July 2014 Highlights

ORNL Fuels, Engines, and Emissions Research Center

TECHNICAL HIGHLIGHTS

The Oak Ridge National Laboratory (ORNL) Contributes to the National Academy of Sciences Review of Medium- and Heavy-Duty Vehicles

Jim Parks participated in a panel discussion at the National Academy of Sciences "Meeting of the Committee on Assessment of Technologies and Approaches for Reducing the Fuel Consumption of Medium- and Heavy-Duty Vehicles." Dr. Parks presented ORNL research in advanced combustion and emissions control that affect the trade-off between NOx emissions and fuel economy.

ORNL and Industry Partners Launch Multiple Predictive Engine-Simulation Efforts on Titan Supercomputer

Over the summer, ongoing efforts by ORNL researchers and industry partners to develop innovative strategies to accelerate advanced engine design have led to several simulation campaigns on the Oak Ridge Leadership Computing Facility's flagship machine, Titan. Work at ORNL supported by the Department of Energy (DOE) Vehicle Technologies Office (VTO) developed a novel approach to use massive parallel simulations on high performance computing resources to study the inherently serial problem of cycle-to-cycle combustion variations in internal combustion engines. ORNL and Convergent Science have partnered with Ford to apply this new approach to investigate highly dilute operation of light-duty engines and with General Electric (GE) to investigate dual-fuel operation of locomotive engines. During June and July 2014, ORNL researchers transferred the knowledge and methodologies developed during the DOE study enabling Ford and GE to launch simulation studies on Titan. Additionally, ORNL, Ford, and Convergent Science received an additional 17.5Mhrs on Titan through a DOE ASCR Leadership Computing Challenge (ALCC) award beginning in July to continue improving the approach and explore the impact of key engine operating parameters on combustion stability. Efforts to accelerate and optimize fuel injector design also continue through a second ALCC allocation of 15Mhrs awarded to GM, ORNL, and Convergent Science. Simulations were launched on Titan in July coupling internal flow and cavitation predictions from GM's OpenFOAM injector model with in-cylinder mixing and spray evolution using Convergent Science's CONVERGE computational fluid dynamic (CFD) software.

ORNL Researchers Discover that Natural Gas Ignition and Combustion is Facilitated with Localized Oxygen Introduction

Researchers at ORNL and the University of Tennessee are evaluating the effects of introducing small quantities of oxygen to the spark plug gap of methane and air mixtures. Recent studies have shown that the introduction of 0.004 grams of oxygen to the flame kernel can increase the pressure rise rates and peak pressures for equivalence ratios of 0.6 and 0.54. For starting pressures of 4.8 bar (70psi) and less, the peak pressure increased from 5.9 bar (85 psi) to 13.9 bar (201 psi) with the introduction of oxygen. At 6.9 bar (100psi), the peak pressure was unchanged, but the pressure rise rate was still much higher when oxygen was added. Analysis of the emitted infrared spectrum indicated the presence of a highly reactive triplet state of oxygen. Raising the ground state of oxygen molecules (in the flame kernel) to one or more excited states is believed to be responsible for the observed increase in combustion pressure rise and peak values.

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HIGH-LEVEL OR NOTEWORTHY VISITS

Nissan Representatives Tour the Fuels, Engines, and Emissions Research Center (FEERC)
Two representatives from Nissan in Smyrna, Tennessee, visited to tour FEERC, Power Electronics and Electric Machinery Research Center (PEEMRC), the Vehicle Simulation and Integration Laboratory, and other ORNL facilities related to transportation. The tour contingent also included local representatives from AUTOXLR8R, a Southern Middle Tennessee Entrepreneur Center dedicated to identifying promising new technologies and helping them get commercialized.

INVITED TALKS AND PRESENTATIONS

FEERC Staff Attend Biomass 2014
Brian West and Stuart Daw attended the Biomass 2014 Conference, "Growing the Future Bioeconomy," sponsored by the Bioenergy Technologies Office. Mr. West spoke during the breakout session on Building the Market for Renewables with High Octane Fuels, highlighting the potential benefits of a future high-octane gasoline that could make better use of biofuels. Dr. Daw presented a poster along with his National Renewable Energy Laboratory (NREL) colleagues detailing the modeling activities being conducted under the Computational Pyrolysis Consortium. In the consortium, computational fluid dynamics are being used to improve the yields and quality of renewable fuels generated by catalytic upgrading of biomass pyrolysis oils.

