

# A Novel Approach for Adjusting the Maxwell Eucken Model and Effective Medium Theory in Computing the Thermal Conductivity of Yttria Stabilized Zirconia Thermal Barrier Coating

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## Abstract

Thermal conductivity is the most important characteristic for thermal barrier coating (TBC) materials, as it determines the performance and quality of these coatings. The thermal conductivity of Yttria Stabilized Zirconia (YSZ) TBC is significantly affected by its porosity percentage. The Maxwell-Eucken (EM) model and the Effective Medium Theory (EMT) model do not predict TBC thermal conductivity accurately. Therefore, correction factors were developed to close the gap between the experimental values of thermal conductivity and the corresponding predicted values using the EM model and the EMT model. These correction factors are connected to the TBC's porosity percentages within the range (0-23.8%), an effect that the classic EM and EMT models do not take into account. The results revealed that the adjustment of EM and EMT models improves their accuracy and applicability in capturing real-world problems. Statistical evaluation showed that the Coefficient of Determination ( $R^2$ ) value increased, accompanied by a substantial reduction in Root Mean Square Error (RMSE) and Mean Absolute Error (MAE). These results validate the robustness of the correction factor in improving predictive accuracy.

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**Keywords:** Thermal barrier coatings; Thermal Conductivity; Maxwell-Eucken Theory; Effective Medium Theory; Correction factor.

## 1. Introduction

Thermal Barrier Coating (TBC) is a refractory material in the form of thick layers that are used to cover a substrate, acting as an insulating material that shields the underlying metallic substrate from high temperatures. These materials are frequently used in turbine engines and power plant components, where the surface needs to be protected from high temperatures for better performance and durability [1, 2].

Yttria Stabilized Zirconia (YSZ) is one of the most popular TBC materials that is created by mixing yttrium oxide ( $Y_2O_3$ ) with zirconium oxide ( $ZrO_2$ ) to impede the undesired monoclinic-tetragonal phase transformation upon heating to temperatures between 1170 °C- 2370 °C. This transformation causes strains and reduces the coating's stability [3].

One of the most crucial characteristics of TBC materials that establishes their quality is their thermal conductivity [4]. Therefore, it has been thoroughly studied since TBC coatings must have a low thermal conductivity in order to shield components operating at extremely high temperatures in applications such as turbine engines and electrical generators.

Consequently, an accurate determination of TBC material thermal conductivity is crucial. However, experimental determination is a very costly and time-consuming job. Therefore, the consideration of theoretical models becomes necessary as they provide cost-effective and efficient means of predicting the thermal conductivity of YSZ TBC material. The theoretical models that fit the structure of TBC materials describe the structure as a porous microstructure embedded in a continuous solid matrix, including the Maxwell-Eucken Model (EM) and Effective Medium Theory (EMT) [5]. Using these theories, the thermal conductivity is computed using the volume fraction and the thermal conductivity of each one of the composite phases. However, the thermal conductivity of YSZ TBC is significantly affected by its porosity percentage. Thus, these models are not yet sufficiently mature to be applicable for YSZ TBC material.

This work attempts to close this gap and improve the accuracy of the EM and EMT models, using the necessary adjustments and proposing correction factors for both models. The findings of these models will then be compared with experimental data that has already been published in the literature.

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## 2. Literature Review

Thermal conductivity of YSZ TBC's has been thoroughly researched. It is influenced by two significant variables which are the amount of yttria added to zirconia, and the percentage of porosity. The impact of varying yttria content in YSZ TBC material on the thermal conductivity has been examined. The results indicated that when yttria content is increased from 0 to 7.7% mol, the thermal conductivity is reduced from 1.85 to 1.22 W/m.K. This is because yttria interferes with zirconia's phase change, causing an effective electron-phonon scattering [6]. The effect of the porosity percentage on the thermal conductivity of TBC has been examined at different temperature levels; and it was found that TBCs with high percentages of porosity have lower thermal conductivity as the electron-phonon scattering increases with increasing porosity percentage [7, 8].

Other studies examined experimentally the effect of both factors (porosity percentage and Yttria content) on thermal conductivity of YSZ TBC at different temperature levels, both factors resulted in YSZ TBC with low thermal conductivity [9]. The air confined in the pores gives a thermal insulation. Hence, the increase in porosity percentage decreases both heat transfer and thermal conductivity of TBCs significantly [10-12].

The study of thermal conductivity in coating materials has attracted significant interest due to its influence on heat transfer, performance, and durability in high-temperature applications. Prior research across materials, mechanical, and industrial engineering has examined how coating composition, microstructure, and processing parameters affect thermal behavior in advanced coating systems. These contributions collectively underscore the continuing need for accurate thermal modeling and predictive tools, such as those pursued in the present study [13].

