Optimization of thermal barrier coatings in a single cylinder diesel engine using thermal analysis and genetic algorithm

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Abstract. A significant portion of the energy produced by combustion inside an engine is rejected as heat. Though it is impossible to prevent heat rejection, reducing the amount of heat rejected will help to increase the useful energy. Low heat rejection engine is a solution to these problems as they supply designers with insulation properties. In the design of adiabatic engines, reducing heat rejection in cylinder requires the use of special type of insulation often referred to as thermal barrier coatings in the combustion chamber of the engine. This insulation especially on engine piston is considered as a solution for the reduction of unburned HC emissions caused by incomplete combustion with respect to crevice volume when engines start. The insulation layer in effect reduces the thermal conductivity and raises the oxidation of the unburned charge such that the metallic substrates are exposed to lower peak temperatures, thus reducing the thermal stress in engine components. In this work piston is modelled using CATIA V5R16. For analyzing the effects of insulation layer on the piston, thermal analysis is conducted using finite element method in ANSYS after applying thermal boundary conditions. By changing the coating thickness and performing thermal analysis on each coating thickness followed by the use of mathematical operations enables the optimization of piston coating thickness. This optimized coating thickness is validated using Genetic Algorithm.

1. Introduction

The theoretical heat engine thermal efficiency is proportional to net heat transfer. However conversely, net heat transfer is proportional to heat rejected. Thus in order to raise the thermal efficiency, we have to decrease the heat rejection from the engine according to 2nd Law of Thermodynamics which is illustrated in figure 1.
Consider the above heat engine receiving an input heat ‘Q\textsubscript{h}’ from a source of temperature ‘T\textsubscript{h}’ and producing a work ‘W’ along with rejection of heat ‘Q\textsubscript{c}’ to a sink of temperature ‘T\textsubscript{c}’.

\[
\eta = 1 - \frac{Q\textsubscript{c}}{Q\textsubscript{h}} \tag{1}
\]

Maximum Efficiency is when \(\frac{Q\textsubscript{c}}{Q\textsubscript{h}} = 0\)

i.e., \(Q\textsubscript{c} = 0\).

Although this is impossible to achieve, efficiency could be increased if the heat rejected from the engine could be reduced, i.e. if \(Q\textsubscript{c}\) could be reduced efficiency improves. A Thermal Barrier coating (TBC) is employed based on this principle to achieve higher efficiency [1].

2. Low Heat Rejection Engine

Low Heat Rejection (LHR) Engine is provided with an insulation to reduce heat rejection [2,29]. It is accomplished by employing a Thermal Barrier Coating (TBC) to engine parts so as to avoid heat flow by increasing the thermal resistance at the contact surface between high-temperature combustion gases and metallic surfaces [14].

Ceramic coatings are widely used in industry to provide valuable wear, corrosion and erosion resistance [4]. Although coatings exhibit excessive variation and unpredictability in nature, thermal barrier coating in internal combustion engines is a subject of research for many investigations, in particular for reducing in-cylinder heat rejection of adiabatic engines because ceramic coatings show strong insulating properties [6]. The thermal barrier coating (TBC) technology is applied successfully in diesel engines, especially to the combustion chamber [11,3]. Thermal barrier coatings on different parts of an internal combustion engine like the piston have advantages including fuel efficiency, multi-fuel capability and high power density [3]. Insulating the combustion chamber can reduce not only the heat release but also promote thermal fatigue protection of the underlying metal surfaces [3].

3. Thermal Barrier Coatings

Usually thermal barrier coatings consist of two layers: bond coat and ceramic topcoat as illustrated in figure 2 [7,15]. Ceramic topcoat consists of Yttria-Stabilized Zirconia (YSZ), which is having very low conductivity and stable at moderate operating temperatures [8,17,18]. This ceramic layer produces
the TBC’s largest thermal gradient and holds the lower layers at a temperature lower than the surface [9,19]. Bond coat binds the ceramic top coat to the metal substrate [21,25].

