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Overview of Thermal Barrier Coatings in Diesel Engines

T.M. Yonushonis

An understanding of delamination mechanisms in thermal barrier coatings (TBCs) has been developed for diesel engine applications through rig tests, structural analysis modeling, nondestructive evaluation, and engine evaluation of various TBCs. This knowledge has resulted in improved TBCs that survive severe cyclic fatigue tests in high-output diesel engines.

Although much conflicting literature now exists regarding the impact of TBCs on engine performance and fuel consumption, changes in fuel consumption appear to be less than a few percent and can be negative for state-of-the-art diesel engines. The ability of the TBC to improve fuel economy depends on a number of factors, including the fuel injection system, combustion chamber design, and initial engine fuel economy. Limited investigations on state-of-the-art diesel engines have indicated that surface- connected porosity and coating surface roughness may influence engine fuel economy.

Current research efforts on TBCs are primarily directed at reduction of in-cylinder heat rejection, thermal fatigue protection of underlying metal surfaces, and possible reduction of diesel engine emissions. Significant efforts are still required to improve the plasma spray processing capability and the economics for complex-geometry diesel engine components.

Keywords diesel engine experience, failure behavior, mullite coating, thermal barrier coating

1. Background

THERMAL BARRIER COATINGS (TBCs) were initially investigated for "adiabatic" diesel engines due to first law thermodynamic predictions of significant fuel economy improvements, reduction in heat rejection, and potential increased power density of the diesel engine. Cummins Engine Company, Inc., conducted an extensive evaluation of existing TBCs using the Cummins V903 diesel engine. These initial exploratory efforts used duplex coatings consisting of a NiCrAlY bond coating and a yttria-stabilized zirconia (YSZ) top layer. Total coating thickness was on the order of 1.5 mm, with a bond coating thickness of approximately 0.1 mm. These investigations, conducted in the early 1980s, revealed that the existing TBCs were insufficient to survive short- duration tests in a high- output diesel engine (1.38 MPa brake mean effective pressures, or BMEPs) (Ref 1). Extensive trial-and-error development efforts using plasma-sprayed zirconia coatings did not result in acceptable or reproducible coating lives.

Efforts sponsored by the Department of Energy/National Aeronautics and Space Administration (DOE/NASA),U.S. Army Tank Automotive Command (TACOM), and Cummins internal funds in the mid-1980s focused on understanding the stresses in the TBCs with a goal of significantly improving the life of coatings in diesel engines. Improvements in TBC life of approximately two orders of magnitude were necessary for utilization of the coatings in advanced diesel engines.

An objective of the DOE/NASA program (Ref 2) was to develop zirconia-based TBCs with a thermal conductance of 410 $W/m^2 \cdot K$ that could survive 100 h of operation in a research single-cylinder engine. The engine chosen for this program was the Cummins V903 direct-injection diesel engine with a 140 mm bore and 120 mm stroke. The V-8 engine was rated at 360 kW at 2100 rev/min for the turbocharged configuration. The geometric compression ratio chosen for this work was 13.5:1, and the peak cylinder pressure was limited to a maximum of 13.8 MPa.

Extensive diesel engine cycle simulation and finite-element analysis of the coatings were conducted to understand the effects of a coating on diesel engine performance and the stress state in the coating and underlying metal substructure. The TACOM programs (Ref 3) expanded the effort initiated with DOE to develop improved TBCs that could survive the high cylinder pressures and thermal loads projected for military applications.

An engineered coatings approach was taken in the DOE program, using existing databases augmented where necessary by collecting additional data, modeling stresses in the coatings by finite-element techniques, and performing extensive rig and engine tests. Cummins and United Technologies Research Center (UTRC) cooperated on this program to modify thick TBCs developed for turbine tip seals for diesel applications.

T.M. Yonushonis, Cummins Engine Company, Inc., MC 50183, Columbus, IN 47202-3005, USA.

2. Coating Development for Diesel Engines

2.1 *Modeling*

Diesel engine performance modeling projected that the maximum benefits of TBCs were obtained by applying the coatings to piston and cylinder head surfaces. The effects of the coatings on valves and cylinder liners were not projected to result in significant fuel economy improvements. Therefore, research efforts in the DOE/NASA and TACOM programs concentrated on cylinder head and piston coating development. With the insulation levels defined by the coating thermal conductance, diesel engine performance models predicted that the in-cylinder heat rejection would be reduced by 38% and that the fuel economy would be improved by 2% for a turbocharged engine and by 3% for a turbocompound version of the engine.