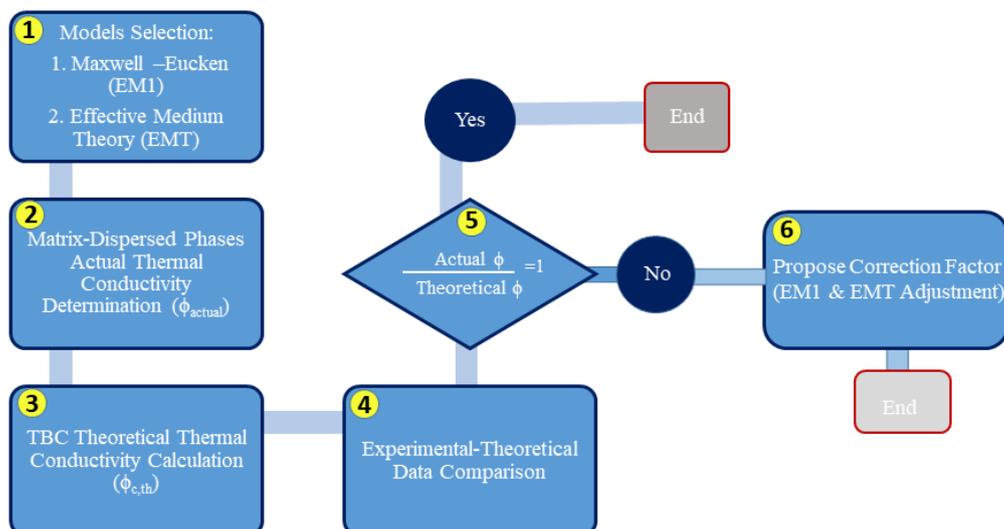
In addition to the experimental methods, finite element analysis (FEA) and mathematical modelling were used to predict thermal conductivity of TBCs. For example, FEA was applied to find the thermal conductivity of zirconia and polyester TBC at different porosity percentages [14]. A model of intermingled fractal units is proposed to estimate

the thermal conductivity of YSZ TBCs for different pore sizes and fractions. The outcomes and the experimental results agree fairly well [15]. The thermal conductivity of porous TBC materials was predicted via a novel mathematical model that is based on the assumption that the coatings' porosity is a major factor influencing its thermal conductivity. According to the findings, the new model outperforms the existing methods in its ability to forecast the thermal conductivity of TBCs [16]. The thermal conductivity of YSZ TBC and lanthanum zirconate (LZO) has been compared using the Effective Medium Theory (EMT) and Maxwell-Eucken (EM1). They discovered that the thermal conductivity of YSZ with LZO is lower than that of a single YSZ, ranging from 0.36 to 0.75 W/m.K [17].

In recent years, advanced computational approaches such as multiscale modeling and machine-learning-based frameworks have gained significant attention for predicting the thermal behavior of YSZ thermal barrier coatings. Multiscale finite element and homogenization models have been developed to explicitly link pore-level features and intersplat interfaces with the macroscopic effective thermal conductivity of TBC systems [18]. Likewise, machine learning approaches—including neural networks and ensemble learning algorithms—have demonstrated promising accuracy in predicting thermal conductivity across diverse microstructural conditions by utilizing both experimental and synthetic datasets [19]. While these approaches offer powerful predictive capabilities, they often require detailed microstructural characterization or large training datasets. In contrast, the present study introduces an empirical correction strategy that enhances classical EM and EMT models using porosity-dependent experimental data, offering a practical and computationally efficient alternative.

## 3. Methodology

The methodology used in this study was in accordance with the steps indicated in the flowchart illustrated in Figure 1. A thorough explanation of every one of these phases is provided in the section that follows:



**Figure 1.** Flowchart of the methodology used to propose a correction factor that adjusts the EM1 and EMT theories for YSZ TBC material.

3.1. Models Selection

Researchers have developed several models to predict the thermal conductivity of the composite materials, five theoretical models are widely used. The mathematical form for each one of these models is shown in Table 1. These models include the series model, parallel model, Maxwell-Eucken model (EM) with two forms, and Effective Medium Theory (EMT). However, the structure of YSZ TBC material is more complex than that assumed in both series and parallel models. It is important to note that the appropriate form of EM model for YSZ TBC is EM1 [17].

3.2. Matrix-Dispersed Phase Actual Thermal Conductivity Determination

Literature and previous studies were reviewed to obtain experimental values for the thermal conductivity of the matrix phase, ZrO<sub>2</sub>, and the dispersed phase, Y<sub>2</sub>O<sub>3</sub>, at 12 different temperatures falling within the range of 0 °C to 1200 °C. These values are listed in Table 2.

3.3. TBC Theoretical Thermal Conductivity Calculation

The prediction of the composite thermal conductivity (K) using the theoretical models is based on k<sub>1</sub>, k<sub>2</sub>, v<sub>1</sub> and v<sub>2</sub> which are the thermal conductivity and the volume fractions of matrix phase and dispersed phase, respectively. In this study, the prediction of thermal conductivity for a 170 input-output dataset of YSZ TBC varying in temperature and content of yttria and zirconia was conducted using EM and EMT models. A sample is shown in Table 3.

3.4. Experimental-Theoretical Data Comparison

In this stage, the results of the theoretical models were compared with the corresponding experimental results [8, 22, and 23]. Experimental results represent real-world observations. Therefore, when the theoretical results are close to these results, then the models are effectively capturing the problem. This comparison shows how well the theoretical models perform in relation to an established real-world framework.

**Table 1.** Mathematical form of the theoretical models that predict thermal conductivity for composite materials

| Model          | Mathematical form  | Reference |
|----------------|--|-----------|
| Series Model   | $K = \frac{1}{\frac{v_1}{k_1} + \frac{v_2}{k_2}}$  | [17]      |
| Parallel Model | $K = k_1 v_1 + k_2 v_2$  | [17]      |
| EM1 Model      | $K = k_1 \frac{(2k_1 + k_2 - 2v_2(k_1 - k_2))}{2k_1 + k_2 + v_2(k_1 - k_2)}$   | [5]       |
| EM2 Model      | $K = k_2 \frac{(2k_2 + k_1 - 2(k_2 - k_1)(1 - v_2))}{(2k_2 + k_1 + (k_2 - k_1)(1 - v_2))}$                             | [5]       |
| EMT Model      | $K = \frac{1}{4} [k_2 (3V_2 - 1) + k_1 [3(1 - V_2) - 1] + \sqrt{(k_2 (3V_2 - 1) + 3((1 - V_2) - 1)k_1)^2 + 8k_1 k_2}]$ | [5]       |