FEERC Staff and Students Participate in University of Alabama Sustainable Fuels Workshop
FEERC director Robert Wagner, FEERC researcher Scott Curran, and two summer research interns Michelle Edwards and Karson Stone participated in the "2014 Technical Workshop on Sustainable Fuels: Production and Combustion" at the University of Alabama's Institute for Sustainable Energy. Robert Wagner was invited to speak on the next generation combustion engines and future fuels opportunities while Scott Curran was invited to present a well-to-wheels analysis of natural gas options for transportation. Michelle Edwards and Karson Stone presented a well-to-wheels analysis of dimethyl ether that is being completed at ORNL over the summer. The workshop was well attended from regional experts in combustion and fuels not only in transportation but in the industrial and energy production sectors.

AWARDS

FEERC Researchers receive two Research and Development (R&D) 100 Awards
Ionic Liquid Anti-wear Additives for Fuel-efficient Engine Lubricants was developed by ORNL, General Motors Research and Development Center, Shell Global Solutions, and Lubrizol Corp. ORNL principal investigators were Jun Qu, Huimin Luo, Sheng Dai, Peter Blau, Todd Toops, Brian West, and Bruce Bunting. The technology employs a group of ionic liquids that can be mixed with common lubricating oils to form a nanostructured protective film on bearing surfaces that effectively reduces friction and wear. This ionic lubricant technology has the potential to save the United States millions of barrels of oil each year. The research was sponsored by DOE's Office of Energy Efficiency and Renewable Energy, VTO. *The RF-DPF Diesel Particulate Filter Sensor* was developed by Filter Sensing Technologies Inc. (FST) and in collaboration with ORNL and Massachusetts Institute of Technology. The ORNL team consisted of James Parks II, Vitaly Prikhodko, and John Storey. The RF-DPF is a radio frequency-based sensor and control system used to measure the amount, type, and distribution of contaminants on filters. This technology provides rapid real-time assessment of soot on diesel particulate filters which allows greater precision in filter control thereby reducing fuel consumption and greenhouse gas emissions. The RF-DPF can be used with light- and heavy-duty diesel vehicles and may enable longer filter life and overall system cost savings. The project was funded by FST and DOE VTO.

FEERC Postdocs Participate and Win Award at ORNL 2nd Annual Postdoc Research Symposium
On July 10, 2014, ORNL held its 2nd Annual Postdoc Research Symposium. Three postdocs from FEERC participated in the symposium through posters and presentations. Ben Lawler presented a poster entitled "High Frequency Vibrations in an Engine Block." Dr. Lawler's work applies signal processing techniques to high speed accelerometer data to study the vibrations in an engine block imparted by engine cycle events (i.e., valve events, fuel injection, combustion, etc.). Chao Xie presented a poster entitled "Impact of Metal Fuel Impurities on Diesel Engine Emissions Control." Dr. Xie's work investigates the impact of metal impurities such as K, Na, and Ca in biofuels on the performance of exhaust aftertreatment catalysts. Will Brookshear presented a poster entitled "Effect of Fuel-borne Sulfur on Cu/zeolite NOx-SCR Catalyst Performance and Material Characteristics." Dr. Brookshear's objectives are to determine the sulfur durability of small-pore Cu-zeolite selective

catalytic reduction (SCR) catalysts for NOx abatement in marine diesel engines. Adam Dempsey gave a presentation entitled "Particulate Matter from Reactivity Controlled Compression Ignition (RCCI)." Dr. Dempsey's talk was on the volatile and solid content of the particulate matter (PM) from RCCI combustion and how the PM composition changes with engine operating conditions. Dr. Dempsey was awarded honorable mention for his presentation out of a total of 34 presentations given.

OUTREACH

FEERC Hosts Appalachian Regional Commission Summer Science Institute

High school students, their teachers, and mentors toured ORNL's National Transportation Research Center this month. The student and teacher researchers are selected from eligible counties in 13 Appalachian Region states from New York to Mississippi. Their time spent at ORNL is designed to motivate the students to continue their science education beyond high school, and to help teachers bring practical examples back to the classroom. The group visited FEERC to learn about the applied R&D aimed at reducing the nation's dependence on petroleum. The tour also included stops at the PEEMRC, the Vehicle Systems Integration Laboratory, the Battery Manufacturing Laboratory, and the Manufacturing Demonstration Facility.