4. Thermal Analysis
Thermal analysis refers to finding out the thermal effects on a particular body. The thermal effects include temperature and heat flux [13]. In this paper, the thermal analysis is done using the Ansys software on a ceramic coated piston.

Steps involved in analysis are:
1. Modelling
2. Material Property selection
3. Meshing
4. Applying Boundary conditions
5. Thermal analysis.

Thermal analysis of a particular thickness is performed. In a similar manner thermal analysis is performed on various coating thickness. With the resulting data collected from each thermal analysis, optimisation of coating thickness is done using suitable mathematical tool for the selected feasible thickness range [10].

4.1 Model
The piston part is modelled in the modelling software CATIA V5R16. Aluminium alloy piston model created using CATIA software of a single-cylinder compression ignition engine with and without thermal barrier coating is shown in figure 3 & figure 4.

![Figure 3](image1.png)  ![Figure 4](image2.png)

**Figure 3.** Uncoated aluminium alloy Piston.  **Figure 4.** Partially stabilised zirconia coated Piston.

The CATIA coated piston models for six different values of coating thickness within the selected feasible range are created. The different thickness values are- 125µm, 300µm, 450µm, 500µm, 800µm, 1000µm [5].

4.2 Material Properties
Piston is made of aluminium alloy and Partially stabilised zirconia (PSZ) is used as the coating material [5,20]. The material properties of aluminium alloy and Partially stabilised zirconia (PSZ) is shown in table 1.
4.3 Convergence Test
When the number of elements in the mesh increases, the results of a finite-element analysis would be more accurate [5]. But if we increase the number of elements beyond certain limit the processing time will be more. So there arises a need to attain an optimum number of elements. A trial and error approach is used to identify the optimal mesh size. The mesh size is varied and the maximum temperature obtained is shown in table 2. As the number of elements increase there is a change in the value of the maximum temperature [12]. Optimal mesh size is that at which the change in temperature is not so significant with respect to change in the element size.

The following table shows the variation in maximum temperature with number of elements and number of nodes.

| ELEMENT SIZE (mm) | NO OF ELEMENTS | NO OF NODES | MAX TEMP AT TOP |
|------------------|----------------|-------------|-----------------|
| 0.4              | 1422931        | 2259673     | 515.18          |
| 0.5              | 1121239        | 1786801     | 515.15          |
| 1.0              | 136965         | 230722      | 514.75          |
| 1.5              | 64382          | 110835      | 512.07          |

It could be inferred from the table that as element size is increased above 0.5 there is a large variation in maximum temperature. But for element size below 0.5mm there is not much change in maximum temperature. Thus it can be concluded that the optimum mesh size is 0.5mm using convergence test.

4.4 Validation of the results
The results obtained by conducting thermal analysis were validated as shown in figure 5 & figure 6 with the results in the reference journal by S.Vedharaj [5]. The maximum temperature and heat flux in the reference journal for 450µm coating thickness were 545.28°C and 1.261W/mm². Applying the same boundary conditions and material properties as in the reference journal we obtained the maximum temperature as 515.15°C and maximum heat flux as 1.411W/mm². The percentage of error is below 10%, so the analysis procedure was validated. The small variation in the obtained temperature and heat flux values may be due to the assumptions made in dimensions of curvatures of the piston model.
4.5 Thermal Analysis for Different Coating Thickness

The coating thickness was varied and the thermal analysis was conducted for each different coating thickness [16]. The thicknesses used within the selected feasible range were: 125µm, 300µm, 450µm, 500µm, 800µm, 1000µm. The models created in CATIA V5R16 were imported into ANSYS and then the analysis was performed. The procedure is same as said hitherto.

4.5.1 Temperature Distribution

The results of Temperature Distribution is shown in the figure 7.

