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Additional Information

Reply to short communication HMT-D-20-01896 'Comment on "Numerical approach to define a thermodynamically equivalent material for the conjugate heat transfer simulation of very thin coating layers" by P. Olmeda, X. Margot, P. Quintero, J. Escalona, International Journal of Heat and Mass Transfer, Vol. 162(2020) 120377" by Jaal Ghandhi and Georgios Koutsakis

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Abstract

In the recent paper "Surface temperature of a multi-layer thermal barrier coated wall subject to an unsteady heat flux" by G. Koutsakis, G. F. Nellis, J. B. Ghandhi, Int. J. Heat Mass Transfer 155(2020) 119645 the authors have proposed an analytical solution to determine wall temperature of surfaces coated with multi-layer coatings. The solutions is obtained by the assumption of one-dimensional heat flux using the matrix method in conjunction with the 1-D Laplace transformed heat diffusion equation. The authors suggest that using this analytical approach a thicker pseudo-material could be found in order to address the 3D conjugate heat transfer problem. This approach is compared with another published methodology that employs a DoE (Design of experiments) in combination with a multiple regression analysis to define a thicker equivalent coating layer.

1. Introduction

Nowadays, important efforts of the Original Equipment Manufacturers (OEMs) are oriented at developing thermal coatings with low conductivities and low heat capacitances to coat the combustion chamber walls of internal combustion engines (ICEs). A material with such characteristics allows to instantaneously follow the in-cylinder gas temperature throughout the engine cycle, reducing the thermal gradient between the gas and the walls. Therefore, a gain in the thermal efficiency is expected. In this regard, there exists a special interest in the industry for developing methods to study the impact of these materials on the engine performance.

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Experimental measurements are complicated and costly. Thus, numerical methods arise as an important alternative to study heat transfer in ICEs. Though the 1D models are very useful, they do not allow studying in detail the physical processes within the engine such as turbulence or combustion. Consequently, 3D CFD-CHT is presented as the most suitable tool for evaluating the heat transfer through the solid walls in ICEs. However, the thin thicknesses of the new generation of thermal coatings ($\sim 100\ \mu m$) are computationally expensive and difficult to model. In this regard, Olmeda et al. recently published the article "Numerical approach to define a thermodynamically equivalent material for the conjugate heat transfer simulation of very thin coating layers", Int. J. Heat Mass Transfer 162 (2020) 120377 [1], where a methodology is proposed to address this problem.

The approach consists in determining the thermal properties (conductivity k and ρc) of a thicker pseudo-material (e.g. 2 mm) whose thermodynamic response is similar to that of the real thin coating. For this, a multifactorial test (DoE) in combination with a multiple regression analysis is employed.

On the other hand, Koutsakis et al. [2] have proposed an analytical solution to determine the wall temperature of the coated surface. According to the authors, the thermal properties of the pseudo-material can be determined for any coating using this approach with a minimum of assumptions.

In this work, both approaches are analyzed and the pseudo-materials obtained with the method proposed by Koutsakis et al. are compared with the one obtained in [1].

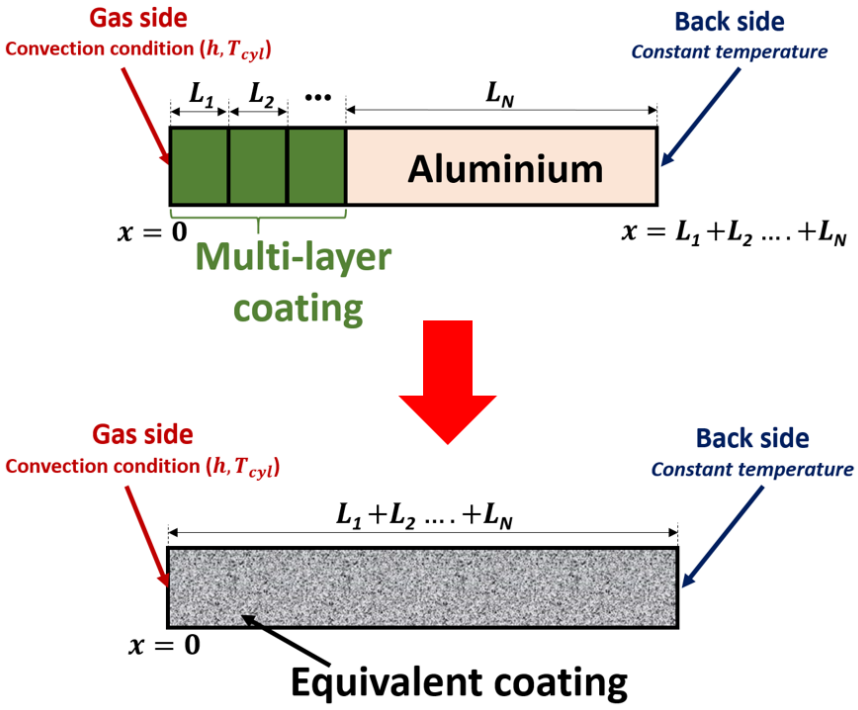

Figure 1: Methodology employed for the calculations.

