports the earlier discussion that TBC is helpful in decreasing heat penetration into the substrate and hence, retaining much of the heat of the working fluid within fluid itself, which ultimately would be useful for enhancing thermal efficiency of the system.

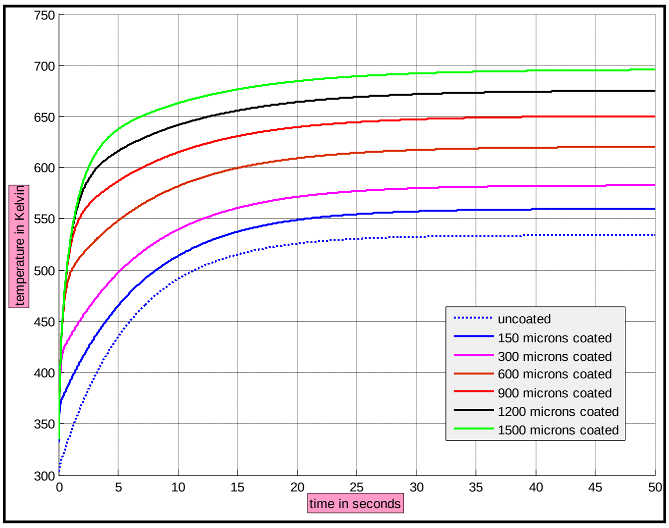


**Figure 5: Effect of Top Coat 8Y-PSZ Layer Thickness on Top Surface Transient Temperature**

Figure 6 shows effect of thickness of 8Y-PSZ layer on the temperature distribution along the thickness after 5 seconds of thermal loading. Solid points on each curve represent the grid points considered in the numerical analysis. The 5 mm thick substrate has been sub-divided into 6 grids, 1 mm apart. The 150 microns thick NiCrAlY bond coat has been sub-divided into 3 grid points, 75 microns apart. Top coat of Y-PSZ has been sub-divided into 2, 3, 5, 7, 9 and 11 grid points, respectively in case of 150/150, 300/150, 600/150, 900/150, 1200/150 and 1500/150 coated models and 150 microns apart in each case. It again shows that the increase in TBC thickness results into increase in the top surface temperature and decrease in the top substrate temperature. Moreover, the figure shows that there is small change in the slope of curve between top ceramic surface and TBC-bond coat interface as the thickness of top coat varies. This implies that temperature gradient with respect to length decreases as the thickness of TBC increases. In other words, more temperature drop occurs in a thick TBC as compared to thin TBC but rate of temperature drop within a thick TBC is lesser than in a thin TBC.

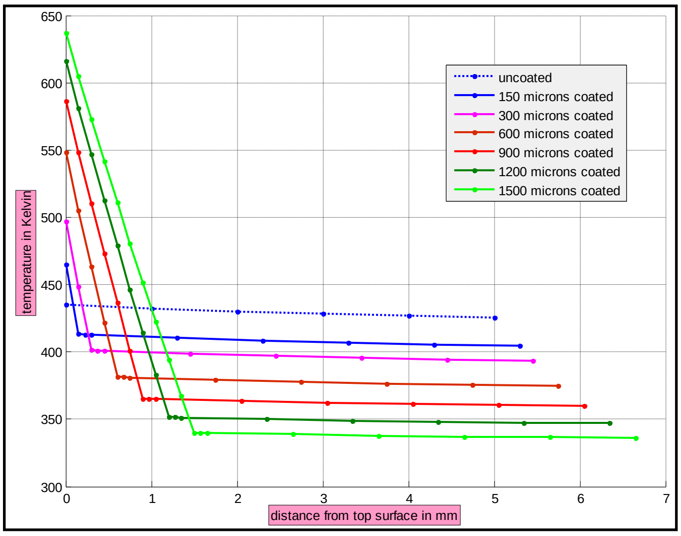


**Figure 6: Effect of Top Coat Thickness on Temperature Distribution along Thickness after 5s of Thermal Loading**

Figure 7 (left) shows percentage increase in top surface temperature and percentage decrease in top substrate temperature (bond coat-substrate interface temperature) for different coating thicknesses after 5 seconds of thermal loading. As compared to uncoated model, top surface temperature increases from 6.97 % for 150/150 coated model to 46.52 % for 1500/150 coated model while top substrate temperature decreases from 5.10 % for 150/150 coated model to 21.87 % for 1500/150 coated model.