![Figure 5. Temperature distribution validation.](image)

![Figure 6. Heat flux distribution validation.](image)

![Figure 7. Temperature distribution for (a)125µm, (b)300µm, (c)450µm, (d)500µm, (e)800µm and (f)1000µm.](image)
Finite element approach is used to find the Yttria-Stabilized Zirconia coated piston temperature distribution. Due to their low conductivity and their comparatively high thermal expansion coefficient, the zirconia-based ceramic coatings are used as thermal barrier coatings which reduce the detrimental interfacial stresses [4]. The most important issue with the coated device is the thermal stresses that arise during operation due to the substantial difference between the metal substrate thermal expansion coefficients and the ceramic coating. Because of the low conductivity and relatively high thermal expansion coefficient TBCs are preferred.

Phenomena of heat transfer in the diesel engine piston are complex. Therefore, it is believed that the main heat transfer mechanism between the combustion chamber and the piston surface is by convection in the thermal stress analysis [1]. A convection heat load like the radiation effect is applied to the surface of the piston crown [1]. That is, the convection heat load is increased to take radiation effect into account [1]. Using ANSYS, thermal analysis was performed to identify the temperature distribution as shown in figure 7 (a)-(f). The highest temperature is at the piston's sharp edge and the lowest temperature at the bottom of the piston bowl [28]. The highest temperature is at the piston's sharp edge since the lip has a much greater heat transfer area [30,28,4].

4.5.2 Heat Flux Distribution
Using ANSYS, thermal analysis was carried out to find the heat flux distribution as shown in figure 8 (a)-(f). Both the heat flux and the temperature were found to have a higher value on the piston's coated surface than on the metallic substrate, because the coated surface does not appear to allow heat transfer to the piston [5]. It is therefore very certain that the thermal efficiency and fuel consumption will be improved due to the reduced temperature and heat flux transfer into the piston [5].

![Figure 8. Heat flux distribution for (a) 125\mu m, (b) 300\mu m, (c) 450\mu m, (d) 500\mu m, (e) 800\mu m and (f) 1000\mu m.](image)

5. Thickness Optimization Using Thermal Analysis
The temperature and heat flux distributions for 125\mu m, 300\mu m, 450\mu m, 500\mu m, 800\mu m and 1000\mu m thickness was analysed. It was observed that as the thickness increases the insulating property of the coating increases, so heat conducted to the piston material decreases and more heat is obtained at the
top of coating. So temperature at the top of coating increases with thickness. So the need arises to find
the optimum coating thickness which would yield the best result. A thickness versus temperature
graph and thickness versus heat flux graph were plotted using MATLAB software using the maximum
temperature and maximum heat flux obtained for each thickness as shown in figure 9 and figure 10
[16]. As the thickness values are taken in unequal intervals, in order to find the maximum temperature
and maximum heat flux values for various thicknesses between the selected ones we use Lagrange’s
interpolation formula:

\[
f(x) = \frac{(x - x_1)(x - x_2) \ldots (x - x_n)}{(x_0 - x_1) \ldots (x_0 - x_n)} f(x_0) + \frac{(x - x_0)(x - x_2) \ldots (x - x_n)}{(x_1 - x_0) \ldots (x_1 - x_n)} f(x_1) + \ldots + \frac{(x - x_0)(x - x_1) \ldots (x - x_{n-1})}{(x_n - x_0) \ldots (x_0 - x_{n-1})} f(x_n)
\]

Taking \(f(x)\) as thickness and ‘x’ as heat flux, using equation 2 of Lagrange equation, it is possible to
express thickness as a function of heat flux by taking values from the results of analysis.

\[
f(x) = 5.90681 \times 10^6 x^5 - 4.09201 \times 10^7 x^4 + 1.13236 \times 10^8 x^3 - 1.56458 \times 10^8 x^2
\]

\[+ 1.07933 \times 10^8 x - 2.97373 \times 10^7\]

Increasing the thickness at the top of the piston reduces the heat conducted to the piston material [27].
The maximum heat flux obtained will decrease as the thickness of the ceramic coating thickness
increases [27]. A Thickness vs. heat flux graph was plotted using MATLAB software as shown in
figure 10.