United Technologies Research Center used one-dimensional thermal-structural modeling to select preferred coating systems for spray fabrication trials and rig tests. A one-dimensional thermal-structural model was established to predict both the temperature gradients across layer interfaces of candidate coating systems and overall coating state-of-stress at maximum operating conditions. Predicted temperatures from the thermal analysis were used to predict stresses within the coating systems under maximum operating conditions of a diesel engine. The modeling indicated that single-layer coating systems were in compression at the top of the coating and in tension at the bond/substrate interface (Ref 4). Previous single-layer coatings have been shown to delaminate in the zirconia coating in this tensile region above the bond coating.

It was determined that multilayer coatings, consisting of multiple layers of ceramic metal mixtures with a top coating of ceramic, reduce in-plane tensile stresses in the ceramic top layers. Figure 1 shows that the thermal stresses were significantly less than the measured coating strength. The coating was in compression at the top surface, which was 2.5 mm from the bond coating/ceramic coating interface. Metal substrates were also analyzed, and it was determined that substrate yielding should not be expected. Additionally, thermal modeling indicated that the metal temperatures were insufficient to result in bond coating oxidation in the short time that engine coating delamination was experienced in previous engine tests.

Two-dimensional finite-element modeling using the cycle average boundary conditions also suggested that a multilayer TBC could survive engine conditions. Efforts concentrated on understanding the performance of a 2.5 mm multilayer coating. This coating consisted of mechanical mixtures of CoCrAlY and zirconia fully stabilized by yttria. The 2.5 mm coating consisted of 0.5 mm layer of 40% zirconia and 60% CoCrAlY, followed by a 0.5 mm layer of 85% zirconia and 15% CoCrAlY, followed by a 1.5 mm thick 100% zirconia layer. The zirconia layer was approximately 85% dense. Processing conditions were developed to generate residual stresses in the TBCs by controlling the substrate temperature during the deposition process.

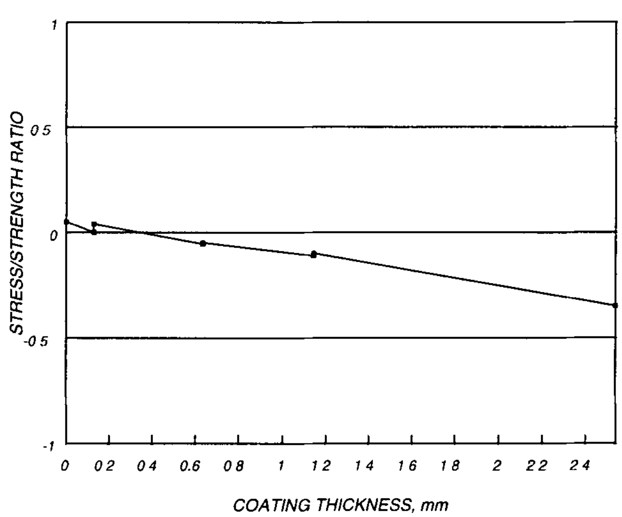

Fig. 1 Coating strength to stress ratio through the thickness of a multilayer zirconia-base coating

It is also important to consider thermal transients when designing with ceramic materials. The low thermal diffusivity of ceramics causes their temperatures to respond quickly to changes in operating environment, whereas the temperatures of the base materials respond much more slowly. This thermal response behavior causes significantly different temperature and thermal stress profiles to be encountered under transient operation than those observed at steady-state conditions.

The first thermal transient considered was a sudden cooling of the combustion face. Calculations were made at steady-state for conditions representative of full-load operation at rated speed. At time zero, the in-cylinder conditions were suddenly changed to those representative of no-load conditions. The resulting transient spatial thermal response within the coating is summarized in Fig. 2, where the surface temperature drops rapidly while the interior temperature reacts more slowly. With increasing time, the coating temperature decreases. The predicted thermal stresses in the coating are shown in Fig. 3. The trend shows a relaxation of the compressive stress at the surface with increasing time. This relaxation results in a slight reduction in the tensile stress experienced in the bond coat adjacent to the substrate. Cycle-to-cycle transients and rapid heating of the coating were also modeled.

