# August 2015 Highlights

## ORNL Fuels, Engines, and Emissions Research Center

### TECHNICAL HIGHLIGHTS

**Journal Paper to Report the Oak Ridge National Laboratory's (ORNLs) Recent Discovery of Incompatibility between Diamond-Like Carbon (DLC) and Zinc Dithiophosphate (ZDDP)**

Y. Zhou, D. N. Leonard, H. M. Meyer, H. Luo, and J. Qu, "Does the Use of Diamond-Like Carbon Coating and Organophosphate Lubricant Additive Together Cause Excessive Tribochemical Material Removal?" in *Advanced Materials Interfaces*, 2015, DOI: 10.1002/admi.201500213. An unexpected but interesting observation at an interface between steel and DLC in the presence of phosphate-based lubricant additives was recently discovered at ORNL. DLC coatings have demonstrated excellent tribological and mechanical properties with great potential in many industrial applications. Phosphate additives, such as conventional ZDDP and newly developed ionic liquids, are known to be very effective in wear protection of steel bearing surfaces. One natural question is what happens when DLC coatings are used together with anti-wear additives? In this study, we discovered significantly increased wear rate on a steel surface that rubbed against DLC when and only when lubricated by phosphate-based anti-wear additives. Very limited literature (only two papers) had touched base with this detrimental effect with an unproved hypothesis that a competition existed between ZDDP-produced tribofilm and DLC-induced carbon transfer. Our experimental results however are clearly contradictory to the literature hypothesis and we instead propose a new mechanism for such excessive material removal based on carbon-catalyzed chemomechanical interactions, which is supported by surface characterization. Such interfacial phenomena is important not only for fundamental understanding but also for technology implementation.

**The Fuels, Engines, and Emissions Research Center (FEERC) Holds Summer Student Research Symposium**

On August 5, 2015, six of FEERC's summer researchers presented brief, summary presentations of their completed work, as well as the future outlook for the projects that will continue under their FEERC mentors. This was a great opportunity for the science and engineering students to succinctly describe their work to our fuels, engines, and emissions-focused audience and thereby understand their research more clearly. What's more, it was a worthwhile chance for the early, mid-, and advanced ORNL-FEERC research professionals to hear about the exciting perspective our student researchers bring to the innovation table. This is the fourth year in a row that FEERC has hosted a dedicated summer student research symposium.

***Mechanical Engineering Magazine* mentions an ORNL Lube Oil Project**

An article in the September 2015 issue of *Mechanical Engineering Magazine* mentions the work of several national laboratories (including ORNL) in the area of lubricant technologies. ORNL is mentioned as a contributor on a collaborative project with Pacific Northwest National Laboratory (PNNL). The project was awarded two years ago through a competitive Funding Opportunity Announcement by the Department of Energy (DOE). PNNL is developing a new oil additive to enable increases in engine efficiency through friction reduction. ORNL's FEERC and High Temperture Materials Laboratory are supporting the project with fundamental friction measurements and

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ORNL is managed by
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demonstration of the fuel efficiency benefit of candidate lubricants in modern engines. ORNL's Scott Sluder and Jun Qu were interviewed for the article.

**ORNL Compatibility Study Reveals Dimethyl Ether (DME) to be Highly Compatible with Many Existing Fuel Components**

A solubility analysis was performed for DME (and its blends with diesel) to assess its compatibility with elastomers and plastics used in fuel storage and delivery systems. Of the elastomer materials, silicone, neoprene, and polyurethane exhibited similar solubility values for both diesel and DME (and blends of each). Interestingly acrylonitrile butadiene rubber (NBR), which is a common seal and fuel hose material, showed pronounced improvement in compatibility with DME content, especially for concentrations exceeding 20%, and in fact, neat DME can be expected to produce only modest swelling in these materials. In contrast, fluorocarbons (which have replaced NBR seals in systems exposed to E10 and E85) were shown to be less compatible in DME. These findings are important because they show that high cost fluorocarbons are less compatible than low cost NBRs when exposed to DME and its blends with diesel. Results for the plastic materials show that for many plastics the compatibility improves with DME content (compared to neat diesel fuel). Notable exceptions include high density polyethylene, polypropylene, and PTFE. PTFE (or Teflon) is a common high performance plastic material and its use may need to be precluded for use with DME and its blends with diesel fuel. The analysis indicates that DME should be highly compatible in existing engines and fuel dispensing infrastructure.

