Technical Highlights for November 2011

Development of a Transient Spaci-IR Technique for Spatially and Temporally Resolved Measurements of Gas Concentrations inside Aftertreatment Catalysts

Researchers at the Oak Ridge National Laboratory's (ORNL's) Fuels, Engines, and Emissions Research Center (FEERC) have added a new tool for investigating the detailed chemistry that occurs inside aftertreatment devices such as selective catalytic reduction (SCR) and lean nitrogen oxide (NO_X) trap (LNT) catalysts. Similar to the Research and Development (R&D) 100 Award winning Spaci-MS technique, Spaci-IR uses a capillary to sample the gas from a specific point inside a catalyst monolith channel. However, instead of a mass spectrometer, Spaci-IR uses a Fourier-transform infrared (FTIR) spectrometer to analyze the composition of the sampled gases. The use of FTIR minimizes the challenges associated with cross-sensitivities that often complicate mass spectrometry measurements. While Spaci-IR was initially developed by one of our university collaborators (Prof. William Epling, University of Houston), the initial implementation suffered from slow instrument response and its utility was limited to measuring steady-state concentration profiles. FEERC researchers developed a new sampling system for Spaci-IR that reduced response time by an order of magnitude, enabling measurement of transient phenomena. Spaci-IR is currently being employed to measure spatial on-board ammonia (NH_3) storage distributions under SCR operating conditions in a commercial NH_3 SCR catalyst.

Emissions Adsorption at Cold Start: An Energy-Efficient Emission-Control Strategy for Hybrid Electric Vehicles and Plug-in Hybrid Electric Vehicles

The emissions control during the cold starting of hybrid electric and plug-in hybrid electric vehicles have been investigated through utilizing low-cost sorbent materials for hydrocarbons (HC) and NO_X pollutants. Cold start emissions account for the majority of emissions emitted from modern vehicles during the transient drive cycles that form the basis for emission compliance. The low-cost sorbent materials are able to temporally trap HC and NO_X at low temperature. At higher temperature, these emissions can be desorbed and subsequently oxidized in a downstream placed conventional catalytic converter. The preliminary results show that a passive hydrocarbon and NO_X adsorber can contribute considerably HC and NO_X emissions removal without any fuel penalty, engine operating change, and configuration modification. The material cost of the sorbent materials is largely less than the precious metal. This type of passive adsorber technology should be technologically practical and low cost in the future.

FEERC Vehicle Laboratory Participates in Round Robin Exercise

During the Department of Energy (DOE) Intermediate Ethanol Blends test program, over 80 vehicles were tested at 3 subcontractor laboratories. In wrapping up the test program, a round robin exercise was commissioned to allow comparison of the laboratories with a common pair of vehicles. Two vehicles, one fueled with E0 and one fueled with E15, were tested on several cycles at Environmental Testing Corporation, Transportation Research Center, Southwest Research Institute, and ORNL. With common vehicles and fuels in each set of tests, the variability due to site variables such as driver, dynamometers, and instrumentation can be assessed. ORNL was last in the rotation and completed testing this month. Preliminary analysis indicates good agreement across the labs, including ORNL. Fuel Economy variation is generally within 5% across all cycles and laboratories.

Invention disclosure submitted on High-temperature DRIFTS reactor

ORNL researchers Josh Pihl, William Partridge and Todd Toops submitted an invention disclosure entitled "High-temperature reactor for Diffuse Reflectance Infrared Fourier-Transform Spectroscopy (DRIFTS)". This reactor is designed to allow the observation of both surface and gas-phase analysis of automotive catalysts under realistic operating conditions. The reactor improves on the state of the art by allowing access for surface and gas-phase analysis at any position along the length of the substrate, providing a well-defined geometry that can be modeled and has minimal dead space, and allowing for good temperature uniformity along the length of the substrate. It is expected that this design will allow for unique and necessary acquisition of data to elucidate key reaction mechanisms that control the emissions control chemistry, and thus enable improved catalytic efficiency.

ORNL Additive Manufacturing Expertise Supporting Advanced Transportation Technologies

Researchers in ORNL's FEERC are collaborating with colleagues in the Robotics and Energetic Systems Group to utilize ORNL's capabilities in additive manufacturing to produce test articles in support of research investigating fouling of EGR coolers. The test articles enable fundamental studies of fouling inside complex heat exchanger tube geometries, including a sinusoidal flow passage that is used in commercial EGR coolers. In commercial EGR

coolers, these passages are formed by metal inserts brazed into the interior of the gas flow tubes, but at sizes that are not conducive to fundamental studies. Additive manufacturing allows test articles to be produced that are suitable representations of these geometries that would not otherwise have been possible to study accurately in the EGR fouling program.