**Table 2.** The experimental reported values for the thermal conductivity of matrix phase (ZrO<sub>2</sub>) and dispersed phase (Y<sub>2</sub>O<sub>3</sub>) at different temperatures ranging 0 °C - 1200 °C.

| Temperature (°C) | k <sub>1</sub><br>Matrix (ZrO <sub>2</sub> )<br>W/m.K <sup>[20]</sup> | k <sub>2</sub><br>Dispersed (Y <sub>2</sub> O <sub>3</sub> )<br>W/m.K <sup>[21]</sup> | Temperature (°C) | k <sub>1</sub><br>Matrix (ZrO <sub>2</sub> )<br>W/m.K <sup>[20]</sup> | k <sub>2</sub><br>Dispersed (Y <sub>2</sub> O <sub>3</sub> )<br>W/m.K <sup>[21]</sup> |
|------------------|---|---|------------------|---|---|
| 0                | 2.3   | 19.0  | 700              | 2.9   | 5.0   |
| 100              | 2.4   | 17.0  | 800              | 2.9   | 4.0   |
| 200              | 2.5   | 15.0  | 900              | 3.0   | 3.7   |
| 300              | 2.6   | 13.0  | 1000             | 3.0   | 3.4   |
| 400              | 2.7   | 10.0  | 1100             | 3.0   | 3.0   |
| 500              | 2.8   | 8.0   | 1200             | 3.0   | 3.0   |
| 600              | 2.8   | 6.0   |                  |   |   |

**Table 2.** Samples of the predicted thermal conductivity of YSZ TBC using EM1 and EMT models

| Temperature (°C) | Matrix (ZrO <sub>2</sub> ) |                    | Dispersed (Y <sub>2</sub> O <sub>3</sub> ) |                    | Composite Coating (YSZ) |                    |
|------------------|----------------------------|--------------------|--|--------------------|-------------------------|--------------------|
|                  | k <sub>1</sub> (W/m.K)     | v <sub>1</sub> (%) | k <sub>2</sub> (W/m.K)                     | v <sub>2</sub> (%) | K from EM (W/m.K)       | K from EMT (W/m.K) |
| 0                | 2.3                        | 0.96               | 19.0                                       | 0.04               | 2.45                    | 3.16               |
| 100              | 2.4                        | 0.96               | 17.0                                       | 0.04               | 2.60                    | 3.29               |
| 200              | 2.5                        | 0.96               | 15.0                                       | 0.04               | 2.64                    | 3.37               |
| 300              | 2.6                        | 0.97               | 13.0                                       | 0.03               | 2.97                    | 3.38               |
| 400              | 2.7                        | 0.97               | 10.0                                       | 0.03               | 2.87                    | 2.42               |
| 500              | 2.8                        | 0.97               | 8.0  | 0.03               | 2.90                    | 3.36               |

### 3.5. Models Adjustment for Enhanced Accuracy

Any significant difference between the results of the theoretical models and the experimental results must be minimized to increase their accuracy and reliability and to achieve a better match with real-world data. It was found that the EM and EMT theoretical models give inaccurate results that are different from the experimental results. Therefore, these models were adjusted by adding correction factors. The correction factors are found based on the assumption that the ratio between the experimental thermal conductivity and the theoretical thermal conductivity must equal one. Therefore, if the ratio is not a unity, the correction factor is utilized to adjust the theoretical values and enhance accuracy.

In this study, 170 YSZ TBC data were gathered at various temperatures, containing varying amounts of pores and varying  $Y_2O_3$  and  $ZrO_2$  ratios. The 170 observations encompass 15 distinct percentages of pores, and knowing that the primary reason earlier theories (the EM and EMT) failed was because they neglected to account for the porosity content when estimating the value of thermal conductivity. This issue has been addressed by proposing a correction factor that is directly related and linked to the porosity content in YSZ coatings.

All of the experimental observations with the same porosity content were gathered, irrespective of the  $ZrO_2/Y_2O_3$  ratio or temperature. Thereafter, the following procedures were used to determine the value of the correction factor:

**Step 1:** For each experimental observation, the correction factor is the ratio between the experimental value of thermal conductivity and the calculated theoretical value and is determined using Equation No. 1:

$$CR_{i,p_j} = \frac{\phi_{exp,i,p_j}}{\phi_{theor,i,p_j}} \quad (1)$$

Where,

$CR_{i,p_j}$ : correction factor for observation,  $i$ , and at the porosity content,  $p_j$ .

$\Phi_{exp,i,p_j}$ : Experimental thermal conductivity for observation,  $i$ , and the porosity content,  $p_j$ .

$\Phi_{theor,i,p_j}$ : Theoretical thermal conductivity for observation,  $i$ , and the porosity content,  $p_j$ .

**Step 2:** As each observation will result in a certain value of the correction factor, the current approach uses the arithmetic mean of the correction factor for all experimental observations with the same porosity content, which is calculated through Equation No. 2:

$$CR_{Avg,p_j} = \frac{\sum_{i=1}^n CR_{i,p_j}}{n} \quad (2)$$

Where,

$CR_{Avg,p_j}$ : Average correction factor for the porosity content,  $p_j$ .

$n$ : number of observations in the gathered dataset that have porosity content,  $p_j$ .

