1. HEAVY VEHICLE PROPULSION MATERIALS

Advanced materials are an enabling technology for fuel-efficient heavy-vehicle truck engines. The Heavy Vehicle Propulsion Materials Project is organized around the following technology issues: fuel systems; exhaust aftertreatment; air handling, hot section, and structural components; and standards.

Materials for Fuel Systems

The fuel systems for diesel engines are complex, expensive systems that are critically important to meeting the efficiency and emissions targets of the Office of FreedomCAR and Vehicle Technologies (OFCVT). Virtually every path to improving control of the combustion process in order to improve efficiency and reduce emissions depends on improvements in the fuel injection system.

Fuel injectors are highly precise. The individual components must fit together with clearances that are sometimes less than 1×10^{-6} meters. Control of the combustion process requires precise control of the size, shape, and surface finish of the injector components.

The current systems for reliably controlling multiple injections are limited by the ability of mechanical and electronic systems to respond precisely and quickly enough to provide additional injection control. Smart materials, such as piezoelectric materials, offer the potential for better control of fuel injection and have been recently introduced for automobiles. However, a number of improvements in materials and manufacturing methods for the materials are yet required for heavy vehicles.

Presently, the fuel system represents a significant portion of the cost of a heavy-duty diesel engine. Enabling materials and cost-effective, precision manufacturing processes are instrumental in developing improved fuel injection systems. In addition to new and improved materials, improved manufacturing and inspection methods for the injector components are being developed.

Manufacturing technology for nickel aluminide–titanium carbide cermet fuel system components continued this year in coordinated efforts at Oak Ridge National Laboratory (ORNL), Southern Illinois University–Carbondale (SIUC), CoorsTek, Inc. and Cummins, Inc. ORNL prepared a large batch of processed powder, which was provided to CoorsTek for injection molding of test components. The injection-molded components were then sintered at ORNL and provided to Cummins for testing in fuel injection systems. In a parallel effort, SIUC evaluated a low-cost, high-throughput process, continuous belt sintering, for manufacturing the cermet components. SIUC determined that rapid heating, at rates up to 750°C/minute, resulted in higher densities and more uniform microstructures and offers the potential to reduce sintering costs by as much as 50% by increasing part throughput.

Materials for Exhaust Aftertreatment

The reduction of nitrogen oxides (NO_x) and particulate emissions is critically important to OFCVT's program and is highly materials dependent. The U.S. Department of Energy (DOE) goals for improved efficiency of heavy vehicles are greatly complicated by engine design and exhaust aftertreatment technologies designed to meet the mandatory U.S. Environmental Protection Agency (EPA) emission regulations for 2007 and 2010. Materials and systems research is being conducted to minimize the potentially negative effects of emission-reduction technologies on fuel economy and to result in cleaner and more efficient engines.

Durability of exhaust aftertreatment systems in heavy vehicles is a concern. A lifetime of at least 500,000 miles is expected, and a 1,000,000-mile lifetime is desired (compared with 100,000 miles for automobiles). Exposure of the aftertreatment systems to high temperatures, vibration, erosion, and chemical attack by species in the oil and fuel results in degradation of performance. The effects of exposure in service on the microstructure and microchemistry of the aftertreatment systems are being characterized, and this research may lead to development of more durable systems. The development of advanced NO_x sensors is being conducted to facilitate optimal engine and aftertreatment control strategies.

Accomplishments this year included significant progress in a collaborative Ford–ORNL program intended to facilitate deployment of a NO_x trap for lean diesel or gasoline exhaust by (1) investigating materials issues related to deterioration of NO_x trap performance upon aging as a result of thermal and sulfation-desulfation cycles and (2) investigating materials that are robust under the lean NO_x trap operating conditions. The latter objective includes the synthesis of new materials. Accomplishments of this effort include completing a study of microstructural changes in a series of model catalysts during aging under lean and rich conditions at 500°C; beginning the updating of the ex-situ reactor to enable transmission electron microscopy (TEM) sampling under lean, rich, or stoichiometric conditions as well as lean-rich cycles; and equipping a new synthesis laboratory for the preparation of NO_x trap materials.

Research conducted at the High Temperature Materials Laboratory at ORNL is focused on the development and utilization of new capabilities and techniques for ultra-high-resolution TEM to characterize the microstructures of catalytic materials of interest for reducing NO_x emissions in diesel and automotive exhaust systems. This research aims to relate the effects of reaction conditions on the changes in morphology of heavy metal species on “real” catalyst support materials, typically oxides. Accomplishments included the characterization via high-resolution annular dark-field scanning TEM (STEM) that imaged the structure of a model NO_x trap material of near-atomic clusters and rafts of platinum atoms 1–3 atomic layers thick; characterization via TEM and STEM of core samples taken from catalyst monoliths removed from vehicles after up to 82,000 km of driving; and taking delivery of the new aberration-corrected electron microscope (ACEM), which will enable imaging of ultra-fine clusters of catalyst species on real catalyst samples of interest.