FEERC Distinguished Research Staff Presents Invited Keynote Lecture for EuropaCatX Conference at University of Glasgow, Scotland

Bill Partridge presented an invited Keynote Lecture for the Environmental Catalysis Session of the EuropaCatX Conference on August 30, 2011 at the University of Glasgow in Glasgow, Scotland. The presentation was titled "Temperature & Hydrothermal Ageing Impacts on Intra-Catalyst SCR-Reaction Distributions" and was the result of ORNL research in collaboration with Cummins, Inc. and Chalmers University of Technology; coauthors were Xavier Auvray, Louise Olsson, Jae-Soon Choi, Josh Pihl, Krish Kamasamudram, Alex Yezerets, and Neal Currier. The presentation highlighted new catalyst insights based on the unique analytical capabilities developed at ORNL for resolving spatiotemporal reaction distributions within operating SCR catalysts; specifically, heretofore not shown nature of a model Cu-Beta catalyst using the entire NH_3 capacity throughout the SCR zone and apparent NH_3 inhibition at the front catalyst sections where gas-phase NH_3 concentration is high. This type of knowledge regarding detailed catalyst nature is necessary for creating the tools required to realize implementation of efficient engine-catalyst systems.

FEERC Researchers Present at NBB Biodiesel Technical Meeting.

FEERC researchers Todd Toops and Scott Curran presented the results of recent ORNL research involving biodiesel at the National Biodiesel Board's (NBBs) Biodiesel Technical Meeting in Kansas City, Missouri. Todd Toops' presentation "Characterization Techniques to Investigate Location and Impact of Biodiesel Metals" showed results of cutting edge techniques used to look at not only the effect of metals found in biodiesel on emissions reduction catalysts but also where the effects take place. This research utilizes materials characterization expertise and the University of Tennessee-Knoxville (UTK) and ORNL's HTML and is part of a collaborative effort between ORNL, UTK, the National Renewable Energy Laboratory (NREL), Ford, and the Manufacturers of Emission Controls Association (MECA). Scott Curran's presentation, "Background on RCCI and B20 RCCI Results with Both Gasoline and Ethanol Blends" gave the biodiesel community an overview of the advanced combustion mode known as RCCI and showed results of how biofuels including biodiesel blends can improve the performance of these modes as compared to their operation using conventional fuels.

FEERC Researcher Participates in 2nd Annual GreenGov Symposium

Tim Theiss participated as a panelist at the 2nd Annual GreenGov Symposium sponsored in Washington, D.C., October 31, 2011. Mr. Theiss was one of four panelists invited to speak in the Clean Energy Session regarding Energy Efficiency Tools & Strategies. Mr. Theiss highlighted the use of "green gas" coupled with on-site power generation and combined heat and power as a means to meet the green electricity mandates included in the Administration's mandate for green government.

FEERC Organizes SAE High Efficiency Heavy Duty Vehicles Symposium

Robert Wagner was the lead organizer and provided opening remarks at the first SAE Symposium on High Efficiency Heavy Duty Vehicles on November 30, 2011. The objective of this symposium was to "…explore cost-effective technologies capable of delivering quantifiable improvements in vehicle efficiency - a critical priority for the medium- and heavy-duty vehicle industry in light of pending fuel economy/GHG regulations and the volatile cost of fuel." Sessions included regulatory overviews, internal combustion engines, hybrid powertrains, vehicle technologies, modeling and simulation, and intelligent transportation systems. Dr. David Smith of the Advanced Vehicle Systems program at ORNL presented on "Coupling Model-based Design with Laboratory Experimentation to Enhance Heavy Duty Vehicle Efficiency".

ORNL Researchers Present at the Global Powertrain Congress

ORNL's FEERC and the High Temperature Materials Laboratory (HTML) were well represented at this month's Global Powertrain Congress in Troy, Michigan, hosted by the Global Automotive Management Council. Dr. Robert Wagner gave a presentation detailing recent advances in dual fuel combustion, also known as reactivity controlled compression ignition (RCCI) combustion. Dr. Wagner's talk explained how the same efficiency as conventional diesel operation can be achieved but with 90% reduction in NO_X and particulate matter (PM) emissions, and showed

the extension of RCCI operation to a wider engine load envelope. Dr. Dean Edwards discussed paths to high efficiency vehicles and his thoughts on the
next generation of advanced powertrains. His presentation included a step-by-step discussion of efficiency opportunities as well as methods for estimating the efficiency potential of the next generation of high efficiency engines. Dr. Michael Lance spoke on his project with John Deere examining fouling in exhaust gas recirculation (EGR) coolers. Dr. Lance performed microstructural analysis of fouling layers in dyno-aged coolers and his images showed vividly how the layer changes under different conditions. Dr. John Storey collaborated with Ford on a presentation about their joint project on exhaust condensate collection for corrosion studies. Dr. Storey and his team collected condensate from a vehicle operating on high sulfur fuel, analyzed the condensate, and developed a new modeling methodology for predicting the pH of the condensate based on exhaust constituents. Dr. Storey's talk was followed by a presentation by Behr who credited the ORNL study for its contribution to developing a rapid aging/corrosion test for charge air coolers.