### 3.6. Porosity Interval Grouping

Due to the limited number of data points in several of the original 15 porosity intervals, individual correction factors computed for these narrow ranges were found to be statistically unstable and unreliable. To overcome this, we combined adjacent intervals exhibiting similar conductivity trends into broader groups, resulting in 7 final porosity intervals. This approach ensured a more statistically robust correction factor for each range. The grouping also preserved the physical consistency of the data and led to measurable improvements in the accuracy of the EM and EMT model predictions, as validated through statistical metrics (see Section 4.4).

It is important to note that the correction factors reflect not only the influence of porosity but also the underlying microstructural characteristics of YSZ coatings, including pore morphology, size distribution, and connectivity. These features introduce scattering mechanisms and anisotropic thermal pathways that are not fully captured by classical EM and EMT models. Consequently, the correction factors account for the combined effects of porosity and microstructural heterogeneity, enabling a more realistic correspondence between theoretical predictions and experimental measurements. Due to the lack of sufficient experimental data covering these variables, their individual contributions could not be explicitly modeled. However, the empirically derived correction factors implicitly incorporate the combined influence of these microstructural and processing-related parameters, as they are intrinsically reflected in the discrepancies between theoretical predictions and measured values.

## 4. Results & Discussion

### 4.1. Models Results Comparison

The experimental and theoretical thermal conductivity values of YSZ TBC obtained using the EM1 and EMT models for the full dataset of 170 samples are presented in Figure 2 and Figure 3, respectively. In these figures, the experimental measurements are shown as blue “+” markers, while the predictions from the EM1 model are shown as red “x” markers and the predictions from the EMT model are shown as green triangular “Δ” markers. As observed, the theoretical predictions are consistently offset from the experimental data, showing considerable deviation across all samples. This wide separation between the experimental and theoretical point distributions clearly demonstrates the limited accuracy of the EM1 and EMT models in capturing the complex thermal behavior of real YSZ coatings. The data points are intentionally not connected by lines, as each index represents an independent discrete measurement rather than a continuous function. This can be explained by several reasons, as these theoretical models do not include the effect of porosity, which has a significant impact on the thermal conductivity values. In addition, these models don't distinguish between bulk and coated materials. The YSZ TBC material is coated, and it is important to study its properties as it is being coated because they might be different from the properties of corresponding bulk materials.

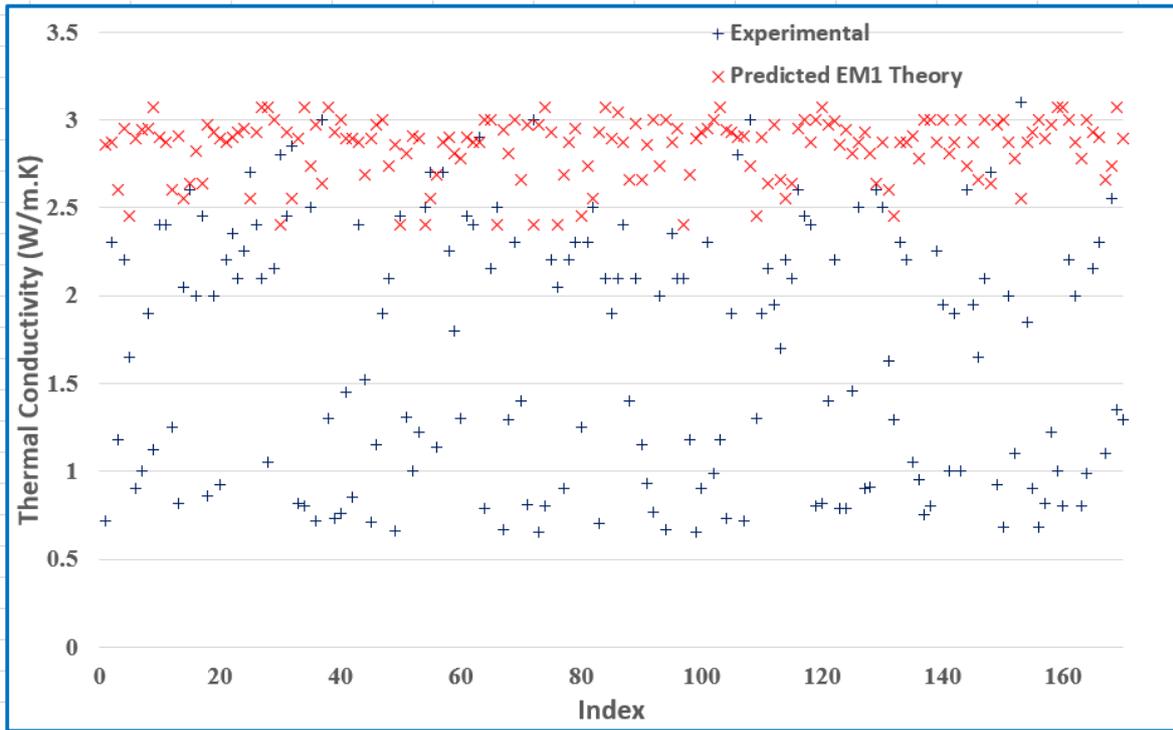


Figure 2. Experimental values of thermal conductivity of YSZ TBC vs. those predicted using EM1 model