It was determined through transient analysis using a simple finite-element model that:

- Temperature and stress profiles under transient conditions were found to be significantly different from those at steady-state conditions.
- Engine load changes, although resulting in a change in stress profiles, were not predicted to result in coating failure for the cases considered.
- Firing-cycle transients resulted in a predicted surface temperature swing of 225 °C and increased compressive stresses in the surface layers of the coating. These compressive stresses were predicted to be less than 0.13 mm into the coating.

2.2 *Spray Fabrication and Rig Tests*

United Technologies Research Center developed a spray fabrication technique to define material properties most representative of actual coating material. Flat-plate substrates were attached to a rotating holding fixture in areas representing the piston crown diameter. Heat was applied to the panels through the use of small propane torches mounted on a ring that surrounded the base plate. A thermocouple placed on the backside of the substrates provided the processing temperature and allowed for manual adjustment of the propane to maintain the desired prestress temperature through the spray run. The actual robot motion control and spray processing parameters used to coat the piston crowns were used to coat the substrates. Test specimens were fabricated from the substrates in locations indicative of the crown rim and center dome areas of the piston.

This approach was needed to verify uniformity of properties across the crown diameter.

Based on preliminary one-dimensional transient analysis performed by Cummins for the baseline multilayer coating on ductile iron, the rig thermal cycle was targeted to achieve a maximum surface temperature of approximately 675 to 730 °C, with a maximum thermal gradient across the coating of approximately 480 to 537 °C at a 7s time point into the cycle.

Test rig conditions were calibrated using the baseline multilayer coating system on a nickel-base superalloy test panel that had been instrumented with embedded thermocouples. A test cycle that closely reflects the predicted diesel engine thermal environment was created with a maximum thermal gradient across the coating of approximately 510 °C in 7 s and a top surface temperature of 675 °C. Two additional test cycles representing maximum thermal gradients of 555 and 705 °C, respectively, were used to further screen thermal strain capability at higher temperatures.

Ductile iron test panels with the baseline multilayer coating system were sprayed at both a medium fabrication temperature and a medium (hybrid) fabrication temperature that incorporated a temperature spike through the bond coat region. These panels were then exposed to the same thermal cyclic test conditions. The panel sprayed at the medium fabrication temperature was initially tested and survived the 510 °C thermal gradient. Examination of the panel after five cycles showed no visible damage. The panel was then subjected to the more severe 555 and 705 °C thermal gradients. No damage occurred after the 555 °C cycle; however, after the 705 °C cycle the coating showed moderate cracking at the 40/60 zirconia/CoCrAlY to 85/15 zirconia/CoCrAlY interface.

The panel fabricated at the medium (hybrid) prestress temperature profile was exposed to the 705 °C thermal gradient and exhibited minimum cracking sensitivity. These test results showed the superior strain capacity of the baseline multilayer coating system fabricated with the medium (hybrid) fabrication temperature control.

A prototype plasma spray facility with the capabilities needed to continuously apply multilayered TBCs was set up to coat Cummins V903 and L10 piston crowns and single cylinder heads (Ref 4). The facility was equipped with a six-axis articulating robot to provide gun motion control. Fixtures for holding diesel engine components were developed for simulations and actual hardware. The fixturing for the piston crown incorporated a flame shroud to allow the piston crown substrate to be heated during the spray processing to control fabrication temperature. A powder-feed delivery system was used to provide continuous feed rate control during coating deposition. This powder system was able to deliver four coating materials sequentially.

Spray process parameters to produce zirconia-base TBCs on V903 piston crowns and cylinder heads were developed by translating UTRC's experience in producing turbine seal coatings on curved duct segments. Fundamental issues included prestressing technology and special processing techniques needed to coat each of the specific diesel engine components.

Initial processing efforts focused on developing robotic control software for the plasma gun motion. Applying the coating system across the piston crown diameter proved difficult and variable due to the complex bowl geometry. Simulated piston crowns were machined and used to assess the magnitude of the coating thickness variation across the piston crown contour. A combination of single-layer and multilayer coating systems were sprayed on the simulated crown. The simulation was then sectioned and polished for metallographic examination of the thickness variation of the individual layers, particularly in the bowl area of the crown. Thickness measurements showed that the deposition was not efficient in areas away from the 90° spray angle. Movement of the plasma gun in a circular arc across the piston diameter and including a gun rotation into the wall area resulted in the highest degree of uniformity of thickness, microstructure, and properties across the crown diameter. Baseline robotic control parameters such as speed and program incre-