Exhaust aftertreatment materials projects are ongoing at both Caterpillar and Cummins. These projects are significant in that they represent a departure from an earlier culture in which the diesel engine companies relied heavily on catalyst manufacturers to provide the needed technologies and did not actively participate in the development of catalyst materials. These diesel engine manufacturers are actively collaborating with catalyst suppliers in the development of improved catalyst materials and are contributing to the development of a fundamental understanding of catalyst performance that is important to both suppliers and users of catalyst systems. In addition to the in-house efforts at Caterpillar and Cummins, Cummins and ORNL collaborated, via cooperative research and development agreements, in characterizing lab and engine-tested catalysts via X-ray diffraction, spectroscopy, and microscopy; and in characterizing diesel particulate filters and developing probabilistic design tools to predict the useful lifetime of the filters.

Ford Motor Co. and ORNL are collaborating on the development of a NO_x sensor that can be used in systems for on-board remediation of diesel engine exhaust. The sensor should have an operating temperature of 600–700° C and be able to measure NO_x concentrations from 1 to 1500 ppm at oxygen levels from 5 to 20 vol %. Prototype sensing elements are fabricated by patterning electronically conductive and catalytic layers onto oxygen-ion–conducting substrates. The sensing elements are characterized for NO_x response, oxygen sensitivity, and response time. Accomplishments this year included demonstrating NO_2 sensing elements with extremely high sensitivity; demonstrating biased NO-selective sensing elements; and constructing both types of elements to consist of co-planar electrodes, one of oxide and the other of a noble metal.

Materials for Air Handling, Hot Section, and Structural Applications

Engine design strategies for meeting EPA emission requirements have resulted in the need for significantly higher turbocharger boost. The higher boost requirements result in higher heat of compression and greater thermal and fatigue loads on turbocharger components.

Caterpillar began a new project in 2003 to design and fabricate a cost-competitive diesel engine turbocharger, using lightweight titanium materials, that provides a reduction in both fuel consumption and transient emissions. Caterpillar has designed a series turbocharger for use on the C15 engine platform. This turbocharger consists of one turbo wheel and two compressor wheels that are attached to a single rotating drive shaft. This compact design will replace the two-turbocharger system that is presently installed in the C15 engine. Titanium aluminide will be used for the turbo wheel, and one of the compressor wheels will be made from a titanium alloy. Accomplishments this year included procuring cast TiAl turbine wheels, developing friction welding technology for joining the turbine wheels to shafts and for realizing a higher joint strength than in the base TiAl wheel, and conducting preliminary turbocharger bench tests.

In a related project, Dynamet Technologies is conducting a research and development project to develop low-cost Ti-6Al-4V billet feedstock using a blend of titanium and alloy powders and inexpensive Ti-6Al-4V machine turnings. Dynamet has evaluated this low-cost titanium alloy feedstock as starting billet material for casting, forging, and extrusion operations and has produced high-density material in each case.

Caterpillar and ORNL won a 2003 R&D 100 Award for the development of CF8C-Plus cast stainless steel. The new high-temperature stainless steel may have near-term applications in diesel engine exhaust manifolds and turbocharger housings. Thermal-mechanical fatigue (TMF) of the initial commercial heats was completed this year, together with aging of various specimens. There was a significant advantage for CF8C-Plus relative to CN-12 or high-SiMo cast iron in TMF testing to 760°C. This year, MetalTek International produced additional static sand-cast and centrifugally-cast heats of CF8C-Plus for testing at Caterpillar and ORNL. That testing began this year and will be completed next year.

Caterpillar, in collaboration with Argonne National Laboratory and ORNL, has a project to design and fabricate prototype engine valves from silicon nitride and titanium aluminide materials that are 30% lighter than steel valves, provide a 200% increase in service lifetime, and potentially increase fuel efficiency in advanced engines by 10%. A probabilistic design approach was developed for the high-hardness valve materials. The friction welding of TiAl valve heads and Ti-6V-4Al valve stems was successfully optimized. The effects of surface finish on the performance of silicon nitride valves was evaluated and indicated that valves with good surface finish performed well in bench tests.

Caterpillar is also developing innovative approaches to thermal barrier and wear-resistant coatings for engines. Durability issues for thermal sprayed coatings, particularly thermal barrier coatings, remain the major technical challenge to their implementation in new engine designs. New approaches to coating design and fabrication are being developed to aid in overcoming this technical hurdle. Specific objectives are (1) to develop laser technology for surface dimpling, cleaning, and laser-assisted spraying to enhance adherence and increase coating strength; (2) to develop phosphate-bonded composites for thermal management coatings; and (3) to evaluate quasicrystalline materials as potential thermal barrier and wear coatings. This year, a cost analysis of laser pre- and post-treatments was conducted, and post-laser tacking was selected as the method for treating coatings to increase adherence. Phosphate-bonded composite coatings survived thermal cycling to 650°C with good residual adherence to the substrate. Quasicrystalline coatings were sprayed using the high-velocity oxygen-fueled technique, and evaluation began. In a collaborative effort, ORNL demonstrated the use of high-density infrared surface treatment as a means of producing hard-metal coatings with low porosity.