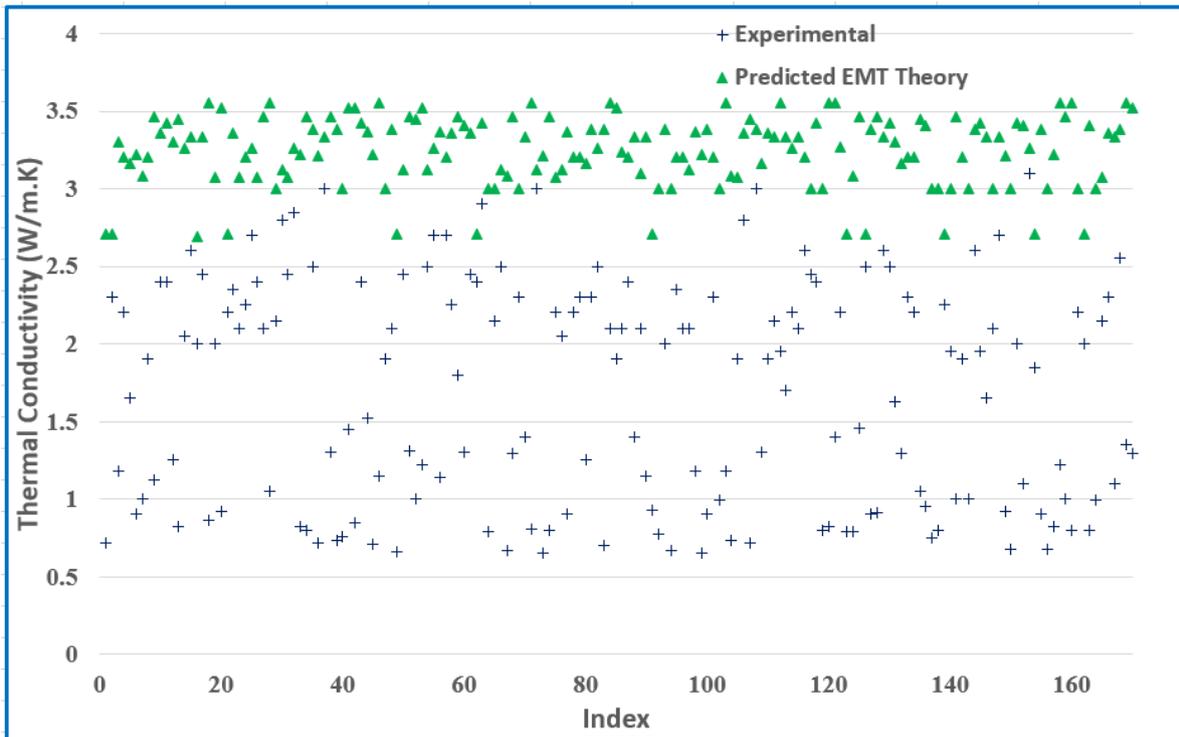


Figure 3. Experimental values of thermal conductivity of YSZ TBC vs. those predicted using EMT model

### 4.2. EM Adjustment

Correction factors were developed to close the gap between the measured values of thermal conductivity and the corresponding predicted values using the EM model. These correction factors are connected to the TBC's porosity percentages because they significantly affect thermal conductivity—an effect that the classic EM model does not take into account. For each porosity content, the two steps procedure that prescribed earlier in Section 3.5 was followed to compute average correction factor. It is important to mention that some porosity content intervals were merged together in one interval when they have close values, this reduces the number of intervals from 15 to 7 in the examined dataset. Table 4 provides a sample of the gathered dataset and gives an example of the values used to calculate the correction factor of thermal conductivity of YSZ TBC found from EM theory for the porosity content 4.8%.

Table 5 shows the values of the correction factor for each specific porosity percentage interval within the range (0–23.8%). Seven different intervals were created. The experimental thermal conductivity values, the predictions

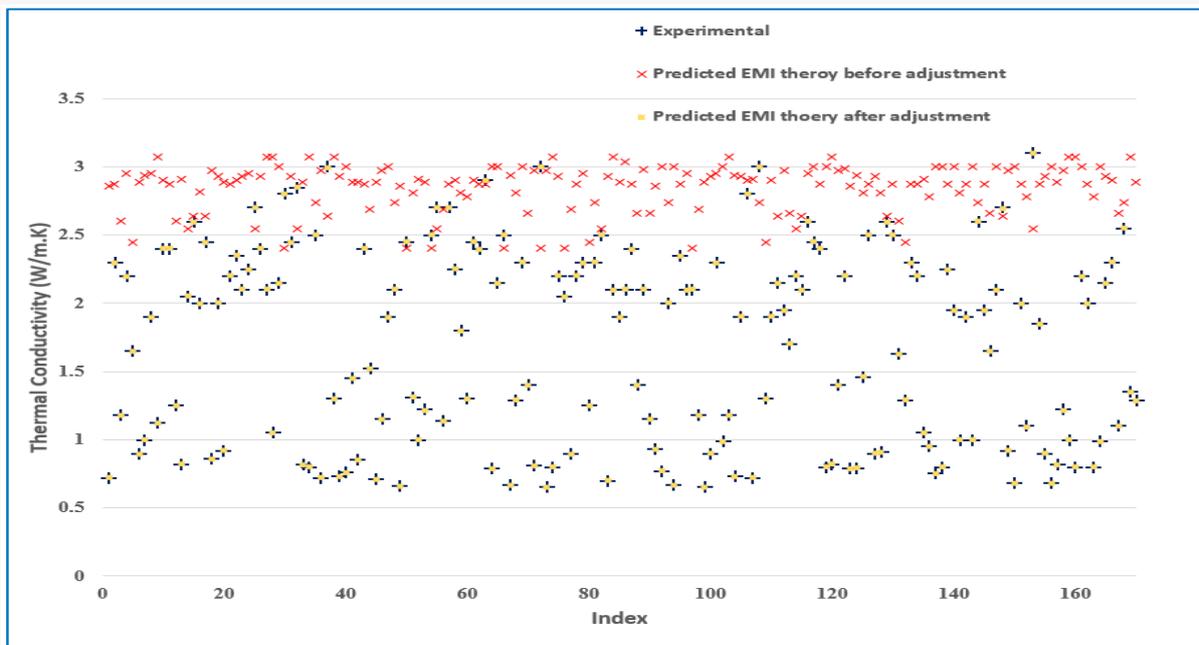
from the EM1 model, and the corrected EM1 results are shown using discrete markers without connecting lines in Figure 4. Each marker represents an individual sample measurement, and the absence of connecting lines reflects the fact that the dataset consists of independent, non-continuous observations. The uncorrected EM predictions exhibit a clear deviation from the experimental measurements, whereas the corrected EM results align much more closely with the experimental data, demonstrating the effectiveness of the proposed adjustment.