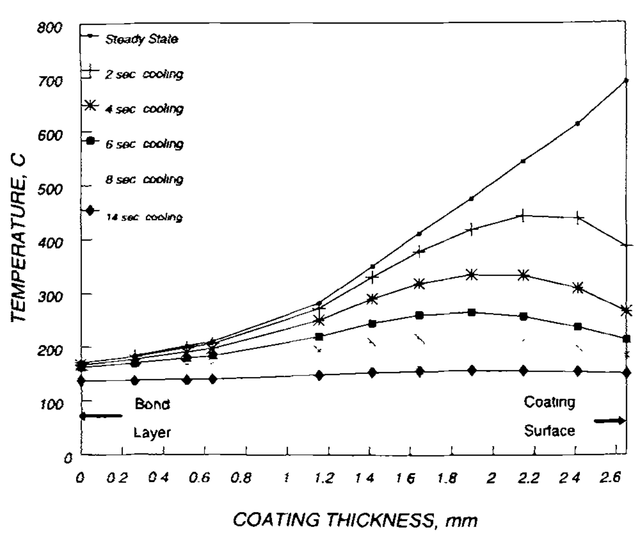

Fig. 2 Coating temperature changes during cooling from steady-state engine conditions

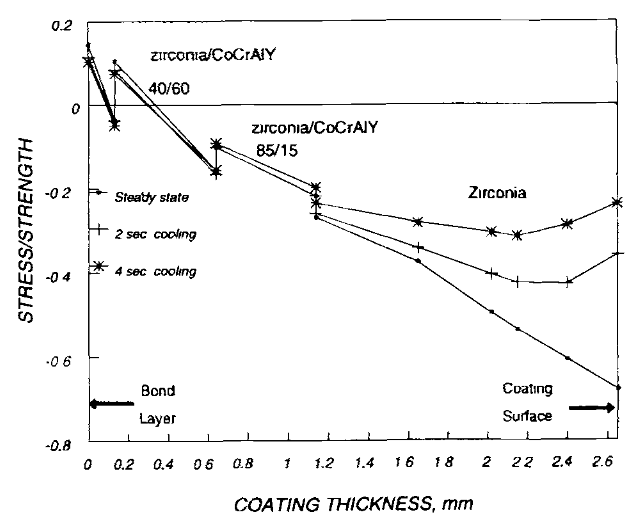

Fig. 3 Estimated stresses in a multilayer zirconia-base coating during cooling

ments were determined empirically by conducting a series of coating trials on piston crown simulations.

3. Engine Evaluation

Single-cylinder engine tests confirmed that the multilayer TBCs exhibited lives approximately an order of magnitude greater than the duplex TBCs. These multilayer zirconia-base coatings achieved the DOE/NASA contractual goals of 100 h at rated engine conditions, approximately 1.38 MPa BMEP, while meeting the thermal conductance goals of 408 $W/m^2 \cdot K$. However, engine fuel economy was not improved, and coating life capability was marginal. Further evaluation of similar multilayer zirconia coatings in a commercial L10 engine revealed that the coatings could survive steady-state operation at 1.38 MPa BMEP. However, cyclic tests resulted in coating deterioration and coating loss. Another problem was the observation that the zirconia coatings had open crack patterns at the surface of the coating, even though finite-element stress calculations predicted the coating to be in compression for the input boundary conditions. Additional improvements in coating life and capability were required for the technology to be commercially viable.

TACOM-sponsored efforts concentrated on the engine evaluation of TBCs on an articulated steel piston in a multicylinder L10 engine to further define coating durability at higher BMEPs, 1.83 MPa. Initial tests at steady-state operation confirmed that multilayer zirconia coatings would survive steady-state conditions for 200+ h. Cyclic tests were conducted between high-idle and full-power conditions. Coating loss was experienced in these cyclic tests. Further coating evaluation focused on the evaluation of the coating in cyclic tests conducted for 75 h, followed by removal of the cylinder head. Various zirconia multilayer coating strategies were evaluated, including varying residual stresses, using partially stabilized zirconia instead of fully stabilized zirconia, varying plasma gun power, and other coating changes. These modifications had essentially no measurable effect on coating life.

