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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

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ABSTRACT

In the recent paper "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, Int. J. Heat Mass Transfer 162 (2020) 120377 the authors develop a procedure to identify a thicker pseudo-material to mimic the dynamic response of a thin thermal barrier coating. A thicker layer is desired to allow efficient conjugate heat transfer analysis. They employ an *ad hoc* procedure for defining the thermal properties of the material to approximate dynamic similarity with low grid resolution. There exists a published analytical solution for this same problem that allows the pseudo-material's thermal properties to be directly determined without a trial-and-error approach. The approach is elucidated and the effects of numerical resolution are explored.

1. Introduction

There is significant interest in the application of thin, low thermal conductivity, k, low heat capacity, ρc, thermal barrier coating to reciprocating internal combustion engine surfaces. Coatings with these properties can follow the rapid gas temperature swings better than previously used coating materials. Because the heat transfer is driven by the gas-wall temperature difference, these coatings reduce heat losses to the chamber surfaces.

Olmeda *et al.* [1] sought to replace the thin coating (0.1 mm) and the top 1.9 mm of the metal substrate with a thicker (2 mm) pseudo-material to enable a more computationally efficient conjugate heat transfer (CHT) analysis. In order to achieve a similar coating surface temperature response, a new set of thermal properties for this thicker pseudo-material were required. Their approach was to undertake a "multifactorial test of possible combinations of heat capacitance and conductivity", which amounts to a trial-and-error, *i.e.*, not analytical, approach to identify k and ρ^c that best match the fully resolved 1D solution for heat flux and surface temperature. They constrained their solution to cases having large node sizes to accommodate the CHT. There are several shortcomings to this approach. The major issue is that the material properties are manipulated to compensate for errors brought on by the lack of adequate numerical grid resolution. In turn, this makes the solution dependent on the applied heat flux and its frequency content, *i.e.*, the solution is not universal.

We have recently published [2] an analytical approach to this same problem in "Surface temperature of a multi-layer thermal barrier coated wall subject to an unsteady heat flux" in Int. J. Heat Mass Transfer 155(2020) 119645. Here we show that using this solution with minimal assumptions the thermal properties of two pseudo-materials that provide full dynamic similarity can be directly obtained for coatings like those of interest for engines, and explore the effects of numerical resolution.

2. Discussion

In [2] a multi-layer wall is considered, but a special-case analytical solution is given for a two-layer (one coating layer and the metal substrate) problem in the limit of $\Lambda \equiv \sqrt{\frac{R_2 C_1}{R_1 C_2}} \to 0$, where $R \equiv \frac{L}{k}$ is the resistance, $C \equiv \rho c L$ is the capacitance, L is the layer thickness, and the subscript 1 and 2 refer to the coating and substrate, respectively. For the conditions of Olmeda *et al.*, listed as

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Table 1
Baseline material properties, pseudo-material properties proposed in [1], and scaled pseudo-material properties from this work.

	Baseline[a]	Proposed	Scaled
k_1 [W/m-K]	0.1	1.546	1.0
k_2 [W/m-K]	144	-	75.8
$(\rho c)_1$ [J/m^3-K]	10^5	3769	10^4
$(\rho c)_2$ [J/m^3-K]	2.3×10^6	-	4.37×10^6
L_1 [mm]	0.1	2.0	1.0
L_2 [mm]	1.9	-	1.0

[a] k_2 and $(\rho c)_2$ based on other published work by same group [3]

the baseline case in Table 1, $\Lambda = 0.0055$, easily satisfying the constraint.

Following the analysis given in [2], 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, which will be referred to using superscripts A and B, respectively, and f is the forcing frequency, which does not affect the results. Because the desire is to match the *dimensional* temperature at the surface, there is also a constraint that the total resistance, $R_1 + R_2$ needs to be matched. The last (fifth) mathematical constraint is that the total length of the wall, $L = L_1 + L_2$, should not change. The (six) unknown values are: $k_1^B, k_2^B, (\rho c)_1^B, (\rho c)_2^B, L_1^B, L_2^B$. The problem is solved by the *a priori* selection of L_1^B to be a value suitable for the conjugate heat transfer analysis, as discussed more fully below. After some simple algebra, one finds

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

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

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

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

There are two ways to apply this analysis to the problem for the application of Olmeda *et al.* The first method, which is not favored, is to assume a single characteristic length for the conduction path through the piston (L_2^A) and a value of L_1^B that provides the desired grid resolution. The procedure above would then give the pseudo-coating and pseudo-piston properties. The piston is, however, three dimensional and defining a single characteristic length will add error.