2. Discussion

The objective of the work proposed in [1] is to replace a very thin coating layer (typically 0.1 mm) applied over some substrate by an equivalent material of larger thickness having the same thermodynamic behaviour as the original configuration, including the substrate. The motivation is to be able to use reasonable mesh sizes for Conjugate Heat Transfer (CHT) computational analysis.

A representative scheme of the proposed methodology employed in [1] is shown in Fig. 1. The equivalent material should have a reasonable meshing thickness and should comprise all the coating layers plus a representative thickness of the metallic substrate layer. In this way it can be integrated into the 3D engine geometry. The equivalent thickness is:

$$L_{eq} = L_1 + L_2 + \cdots + L_N$$

where L_N is the metal substrate.

The latter value takes into account the limit at which the temperature oscillations in the solid near the back side are vanished.

Although in [1] an equivalent material was found considering a one-layer coating, the approach can easily be extended to multi-layer coatings. The characteristics of the coating and the metallic substrate of the baseline case are presented in Table 1 (see column termed Baseline):

As explained in [1], first the real material was discretized in the 1D-HTM model with 1024 nodes for the coating layer (thickness 0.1 mm) and 512 for the aluminium substrate (thickness 1.9 mm). Surface temperature and heat fluxes were then calculated with the model. In order to validate the accuracy of the baseline results a mesh independence study was also carried out and demonstrated that about 500 nodes were needed minimum.

Then, a new discretization with only 4 nodes for the total 2 mm thickness was performed and the equivalent material defined by means of the multi-factorial statistics methodology described in the paper (DoE with 1D-HTM [3] and multiple regression analysis).

As also discussed in the paper, if the number of nodes for the new discretization changes, then so will the properties of the equivalent material. But mesh independence in the 1D-HTM model was not the issue once the thermodynamic behaviour of the baseline material was properly represented.

The target was to ensure that 2 mm equivalent material with 4 nodes accurately reproduced the behavior of the baseline coating + metal substrate (layer of 0.100 mm with 1024 nodes + layer of 1.9 mm with 512 nodes) for its application in the 3D CFD-CHT calculation.

The properties of the single equivalent material calculated for the 4 nodes discretization are presented in the column termed Equivalent in Table 1.

On the other hand, Ghandhi and Koutsakis argue in their short communication [4] that this approach is a trial-and-error method that can be much better solved using their analytical scaling method described in a very recently published paper [2]. They explain that "Full dynamic similarity is achieved when the independent dimensionless parameters $\Xi \equiv R_1/R_2, \Omega_1 \equiv fR_1C_1$ and $\Omega_2 \equiv fR_2C_2$ are matched between the baseline and scaled cases". And they add that two additional constraints should be satisfied, namely that the total resistance and total length of the baseline and scaled cases should be the same. Using their method with the data provided in [1], the authors calculated the properties of a 'pseudo-material' which are listed in Table 1

in the column named Scaled. They then calculated the surface temperature with both sets of values (Equivalent and Scaled) using a finite difference code with 1024 nodes for the coating layer and 512 for the substrate layer. By comparing both solutions, they showed that there were significant discrepancies between both methods.

Table 1: Equivalent material properties

	Baseline	Scaled	Scaled new	Equivalent
k_1 $[\frac{W}{m\cdot K}]$	0.1	2.0	1.0	1.546
k_2 $[\frac{W}{m\cdot K}]$	144	116.6	75.79	—
$(\rho c)_1$ $[\frac{kJ}{m^3 K}]$	100	5	1000	3.769
$(\rho c)_2$ $[\frac{kJ}{m^3 K}]$	2316	2840	1219	—
$L_1[mm]$	0.1	2.0	1.0	2.0
$L_2[mm]$	1.9	8.1	1.0	—

The method of Koutsakis et al.[2] is certainly very interesting, but it is not adequately applied to the Olmeda et al. case. Indeed, as shown in the column 'Scaled' of Table 1, two pseudo-materials were defined (one for the coating layer, one for the substrate layer) instead of only one in the 'Equivalent' column (coating + substrate). For the purpose of a CFD-CHT calculation, this is not practical. In addition, the authors of the short communication assumed that the equivalent coating layer calculated in [1] did not include the substrate layer. This is understandable, as Fig. 1 was not included in the paper. Nonetheless, the method of Koutsakis et al. is applied here using the real data employed in [1] to illustrate the differences between both methods.