The feasibility of reducing the weight of a heavy-duty engine by substituting a lighter material for the cast iron engine block and cylinder head was evaluated by ORNL and Ricardo, Inc. Finite element analysis was used to compute the stresses, temperatures, and fatigue safety factors of a 5.9-L diesel engine, run at the maximum design power, for three lightweight casting alloy systems: titanium, aluminum, and magnesium. The analysis indicated the feasibility of simple material substitutions in all cases, with the exception that the titanium alloy cylinder head will require inserts to reduce the temperature in the valve bridge area. Reducing the weight of the entire engine by up to 33% for the magnesium alloy and 20% for the aluminum alloy, and up-rating the power of the engine by 50% while reducing the weight by 15% for the titanium alloy, were predicted to be feasible.

Efforts in cost-effective manufacturing were carried out by ORNL, the University of Michigan, and Purdue University. Technology for machining difficult materials, such as titanium alloys, was developed in the ORNL/University of Michigan collaboration. ORNL investigated surface modification of lubricated ceramic parts for applications in fuel systems and related applications. Purdue University is investigating the consolidation of low-cost machining chips to produce nanocrystalline components with high strength and hardness.

In a new effort this year, ORNL is investigating the plastic deformation behavior of industrial ceramics and the potential for low-temperature forming of components. In collaboration with Pennsylvania State University, a novel sintering method was developed to fabricate nanocrystalline (less than 100-nm grain size) zirconia ceramics. Enhancement of the plastic deformation of sub-micron zirconia in applied electric fields was observed in collaborative work with North Carolina State University. ORNL also established dynamic indentation and instrumented scratch testing facilities and associated finite-element analysis models to characterize and model contact-induced damage and its links to wear performance and to the optimization of machining and rolling contact fatigue.

Materials and Testing Standards

OFCVT has an International Energy Agency (IEA) “Implementing Agreement for a Programme of Research and Development on Advanced Materials for Transportation Applications” (IA-AMT). The objectives of the IA-AMT are as follows:

1. to identify and evaluate promising new processing and surface engineering technologies capable of improving materials performance in transportation systems and
2. to promote and implement pre-competitive development and verification of advanced characterization methods appropriate for advanced materials for transportation applications.

Annex III, which was approved in July 2002, consists of two subtasks on contact reliability of advanced engine materials including structural ceramics, composites, and nanostructured friction/wear coatings. Subtask 1 is an information exchange, and Subtask 2 focuses on the development of standard test methods and procedures for determining the rolling contact fatigue resistance of advanced materials. At present, the active contracting parties for the IA-AMT are Germany (Bundesanstalt für Materialforschung und–prüfung), Canada (CANMET), United Kingdom (Department of Trade and Industry), and the United States (DOE).

A new activity to be conducted under the IEA program was initiated last year by the National Institute of Standards and Technology (NIST). The objectives of this new effort are as follows:

1. organize an international cooperative research program on an integrated surface modification technology under the auspices of the IEA
2. design and identify surface features and patterns that can achieve friction reduction and enhanced durability for heavy-duty diesel engine components
3. develop understanding and appropriate models to explain texturing effects on frictional characteristics
4. develop appropriate thin films and coatings to achieve a synergistic and complementary relationship with texturing to enhance performance
5. discover and develop surface chemistry for protecting the films and coatings that work in synergy with the textures

Accomplishments this year include the development of a new design principle for surface texture design to enable friction reduction under boundary lubrication conditions.

NIST also leads a project to develop standard testing methods for advanced materials, primarily ceramics. Step by step, we are building a national and international standards infrastructure to facilitate the commercial utilization of new advanced materials in engine applications. The generic test method standards developed to date have proved to be so practical, reliable, and versatile that they are now being used to support a wide range of applications, including surgical implants in humans and even ceramic military body armor. In FY 2004, the pre-standardization work on the flexural strength of split cylinders was completed, a NIST *Guide to Practice on Fractographic Analysis of Brittle Materials* was 50% completed, and several standards from the American Society for Testing and Materials and the International Organization for Standards were revised.

The rolling contact fatigue (RCF) effort is led by ORNL. Its objectives include the characterization of the RCF performance of ceramics and tribological coatings; determination of the effects of subsurface damage, microstructure, material properties, and contact stress on RCF performance; and correlation of RCF performance measured by different internationally-used RCF test techniques. In FY 2004, a three-ball-on-rod test facility was established and informal collaboration was initiated with Bournemouth University in the United Kingdom.

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