The second approach, which will be demonstrated below and follows the example of Olmeda *et al.*, just replaces the piston material near the surface with pseudo-materials 1 and 2 and leaves the remainder of the piston as its original material. In accordance with [1], a 2 mm zone will be replaced; they deemed that 2 mm was large enough to provide reasonably shaped finite element nodes but small enough to not adversely affect the prediction of the energy flow through the piston in the CHT solution. Further, to enable the most efficient possible meshing, the two pseudo-materials are chosen to have the same thickness. Table 1 shows the properties of the pseudo-materials resulting from the dimensional analysis, termed *Scaled*, and the values proposed by Olmeda *et al.*, termed *Proposed*.

A simple 1D example is used to illustrate the differences in these approaches. The domain length was 2.0 mm with one edge of the domain held at 430 K and the other subjected to a periodic

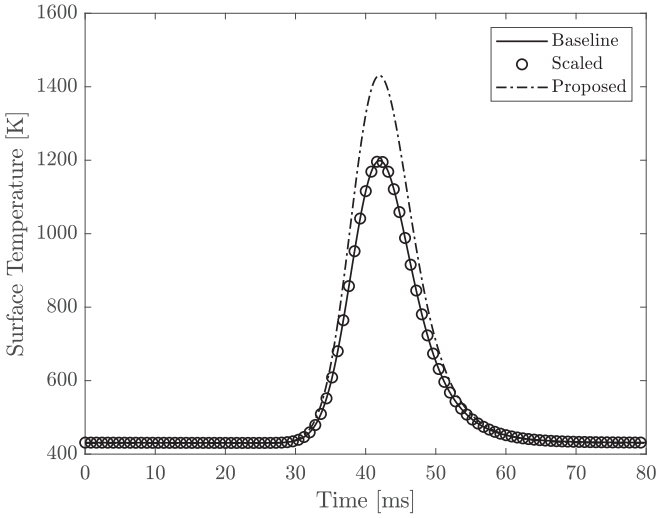

Fig. 1. Comparison of fully resolved results for baseline coating, scaled solution, and proposed single pseudo-material from [1]

(in time) Gaussian heat flux pulse

$$\frac{q''}{q''_{max}} = exp\left[-\left(\frac{t - \tau/2}{\tau/\alpha}\right)\right] \tag{5}$$

where τ is the cycle time, taken as 80 ms to match [1], and the width parameter, α, was included to allow frequency content of the forcing function to be varied. The fully resolved cases utilized 1024 nodes in material 1 and 512 nodes in material 2 (when present). Under-resolved cases will be described in terms of dx_1/L and dx_2/L, where dx_i is the node size in material i. For example, dx_1/L=0.125 and dx_2/L=0.25 corresponds to four nodes in material 1 and two nodes in material 2. In order to achieve a converged result, the cycle was repeated until the maximum difference in surface temperature relative to the prior cycle was less than 10^{-6} K. Unless otherwise stated, $q''_{max} = 10^6$ W/m^2 and $\alpha = 16$.

Figure 1 shows the fully resolved surface temperature for the baseline, scaled and proposed cases from Table 1. It can be seen in Fig. 1 that the baseline and scaled cases match perfectly. The proposed case, however, shows substantial differences; the dynamic response of the wall is incorrectly predicted. This is a result of the incomplete dynamic similitude provided by the proposed solution. The principal argument of Olmeda *et al.* is that at lower spatial resolution the numerical errors will compensate for this mismatch in the physics.

Figure 2 shows the surface temperature error, relative to the fully resolved baseline case, for the scaled properties. These cases were run with dx_2/L=0.25, *i.e.*, 0.5 mm node size, which represents the worst case of just two nodes in material 2. As seen from the very low error for dx_1/L=0.03125 (less than 0.1%), the material 2 spatial resolution has a very small effect on the results. Figure 2 shows that better than 1% error can be achieved with a resolution of just dx_1/L=0.125, which corresponds to just six nodes across the two materials. The same results for the proposed material (recall that there is only a single material for this case) are shown in Fig. 3. The error is significantly larger, which is consistent with Figure 1, but does not show a strong sensitivity to numerical resolution. There is a delay in the peak as the resolution decreases, which will feed back error when a prescribed gas temperature and heat transfer coefficient boundary condition are used.