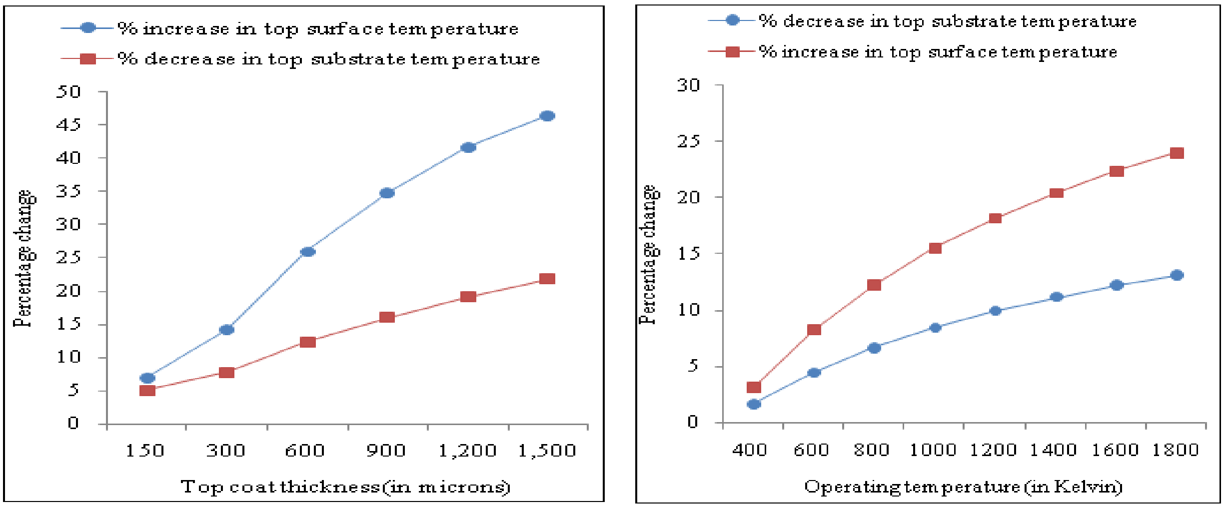


**Figure 7: Percentage Changes in Top Surface Temperature and Top Substrate Temperature after 5s of Thermal Loading at Different Coating Thicknesses (left) and Different Operating Temperatures (Right)**

Figure 7 (right) shows the effect of increase in the operating temperature of the hot environment over percentage reduction in top substrate temperature and percentage increase in top surface temperature after 5 seconds of thermal loading and for 300/150 coated model. The results indicate that same TBC set up works more effectively at higher operating temperatures. As compared to uncoated model, a TBC of 300 microns thick YPSZ over 150 microns thick NiCrAlY causes 1.7 % reduction in top substrate temperature at hot fluid temperature of 400 K while same set up causes 13.1 % reduction in the top substrate temperature at working temperature of 1800 K. Similarly, same 300/150 coating results into an increase of 3.1 % in top surface temperature at operating temperature of 400 K while this value increases to 24.0 % at operating temperature of 1800 K.

Further, overall temperature drop within the TBC layer itself increases from 52.5 degrees in case of 150/150 coated model to 297.4 degrees in case of 1500/150 coated model, as it is clear from Figure 8, showing a plot for variation of overall temperature drop within the Y-PSZ/NiCrAlY TBC set up at different top coat thicknesses.

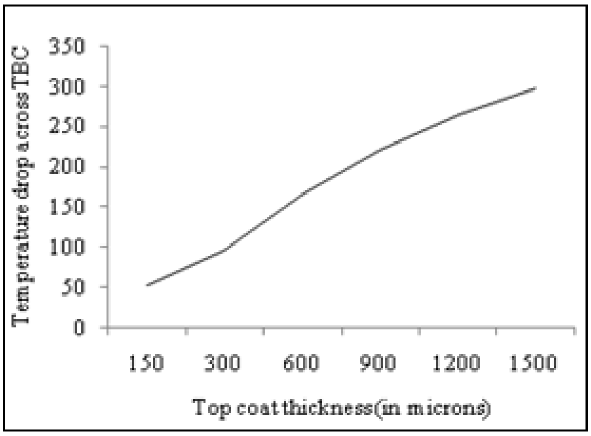


**Figure 8: Temperature Drop in Y-PSZ/NiCrAlY TBC Set Up after 5s of Thermal Loading at Different Y-PSZ Coating Thicknesses**

## CONCLUSIONS

Finite volume based fully implicit one-dimensional numerical modeling was carried out to analyze the thermal behavior of a well known thermal barrier coating material, zirconia, partially stabilized with yttria (8% by wt.) and overcoated over a substrate material of AlSi alloy (12% Si by wt.) using an intermediate bond coat of NiCrAlY. The model was solved in MATLAB 7.10.0 (R2010a) for different top coat thickness values with same bond coat thickness

(150 microns) by choosing typical values of thermal properties of the materials and typical convection conditions of extreme nodes as 923 K, 800 $W/m^2K$ for hot side and 300 K, 1392 $W/m^2K$ for coolant side.

Time marching solution was obtained taking time step of 0.025s and initial throughout uniform temperature consideration of 300 K. It was found that deposition of 8Y-PSZ as TBC resulted into significant decrease in the top substrate temperature, thereby lowering down of within temperatures. Increase in the top surface temperature as compared to the uncoated case further supported the fact that this TBC set up would be responsible in permitting most of the heat of the working medium to be there only by reducing its penetration. More thickness of Y-PSZ coating was found to give better results in this aspect of decreasing heat penetration within the substrate. After 5s of the thermal loading, it was found that as compared to uncoated model, 150 microns Y-PSZ coating caused an increase in top surface temperature of 6.97% while the value rose to 46.52% for 1500 microns top coated model. Similarly, decrease in the top substrate temperature was 5.10% for the former case and 21.87% for the later one. A typical model of 300 microns 8Y-PSZ was also solved for a range of operating temperatures keeping all other conditions unchanged so as to determine the behavior of a particular thickness of coating at different temperatures of operating conditions. It was concluded that same thickness of coating served to be better at elevated temperatures. It is worth noting here that elevated temperatures of working medium are basically desirable so as to make the system thermally more efficient. It is further worthy to be mentioned here that a thicker coating is more prone to degradation in high temperature environment than a thinner one, however the stability aspect of TBC has not been worked out in this paper.

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