New scaled pseudo-materials (see column named 'Scaled new' in Table 1) are determined with the equations 1, 2, 3 and 4, in order to compare with the equivalent material approach developed in [1].

$$k_1^B = \frac{L_1^B}{L_1^A} k_1^A \tag{1}$$

$$k_2^B = \frac{L_2^B}{L_2^A} k_2^A \tag{2}$$

$$(\rho c)_1^B = \frac{L_1^A}{L_1^B} (\rho c)_1^A \tag{3}$$

$$(\rho c)_2^B = \frac{L_2^A}{L_2^B} (\rho c)_2^A \tag{4}$$

Using the same nomenclature as in [4], the superscripts A and B refer to the baseline and scaled cases, respectively. The subscripts 1 and 2 refer to the coating layer and the metallic substrate, respectively. A 1 mm thickness was selected for both the new scaled coating (L_1^B) and the metallic (L_2^B) layers, so that the total thickness of 2 mm defined in [1] was respected.

For the comparison, the transient values of gas temperature and heat transfer coefficient (HTC) displayed in Fig. 2 were considered on the gas side. A constant temperature value of 430 K was used as boundary condition on the back side (Fig. 1).

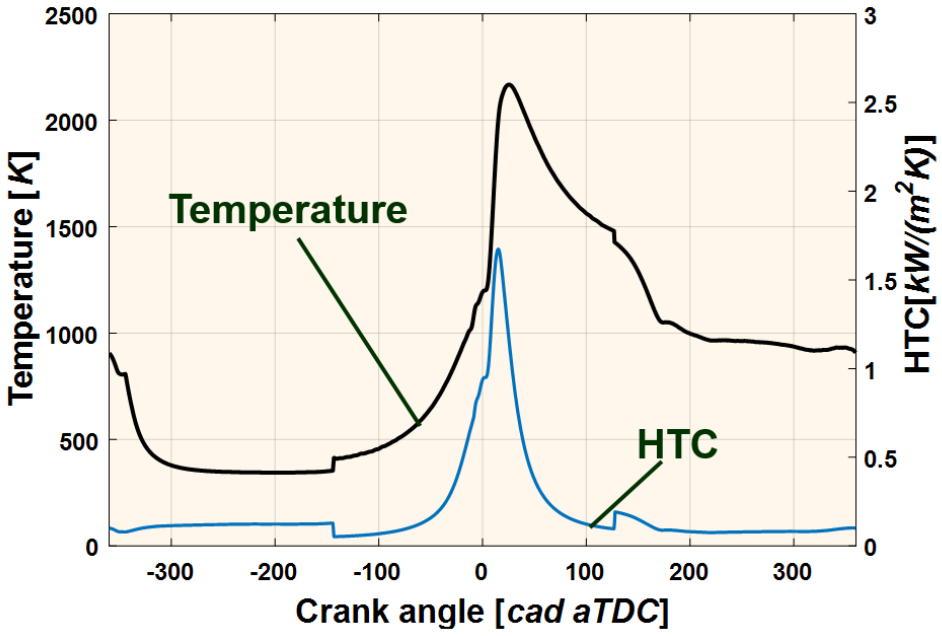

Figure 2: Gas temperature and heat transfer coefficient as boundary conditions for the gas exposed surface.

The temporal evolution of the temperature on the gas exposed wall and of the heat flux through the wall were calculated with the 1D-HTM model for the scaled pseudo material (scaled new). These are shown in Fig. 3 and compared with the baseline results. For this a total of 1536 nodes were employed in the discretization (768 nodes for the scaled material 1 and 768 nodes for the scaled material 2), a number very similar to the one used in [4]. The results confirm that indeed the method of "scaling materials" [2] allows obtaining temperatures and heat flux evolutions in agreement with the baseline case. However, the accuracy of the approach depends on the number of nodes employed in the 1D-HTM discretization, as is demonstrated below.