The effect of the frequency content of the applied heat flux is demonstrated in Figure 4 where the parameter α was adjusted while τ was held constant. It should be noted that the highest value of α in Fig. 4 corresponds to a Gaussian pulse of 65

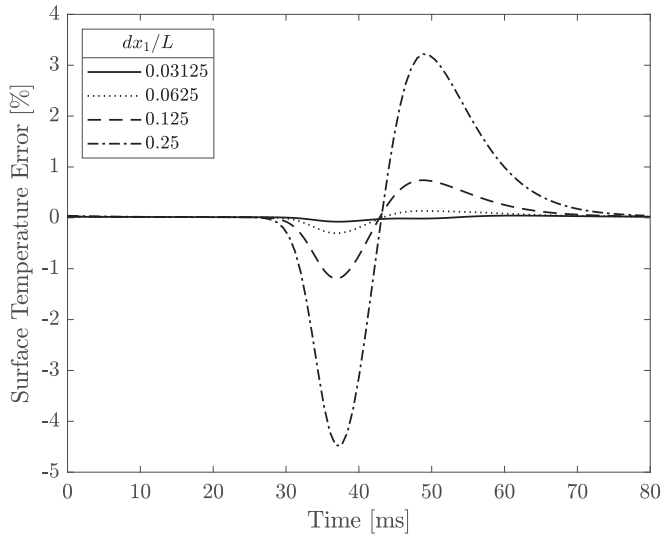

Fig. 2. Surface temperature error for the scaled properties at the given nodal resolutions. All data have dx_2/L=0.25.

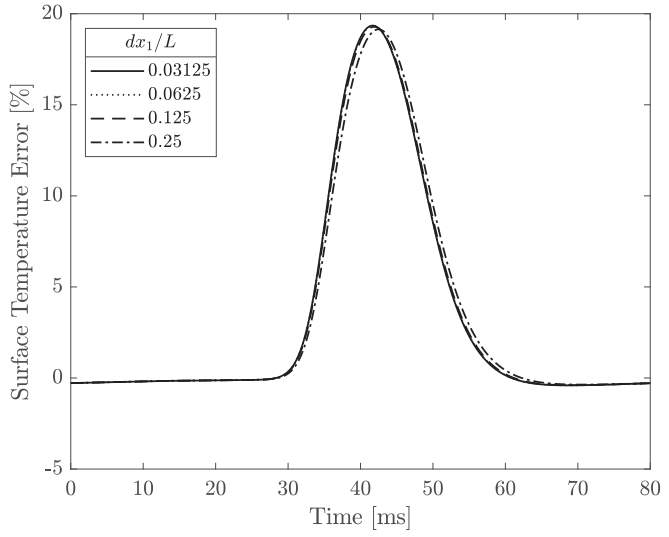

Fig. 3. Surface temperature error for the proposed properties at the given nodal resolutions.

μs full width at half maximum, which is much faster than standard engine conditions. The scaled results were all performed with dx_2/L=0.25. The scaled results show an expected pattern of increased error as the forcing frequency increased, and that this error is mitigated by increasing the grid resolution. Based on these results, one would say that excellent results could be obtained for all

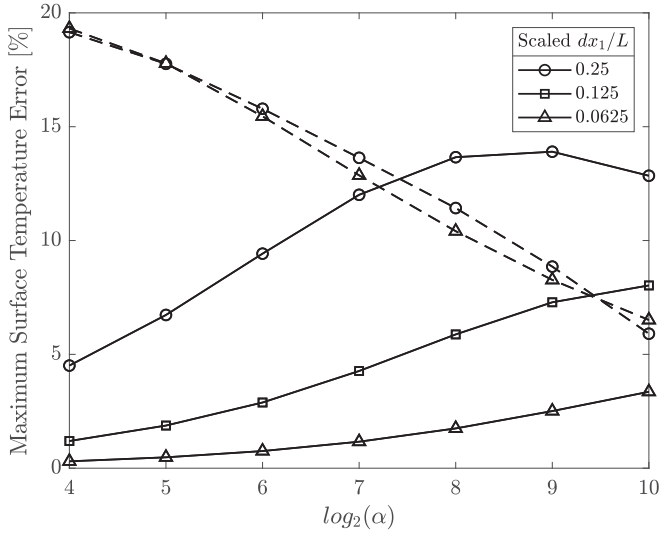

Fig. 4. Maximum surface temperature error as a function of forcing frequency for different spatial resolution, denoted by symbol shape. The scaled results are shown in solid lines and the proposed results are in dashed lines.

practical engine conditions with dx_1/L=0.0625, which corresponds to 10 total nodes in the 2 mm nearest the surface. The single-layer proposed method of Olmeda *et al.* shows a beneficial response of reducing error with increasing forcing frequency, but the results are not improved with increasing spatial resolution. In fact, Olmeda *et al.* define different material properties as the grid resolution is changed [1].

Overall, the method described herein is an improvement on that of Olmeda *et al.* because: its application only involves applying Eqs. (1) thru (4); it is based on the fundamental physics of the problem as compared to an *ad hoc* optimization procedure; and it performs better over all conditions tested.

Declaration of Competing Interest

There are no conflicts of interest to report.

References

[1] P. Olmeda, X. Margot, P. Quintero, J. Escalona, Numerical approach to define a thermodynamically equivalent material for the conjugate heat transfer simulation of very thin coating layers, International Journal of Heat and Mass Transfer 162 (2020) 120377.

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