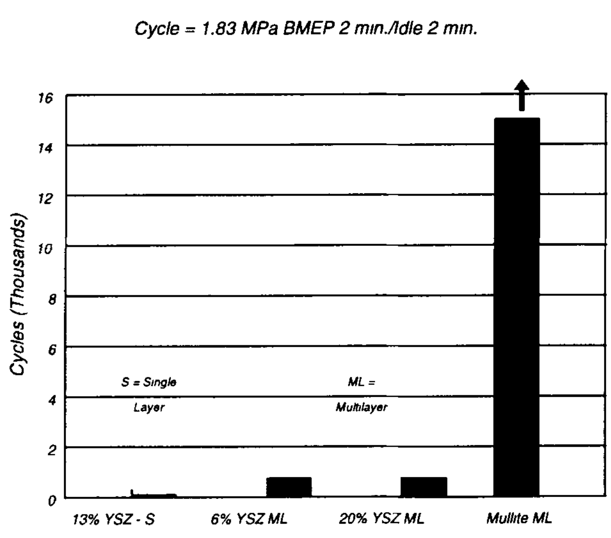

Fig. 4 Lifetime improvements in TBCs in cyclic diesel engine tests

Contrary to intuition and predicted stresses, a mullite-base multilayer coating was tested. Mullite was selected due to its lower thermal expansion and higher thermal conductivity compared to zirconia coatings. The mullite-base coatings had significantly improved performance compared to the zirconia-base coatings (Fig. 4). Diesel engine evaluation of zirconia- and mullite-base coatings has demonstrated that mullite coatings significantly outperform zirconia coatings in steady-state and cyclic engine tests. In multiple engine builds, the mullite multilayer coatings have survived transient conditions that have extensively damaged zirconia-base coatings.

4. Nondestructive Evaluation

Although state-of-the-art plasma control systems and robotics have been used to deposit TBCs, minor errors in plasma gun manipulation, concentric powder feed, and plasma alignment and slight changes in coating deposition rates can alter the coating structure and coating performance. Since TBCs are applied individually to the pistons and limited production studies have been conducted, a reliable coating inspection process is required. While the coatings were being developed, Cummins initiated efforts with Wayne State University to apply infrared imaging techniques to investigate and understand coating appearance before and after engine tests. Thermal wave imaging was found to offer significant advantages, including speed of data collection and user-friendly interpretation of the images (Ref 5). Destructive evaluation of the coatings confirmed that delaminations or coating inconsistencies were detected by the thermal wave imaging technique. Infrared imaging is currently used to inspect the TBC before and after engine evaluation at Cummins. This nondestructive evaluation technique has opened new areas of research and confirmed several hypotheses—one of which was that the center portion of the piston is difficult to coat and in selected cases was delaminated in the region prior to engine evaluation. Another hypothesis was that peak temperatures were critical in defining coating life.

5. Coating Crack Initiation

Although a gradual increase in coating durability was realized, coating life was still inadequate for many advanced diesel applications. A critical factor missing in many investigations was an understanding of the crack initiation and propagation mechanisms in TBCs. Purdue University and Cummins began an investigation to determine the mechanisms responsible for surface crack initiation at conditions that simulate the engine thermal loading conditions in a diesel engine (Ref 6-8).

A simple experiment was designed to simulate the boundary conditions imposed during diesel engine combustion. In direct-injection diesel engines, combustion of the fuel results in localized high heat flux regions on the piston and cylinder head. These areas of high heat flux concentration correlate with coating damage observed during diesel engine evaluation of TBCs. Previous analytical modeling had predicted that the TBC was in compression through all engine operating conditions. This resulted in a paradox, since crack opening due to tensile stresses was observed in TBCs. To understand the observations from diesel engine tests, an experiment was designed as a two-dimensional representation of the diesel engine combustion. An advantage of this specimen design was that during crack formation, the depth of the surface crack and the presence of interface cracks could be determined by low-power optical inspection. The specimens consisted of multilayer beam specimens with a concentrated heat flux in the center of the sample. The experiments and analysis were conducted on three specimen configurations.

The concentrated heat flux region was created by high-power infrared lamps. Temperature measurements were recorded at multiple points on the coating surface and the substrate. Tests were conducted by heating the specimen by turning the lamps on at full power and then maintaining a steady-state temperature for 2 h. A 2 h test time was used in order to allow the surface stresses to equilibrate. At the end of the test, the specimen was cooled to room temperature under natural convective cooling.