**Figure 9.** Thickness vs. Temperature. **Figure 10.** Thickness vs. Heat flux.

Figure 9 shows that the maximum temperature at the top of the coated piston increases as the coating
thickness increases [3]. From the thickness vs. temperature graph, due to the approximate
proportionality between the temperature and thickness we are unable to obtain the accurate trend of the
graph. From the thickness vs. heat flux graph, we are able to determine the trend of the graph
accurately and obtain the optimum value of thickness as 125µm for a heat flux of 1.52 W/ mm².
Because although the maximum heat flux across the coated piston decreases with increase in
coating thickness from 125µm to 1000µm coating thickness, there is little variation in the 124-125µm
range. 125µm was identified as the local minima which is also the global minima in this case. So it
would not be economical to proceed with a higher thickness although there is more reduction in heat
flux at even higher thickness. Thus optimum thickness was obtained as 125µm. From thickness vs.
temperature graph the optimum temperature for corresponding optimum thickness value of 125µm was
found as 473.65 °C.
6. Optimization Using Genetic Algorithm

Genetic algorithms are heuristic searches that are inspired by Charles Darwin's theory of natural selection. It is based on the natural selection process in which the most suitable people are chosen by reproduction to create next-generation offspring in order to obtain the optimal solution [23, 26].

Objective function:

\[ f(x) = 5.90681 \times 10^6 \times x^5 - 4.09201 \times 10^7 \times x^4 + 1.13236 \times 10^8 \times x^3 - 1.56458 \times 10^9 \times x^2 + 1.07933 \times 10^{10} \times x - 2.97373 \times 10^7; \]

Optimization:

Optimizing using Genetic algorithm (GA) with lower bound = 1.18 & upper bound = 1.6.

\[ \text{heatflux} = ga(@\text{thickness}, 1, [], [], [], 1.18, 1.6); \]

Output:

\[ \text{heatlux} = 1.52 \# \text{optimum value of thickness was 125 µm for a heat flux of 1.52 W/mm}^2. \]

This type of search algorithm simulates a “Survival of the Fittest” scenario for each individual data generated. These generated data’s consists of individual points that contain possible solutions within the search space of the algorithm. Since genetic algorithm is an adaptive search algorithm, it is used for selecting the optimal value from a given set of values. In this case, we carry out Static thermal analysis of the piston with and without coating and determine a set of values for the heat flux and piston temperature with respect to the specific thickness of the coating applied to the piston. From this set of values, we use Genetic Algorithm method to obtain optimum value [23]. Optimum value of thickness was obtained as 125 µm for a heat flux of 1.52 W/mm² using Genetic Algorithm, which also validates the thermal analysis results.

7. Results

- By convergence test the optimum mesh size is found to be 0.5mm. The corresponding number of elements and nodes are 1121239 and 1786801 respectively.
- The temperature and heat flux values obtained was validated as shown in table 3 with the results obtained in the journal “Element and finite element analysis of coated diesel engine fuelled by cashew nut shell liquid biodiesel” by S.Vedharaj [5].

| Table 3. Convergence test results |
|----------------------------------|
| JOURNAL | RESULT OBTAINED |
|---------|----------------|
| Temperature(°C) | 545.28 | 515.15 |
| Heat Flux(W/mm²) | 1.261 | 1.411 |

- From the thickness vs. heat flux graph as shown in figure 10 and the genetic algorithm optimization method, the optimum thickness was found to be 125µm.

8. Conclusions

Greenhouse gas emission is a major threat to the very survival of planet Earth. According to NASA in the last 10 years the average global temperature has risen at the fastest rate. By incorporating an LHR engine we could solve two impending issues, increasing pollution and the alarming rate of depletion of fossil fuel [22]. The former is reduced by the reduced emission level of an LHR engine, albeit with a
caveat that NOx emission rises, and the latter is regulated due to reduced SFC of an LHR engine [24]. By conducting a thermal analysis on the piston, the optimum value of thickness was obtained as 125 µm for a heat flux of 1.52 W/ mm² and corresponding optimum temperature was found as 473.65 °C. The same optimum thickness was obtained using Genetic algorithm optimization method, which validates the thermal analysis results.

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