**Table 5.** The proposed correction factors for thermal conductivity of YSZ TBC predicted from the EM1 model

| Porosity percentage      | Correction factor |
|--------------------------|-------------------|
| Fully dense              | 0.840             |
| 0 < porosity ≤ 4.8%      | 0.377             |
| 4.8% < porosity ≤ 5.9%   | 0.859             |
| 5.9% < porosity ≤ 9.6%   | 0.392             |
| 9.6% < porosity ≤ 11.5%  | 0.830             |
| 11.5% < porosity ≤ 14.2% | 0.316             |
| 14.2% < porosity ≤ 23.8% | 0.761             |

**Table 4.** A sample of the used dataset shows the values used to calculate the correction factor of thermal conductivity of YSZ TBC found from the EM theory for the porosity content 4.8%.

| Index | V2 (Y <sub>2</sub> O <sub>3</sub> ) | V1 (ZrO <sub>2</sub> ) | K2 (Y <sub>2</sub> O <sub>3</sub> ) | K1 (ZrO <sub>2</sub> ) | EM adjustment before | Experimental K | correction Factor | porosity % | EM adjustment after |
|-------|-------------------------------------|------------------------|-------------------------------------|------------------------|----------------------|----------------|-------------------|------------|---------------------|
| 5     | 0.04                                | 0.96                   | 19                                  | 2.25                   | 2.450                | 1.65           | 0.674             | 0.048      | 0.923               |
| 33    | 0.04                                | 0.96                   | 6                                   | 2.8                    | 2.550                | 0.82           | 1.119             | 0.048      | 2.189               |
| 40    | 0.04                                | 0.96                   | 3                                   | 3                      | 3.000                | 0.76           | 0.253             | 0.048      | 1.088               |
| 44    | 0.04                                | 0.96                   | 15                                  | 2.5                    | 2.690                | 1.52           | 0.565             | 0.048      | 1.015               |
| 60    | 0.04                                | 0.96                   | 13                                  | 2.6                    | 2.780                | 1.3            | 0.467             | 0.048      | 1.049               |
| 119   | 0.04                                | 0.96                   | 3                                   | 3                      | 3.000                | 0.8            | 0.267             | 0.048      | 1.088               |
| 123   | 0.04                                | 0.96                   | 2                                   | 2.9                    | 2.860                | 0.79           | 0.276             | 0.048      | 1.036               |
| 124   | 0.04                                | 0.96                   | 4                                   | 2.9                    | 2.940                | 0.79           | 0.269             | 0.048      | 1.066               |
| 131   | 0.04                                | 0.96                   | 17                                  | 2.4                    | 2.600                | 1.63           | 0.627             | 0.048      | 0.979               |
| 135   | 0.04                                | 0.96                   | 10                                  | 2.75                   | 2.910                | 1.05           | 0.361             | 0.048      | 1.096               |
| 138   | 0.04                                | 0.96                   | 3                                   | 3                      | 3.000                | 0.8            | 0.267             | 0.048      | 1.088               |
| 155   | 0.04                                | 0.96                   | 8                                   | 2.8                    | 2.930                | 0.9            | 0.307             | 0.048      | 1.105               |
| 157   | 0.04                                | 0.96                   | 6                                   | 2.8                    | 2.890                | 0.82           | 0.283             | 0.048      | 1.091               |



**Figure 4.** Comparison between the theoretical values of thermal conductivity of YSZ TBC attained from the EM model before and after adjustment.

### 4.3. EMT Model Adjustment

The method used to find correction factors for the EM model was also utilized to find the correction factors for the thermal conductivity of the YSZ TBC predicted from the EMT model. Table 6 shows the values of the proposed correction factor for each porosity percentage interval. Figure 5 presents a comparison between the experimental thermal conductivity values and the predictions obtained from the EMT model before and after applying the correction factor. The results are plotted as discrete markers using different colors to distinguish the experimental data, the original EMT predictions, and the corrected EMT predictions. The corrected EMT results align much more closely with the experimental measurements than the uncorrected predictions, demonstrating a substantial improvement in the model's accuracy after adjustment.

**Table 6.** The proposed correction factors for thermal conductivity of YSZ TBC predicted from the EMT model

| Porosity percentage      | Correction factor |
|--------------------------|-------------------|
| Fully dense              | 0.741             |
| 0 < porosity ≤ 4.8%      | 0.328             |
| 4.8% < porosity ≤ 5.9%   | 0.745             |
| 5.9% < porosity ≤ 9.6%   | 0.326             |
| 9.6% < porosity ≤ 11.5%  | 0.724             |
| 11.5% < porosity ≤ 14.2% | 0.280             |
| 14.2% < porosity ≤ 23.8% | 0.667             |