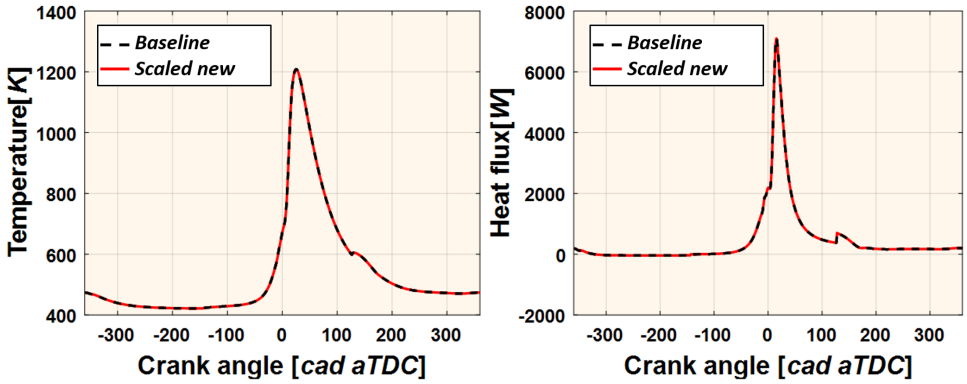

Figure 3: Wall temperature evolution (left) and heat flux evolution (right) of the scaled pseudo-materials meshed with 1536 nodes compared with the baseline.

When the scaled materials approach is employed by considering a total of 4 nodes only, a poor response for the wall temperature and heat flux is observed as shown by the 'scaled new' curve in Fig. 4. In this case, the scaled material layers 1 and 2 were discretised with only 2 nodes each. Fig. 4 also shows the results for the equivalent material found in [1] for 4 nodes. Clearly, the latter approach yields a better estimation of the heat flux and the instantaneous wall temperature. The differences on the heat transfer for all the cases are shown in Table 2.

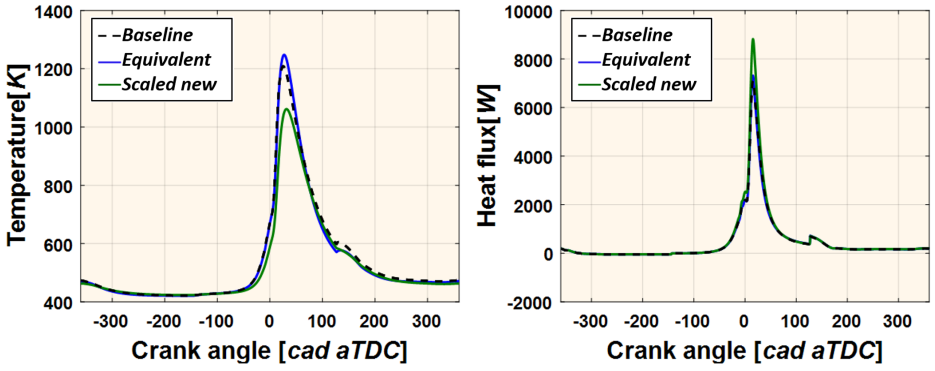

Figure 4: Wall temperature evolution (left) and heat flux evolution (right) of the scaled pseudo-materials meshed with 4 nodes and the equivalent coating also meshed with 4 nodes, compared with the baseline.

Table 2: Heat transfer differences of the pseudo-material respect to the baseline case.

Pseudo-material	$Q^{error}_{negative}[\%]$	$Q^{error}_{positive}[\%]$	$Q^{error}_{mean}[\%]$
Equivalent	-0.004	0.03	-0.08
Scaled new (4 nodes)	-4.15	-11.86	-12.03
Scaled new (1536 nodes)	0	0	0

The methodology proposed by Olmeda et al. prioritizes the heat flux over the wall temperature. However, it is important to keep the errors on the surface temperature as low as possible. In this regard, the instantaneous wall temperature error with respect to the baseline case is shown in Fig. 5 for all the considered cases. The results show that for a discretization of 4 nodes the equivalent coating defined with the method described in [1] gives the lowest temperature error with respect to the baseline.