In order to understand the stress distribution in the specimens, analytical models of the specimens were developed using the finite-element method. The magnitude of the in-plane stress in the top layer governed the formation of the surface crack. The temperatures and stresses were calculated in four discrete steps:

- The residual stresses were calculated by assuming a uniform, stress-free temperature of 618 °C, which approximates the manufacturing temperature used in the coating deposition for the test specimens.
- The thermal stresses were calculated at steady-state temperatures based on measurements of the heat flux generated by the lamps.
- Stress relaxation was allowed to occur for a 2 h period.
- The specimen was uniformly cooled back to room temperature.

The stress relaxation of the zirconia was estimated using a strain gage mounted to the bottom of the substrate to measure the strain change as a function of time during steady-state heating.

Experimental measurements showed that the temperature of the coating surfaces reached approximately 870 °C for a thick zirconia specimen and 760 °C for a comparable mullite coating thickness. The stress relaxation was modeled (Ref 9) as $\varepsilon = A\sigma^n$, where $A = 4.03 \times 10^{-19}$ and $n = 1.59$ for zirconia at 870 °C, and $A = 2.98 \times 10^{-17}$ and $n = 1.1$ for mullite at 760 °C. Surface crack formation was observed in the thicker zirconia specimen, but was not observed in the thick mullite. Crack formation started at the zirconia surface, thus indicating that a tensile stress at the surface governs crack initiation behavior. In order to understand the thermal crack initiation behavior in the zirconia, the stress distributions were calculated analytically. The stress in the thick zirconia coating is compressive (at 200 MPa) near the surface. During heating of the zirconia surface, the zirconia coating surface reaches a much higher temperature than the metal underlying surface. The result of this thermal gradient is that the zirconia coating expands more than the underlying metal, which results in a large calculated compressive stress in the ceramic coating. However, at the higher temperatures, stress relaxation locally reduces the magnitude of the compressive stress. This stress relaxation results in a local tensile residual stress in the coating at room temperature. This operational-induced residual tensile stress is sufficient to crack the zirconia coatings.

The model suggests that the stress relaxation properties should be reduced to extend the service life of the coating. Since stress relaxation is highly temperature and material dependent, analysis was conducted for a mullite coating. The model predicts that the temperatures were not sufficient to induce cracking for the lower temperature and different mechanical properties of mullite.

6. Emissions and Engine Fuel Economy

An extensive data set of engine performance measurements has been made comparing a single-cylinder 1.67 liter diesel engine using steel articulated pistons with an insulated coating of YSZ or mullite (Ref 10). Measurements made on back-to-back

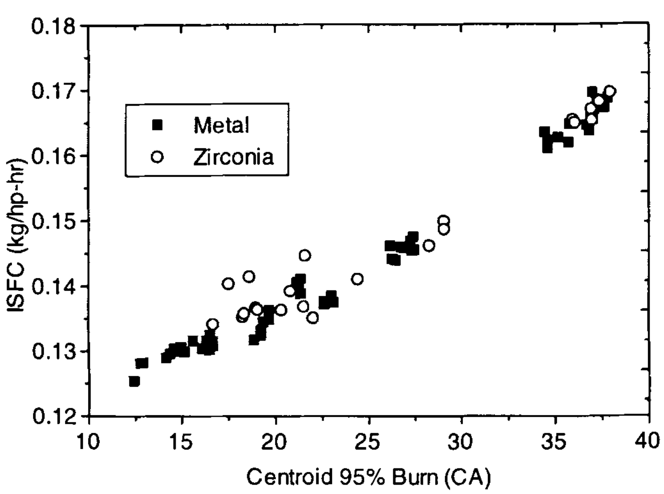

Fig. 5 Comparison of metal- and zirconia-coated pistons at 1800 rev/min and rated load. Indicated specific fuel consumption (ISFC) versus centroid of area where 95% of heat release has occurred.