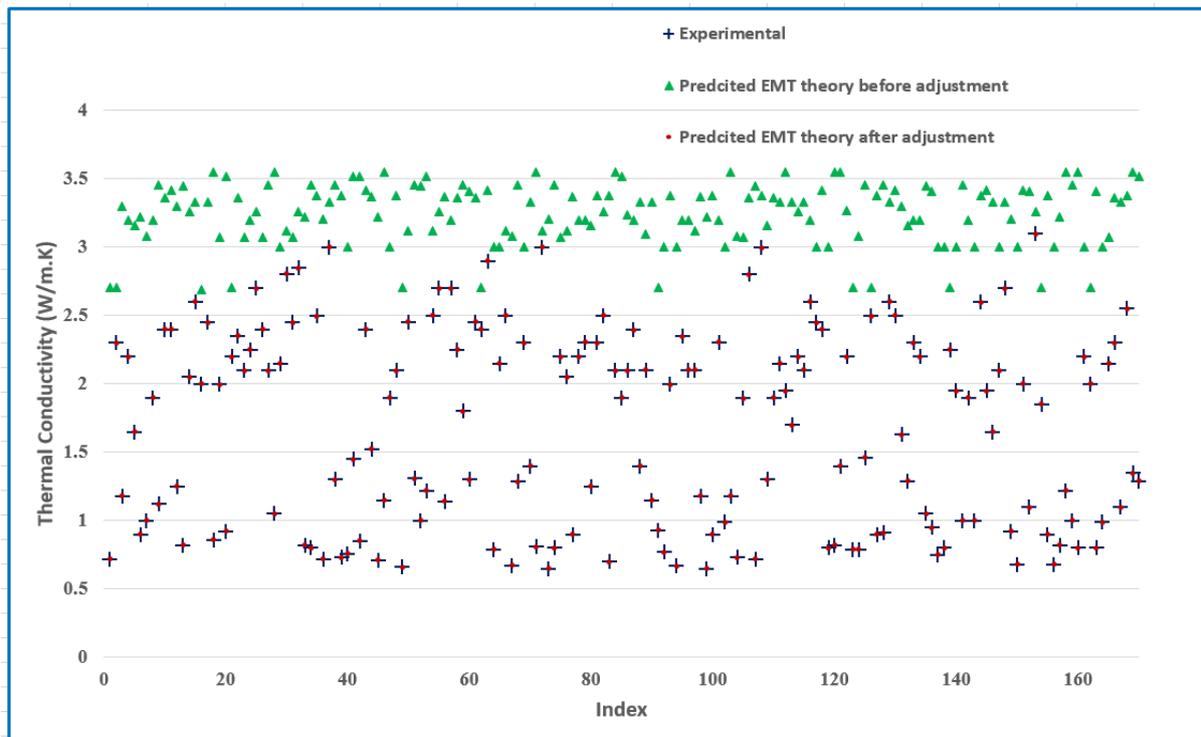
In this analysis, we combine data from three different studies on the thermal conductivity of YSZ TBC, despite variations in porosity content and experimental procedures. All of these studies come to the same conclusion regarding the impact of porosity on the thermal conductivity of YSZ

TBC: as porosity content increases, thermal conductivity decreases. Multiple linear regression was utilized in these studies to assess the porosity data and ascertain the correlation between porosity content and thermal conductivity. The agreement between these studies ensures that our combined dataset provides a robust representation of the material properties. Combining the data from several investigations has the major benefit of creating a dataset with a broad range of temperature and porosity content. A comprehensive understanding of the thermal conductivity behavior of YSZ TBC under various experimental settings is made possible by our coherent framework.

### 4.4. Statistical Evaluation of Model Performance

To provide a quantitative assessment of the predictive capability of the EM and EMT models, a statistical evaluation was conducted using the coefficient of determination ( $R^2$ ), the root mean square error (RMSE), and the mean absolute error (MAE). These metrics were computed with respect to the experimental thermal conductivity values for all 170 YSZ samples.

Prior to applying the correction factor, both analytical models (EM and EMT) exhibited substantial deviations from experimental measurements. The EM model yielded an  $R^2$  value of 0.74557, together with RMSE and MAE values of 1.97423 W/m·K and 1.16435 W/m·K, respectively. The EMT model showed even poorer performance, with an  $R^2$  of 0.83406, RMSE of 1.5649 W/m·K, and MAE of 1.5649 W/m·K. These results indicate that the original theoretical formulations significantly overestimated the thermal conductivity and were unable to track the experimental trends.



**Figure 5.** Comparison between the theoretical values of thermal conductivity of YSZ TBC attained from the EMT model before and after adjustment

After applying the proposed correction factor, both models demonstrated dramatic improvement in predictive accuracy. The corrected EM model achieved an  $R^2$  of 0.99999, and the RMSE and MAE values dropped to 0.00000335 W/m·K and 0.00042 W/m·K, respectively. Similarly, the corrected EMT model achieved an  $R^2$  of 0.99999, with RMSE and MAE values of 0.00029 W/m·K and 0.00029 W/m·K. These very low error values and near-unity  $R^2$  confirm that the correction factor effectively aligns model predictions with experimental data, resulting in almost perfect agreement. The statistical results are summarized in Table 7.