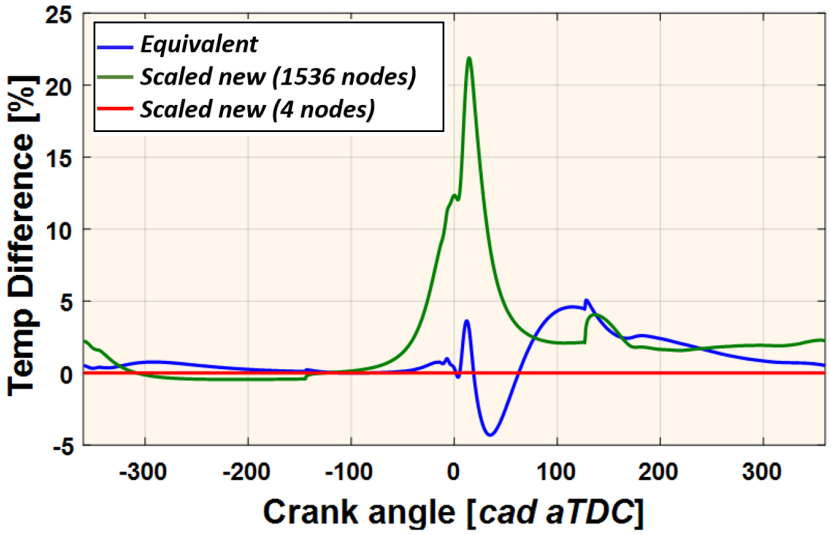

Figure 5: Wall temperature difference error for the four pseudo-materials.

This low number of nodes was selected considering the different restrictions imposed by a 3D coupled CFD-CHT transient calculation in an engine, such as grid size in the fluid domain, adaptive mesh refinement, relative size of cells close to and in the solid parts of the engine. These calculations are computationally very costly, in time and memory resources, and it is simply not possible to discretize a coating layer with even 100 nodes, let alone with 1000. To illustrate this, two meshes of a piston with a coating layer of 2 mm on the piston top surface are shown in Fig. 6.

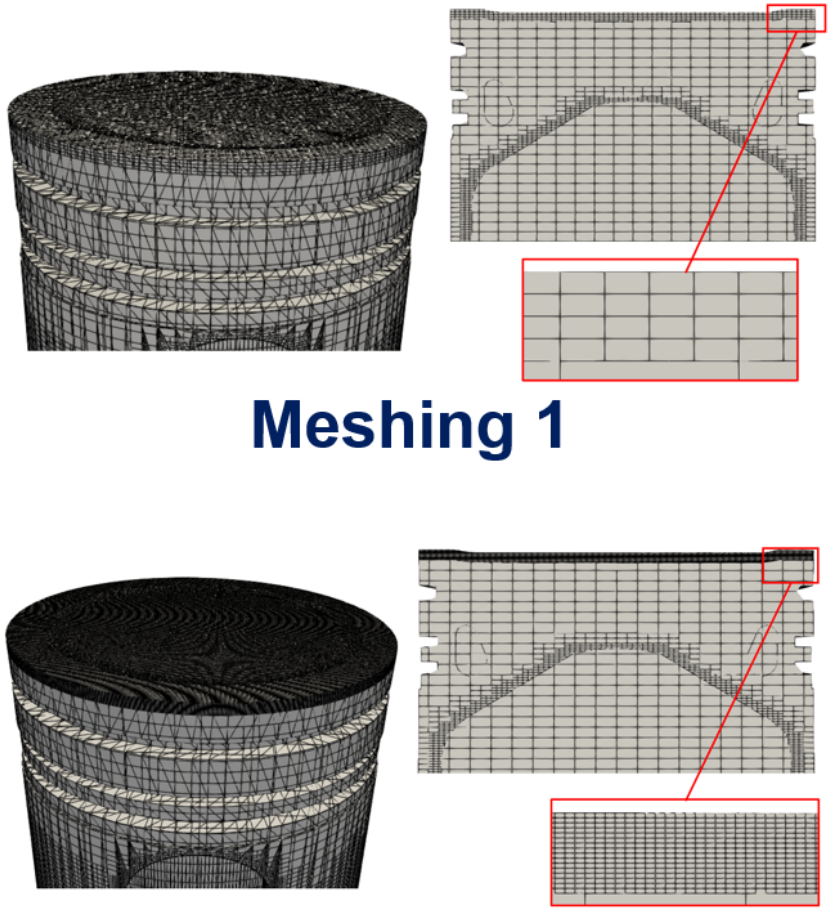

Figure 6: CHT mesh for a piston with 2 mm coating layer on the top surface: 4 nodes (top) and 16 nodes (bottom).

Mesh 1 has 25673 cells in the coating layer with 4 axial nodes; increasing the number of axial nodes to 16 yields mesh 2 with 1247562 cells. This increase in the cells number has an important impact on the computational requirements. Thus, it results impossible and inefficient to consider about 1000 axial nodes for the coating layer in the 3D computational domain.

3. Conclusion

In conclusion, the analytic method presented in [2] is very interesting to reduce the computational time in parametric studies concerning coating layers and may replace with advantage 1D-HTM calculations. However, it cannot be used for the purpose of 3D CFD-CHT calculations, as the number of cells has to be minimized for computational costs reasons. The statistical method proposed in [1] has been successfully applied in the 3D CFD-CHT calculations to study the heat transfer losses in an engine [5].

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