## High-Level or Noteworthy Visits

**FEERC Hosted Professor William Epling from the University of Houston**

Professor William Epling, from the University of Houston's Department of Chemical & Biomolecular Engineering, visited ORNL's FEERC on August 19 and 20. Prof. Epling has been working with FEERC staff for over a decade on emissions control technologies for high efficiency engines. During his visit, he met with FEERC's Melanie DeBusk and Jim Parks to discuss results related to their DOE-National Science Foundation (NSF) joint project on Pt-Pd bimetallic diesel oxidation catalysts (DOCs). He also met with Josh Pihl to discuss synthetic exhaust flow reactor designs for measuring the performance and properties of three-way catalysts (TWCs). Professor Epling also gave a seminar on ongoing research at the University of Houston and participated in a discussion of future collaboration opportunities.

**Korea Electric Power Corporation (KEPCO) Research Institute visits ORNL to Discuss Collaboration Opportunities in Diesel DeNOx/DeSoot System Research**

KEPCO visited FEERC on August 26 and presented their project on development of NOx and soot abatement technologies for diesel generators deployed in South Korean islands. The visitors toured FEERC laboratory facilities, learned about ORNL expertise and programs related to diesel catalyst research and development, and discussed collaboration opportunities. ORNL participants included Jim Parks, Bill Partridge, Todd Toops, Josh Pihl, and Jae-Soon Choi.

**Sandia Senior Manager Visits ORNL**

Dr. Art Pontau, Senior Manager of Combustion and Industrial Technology at Sandia National Laboratories, visited FEERC and the Buildings Technology Integration Center. The purpose of his visit was to discuss ongoing and new collaborations between ORNL and other national laboratories as part of the DOE Optima Initiative and to explore future collaborative opportunities in the buildings area.

## Invited Talks and Presentations

**FEERC Researcher Invited to Present Historical Analysis of the Co-Evolution of Light-Duty Fuels and Engines to Fiat Chrysler Automobiles (FCA)**

FEERC researcher, Derek Splitter, was invited to FCA to present results from a deep literature review encompassing engine, vehicle, and fuel data since 1925. The findings examined historical and recent coupling between compression ratio and fuel antiknock properties (i.e., octane number) in the United States (U.S.) light-duty vehicle market. The analysis identified historical timeframes, trends, and illustrated how three factors affect personal mobility: consumer preferences, technical capabilities, and regulatory legislation. Data showed that throughout history these three factors have a complex and time sensitive interplay. Long term trends in the data were identified where interaction and evolution between all three factors was observed. Specifically, transportation efficiency per unit power (gal/ton-mi/hp)

was found to be a good metric to integrate technical, societal, and regulatory effects into the evolutional pathway of personal mobility. From this framework, discussions of future evolutionary changes to personal mobility are also presented, including potential opportunities to increase fuel octane though bio-fuels.

**FEERC Staff Member Presents at an International Energy Agency (IEA) Meeting in Scotland**
Jim Szybist presented his research at the IEA Task Leader Meeting on Combustion in St. Andrew's, Scotland. The well-received presentation highlighted the original approach to fuel reforming to support highly dilute combustion for high efficiency. Participation in the 4-day meeting included representatives from 14 member countries on a wide array of combustion-related topics.

**FEERC Staff Present Results at Advanced Engine Combustion Program Review Meeting**
FEERC researchers presented four technical presentations at the Advanced Engine Combustion Program Review Meeting in Southfield, Michigan, on August 18–21, 2015. This semi-annual meeting is organized by Sandia National Laboratory and provides opportunity for researchers to present results from ongoing DOE-funded efforts to DOE and industry stakeholders and to receive vital feedback on the direction of their efforts. Dean Edwards presented work from FEERC efforts supporting the Daimler SuperTruck Program entitled "Exploring the Potential Benefits of High Efficiency Duel-Fuel Combustion on a Heavy-Duty Multi-cylinder Engine." Adam Dempsey presented results from recent simulation efforts entitled "Computational Fluid Dynamics Modeling of Gasoline Compression Ignition Combustion." Brian Kaul presented "Impact of Temporal Variations of EGR Gas Properties on Feedback Timescales for Next-Cycle Control of Cyclic Variability" with results from recent experimental studies. Derek Splitter provided an update on recent injector visualization campaigns at ORNL's High Flux Isotope Reactor (HFIR) entitled "Dynamic Neutron Imaging of GDI-based Fuel Injection."

**FEERC Presents to DOE Transportation Working Group (TWG)**
FEERC Director Robert Wagner presented on the ORNL-led Virtual Vehicle Initiative to the DOE TWG. The TWG consists of transportation leads from the national laboratories. He presented on the opportunities and challenges of developing a vehicle systems simulation framework which makes use of DOE Leadership computing resources such as Titan. Robert, Ron Graves, and Sreekanth Pannala led a stakeholder meeting on this topic in Southfield, MI earlier this year. They are currently planning a broader industry workshop for this fall.

## AWARDS

## OUTREACH