**Table 7.** Statistical performance metrics for EM and EMT models before and after applying the correction factor.

| Model                   | $R^2$   | RMSE (W/m·K) | MAE (W/m·K) |
|-------------------------|---------|--------------|-------------|
| EM (before correction)  | 0.74557 | 1.97423      | 1.16435     |
| EM (after correction)   | 0.99999 | 0.00000335   | 0.00042     |
| EMT (before correction) | 0.83406 | 1.56494      | 1.5649      |
| EMT (after correction)  | 0.99999 | 0.00029      | 0.00029     |

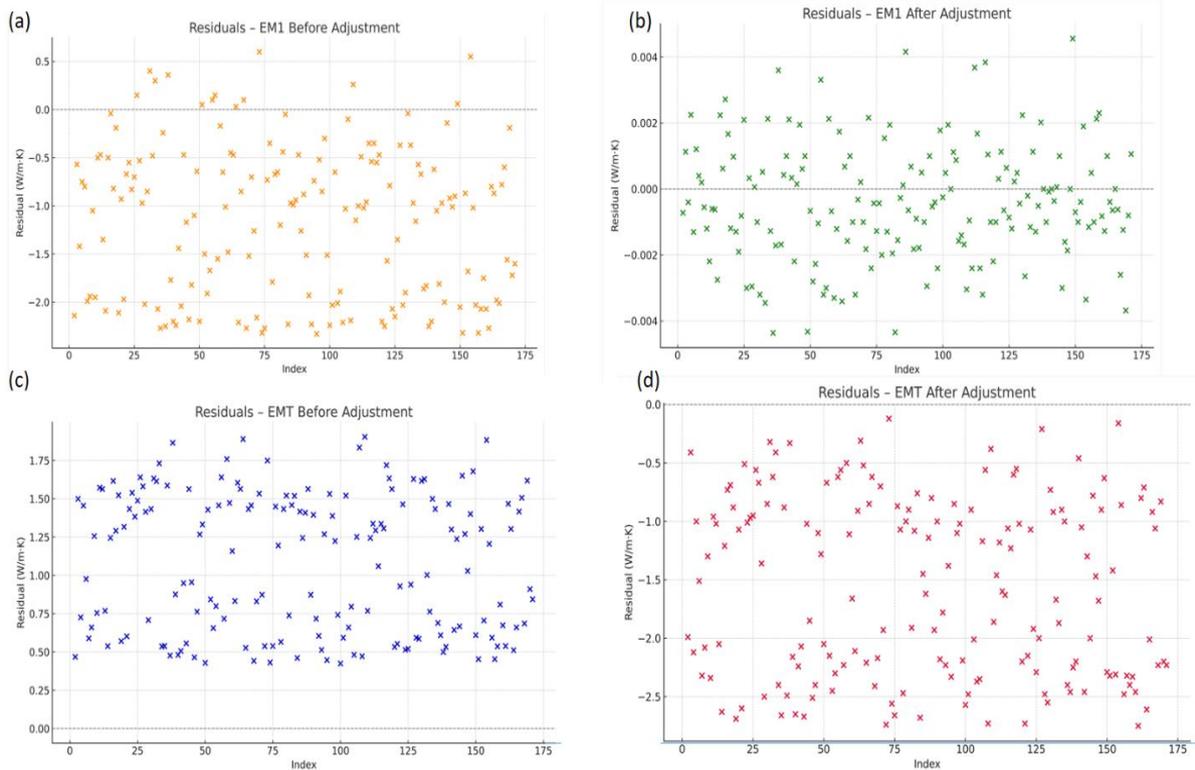
This analysis validates the significant improvement introduced by the correction and supports the trends observed in Figures 2–5.

#### 4.5. Residual Analysis of Theoretical Models

To further quantify the deviation between theoretical predictions and experimental data, residual plots were generated for both the EM1 and EMT models, before and after applying the proposed correction factor. Residuals are calculated as the difference between predicted and experimental thermal conductivity values for each data point.

As shown in Figures 6a–6d, the uncorrected models (Figures 6a and 6c) exhibit large residuals with systematic biases, especially at lower conductivity values. In contrast, the adjusted models (Figures 6b and 6d) show residuals tightly clustered around zero, indicating a substantial improvement in predictive accuracy.

These plots support the correction factors' effectiveness in aligning classical theoretical models with experimental measurements for YSZ TBCs. The results are also consistent with the improved statistical indicators (e.g., RMSE,  $R^2$ ) discussed earlier.



**Figure 6.** Residual plots for EM1 and EMT models before and after adjustment. (a) EM1 model before adjustment; (b) EM1 model after adjustment; (c) EMT model before adjustment; (d) EMT model after adjustment.

## 5. Conclusions

In this study, the EM1 and EMT models were examined for their capabilities to predict the thermal conductivity of YSZ TBC material and then adjusted to enhance their accuracy and applicability. The study comes with the following conclusions:

- The theoretical models (EM and EMT) cannot predict the thermal conductivity of YSZ TBC material accurately.
- The EM1 and EMT models used to predict the thermal conductivity of TBCs can be significantly improved by incorporating correction factors that take into account the impact of porosity content on the thermal conductivity.
- It should be noted that the proposed correction factors are applicable within the porosity range of 0–23.8%, as defined by the dataset used in this study. The behavior of the model beyond this range has not been verified and may require separate investigation.
- While porosity was the primary focus of this study, other microstructural parameters such as pore morphology, anisotropy, coating thickness, and deposition method may also significantly influence thermal conductivity. Due to the lack of sufficient data on these factors, they were not explicitly included in the current model. Future studies incorporating broader porosity ranges and detailed microstructural descriptors will be essential to enhance the predictive power and universality of the correction scheme.
- This adjustment enhances the applicability of EM and EMT models in capturing real-world problems.
- Statistical evaluation showed that the Coefficient of Determination ( $R^2$ ) value increased, accompanied by a substantial reduction in Root Mean Square Error (RMSE) and Mean Absolute Error (MAE). These results validate the robustness of the correction factor in improving predictive accuracy.

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## Data availability

Supplementary materials related to this study are available from the corresponding author upon reasonable request.

## Declaration of interest Statement

The authors certify that the data they have provided is accurate and that they are not aware of any event that involves conflict of interest.

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