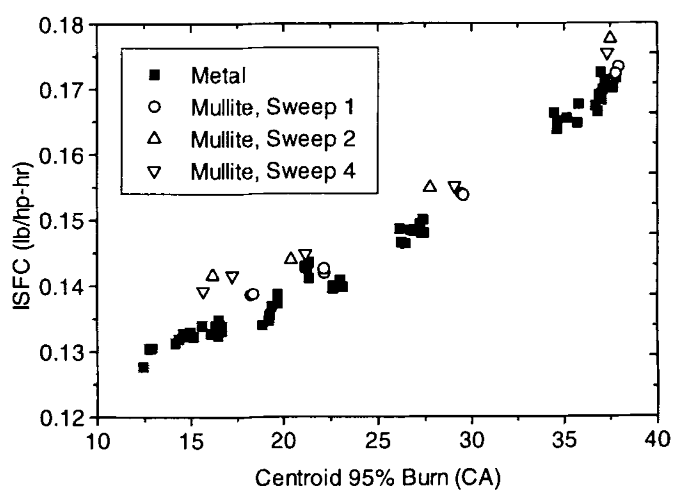

Fig. 6 Comparison of metal- and mullite-coated pistons at 1800 rev/min and rated load. Sweeps refer to specific timing sweeps when data were collected.

single-cylinder tests included cylinder pressure, brake torque, NO_x, unburned hydrocarbons, and particulates as a function of timing at four speed/load operating conditions. The effect on heat transfer of insulated pistons was determined based on indicated fuel consumption versus centroid of heat release curves. Engine performance using the zirconia-coated piston was measured to have 1 to 3% higher indicated and brake-specific fuel consumption in comparison to the baseline (Fig. 5). The difference between the two pistons was greatest at the most advanced injection timings.

The mullite-coated pistons displayed a fuel consumption increase that was as much as 8% at advanced timings (Fig. 6). Heat release was slightly extended for the zirconia pistons and extended even longer on the mullite pistons.

Error analysis of the measurement methods showed an uncertainty of ±3% in the indicated specific fuel consumption, and ±2 crank degrees in the centroid could be expected for this set of measurements. The data was thus inconclusive on the effect of insulation on heat transfer for the zirconia-coated pistons, but the mullite-coated pistons displayed a measurable reduction in indicated mean effective pressure, which was judged to be caused by increased heat transfer. Emissions for the insulated pistons showed similar NO_x particulate trade-off curves at retarded timings, but the particulate increased at advanced timings on the mullite-coated pistons. The zirconia-coated pistons displaced a slight increase in particulate and NO_x at advanced timings (Fig. 7).

7. Summary

Thermal barrier coating life has been significantly enhanced by understanding its control mechanisms. Initial diesel cycle average boundary conditions did not adequately represent the thermal loading applied to the TBC. Nondestructive evaluation based on the infrared imaging technique was instrumental in understanding the TBC structure as deposited and after engine evaluation. Thermal wave imaging confirmed that some coatings were delaminated prior to engine evaluation. This technique also confirmed that local thermal gradients tied to the diesel combustion process were causing localized damage. This information led to the development of a low thermal expansion mullite-base coating system (Ref 11), which had better thermal fatigue resistance than the zirconia coatings.

Use of robust TBCs permitted engine fuel economy and emissions data collection without complications from combustion chamber changes due to coating loss. Improvements in engine fuel economy and emissions performance were not realized for the state-of-the-art diesel engines evaluated. Metal temperatures underneath the coatings have been shown to be reduced, and this impacts the thermal fatigue life of these components.

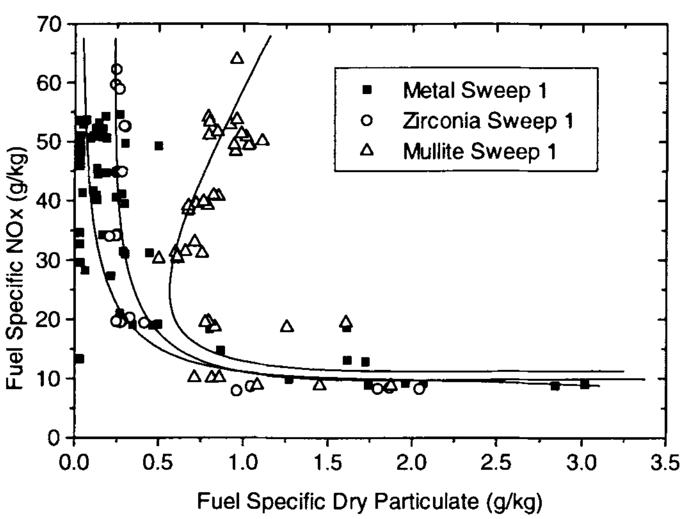

Fig. 7 Fuel-specific NO_x and particulate trade-off curve for metal-, zirconia-, and mullite-coated pistons at 1800 rev/min and part load conditions

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