TECHNICAL HIGHLIGHTS FOR OCTOBER 2013

Improved Ammonia Storage models will Support the Development of Next Generation Selective Catalytic Reduction (SCR) Systems that Allow High Efficiency Lean Burn Engines to Comply with Emissions Regulations

The ability of ammonia SCR systems to remove NO_X from the exhaust of lean-burn engines depends directly on how much ammonia covers the catalyst surface. Development of ammonia dosing strategies that maintain high NO_X conversion with minimal ammonia slip relies heavily on simulation tools that must accurately model catalyst ammonia storage over a wide range of operating conditions. Researchers at the Oak Ridge National Laboratory's (ORNL's) Fuels, Engines, and Emissions Research Center (FEERC) have developed a new methodology for measurement and analysis of ammonia storage on zeolite-based SCR catalysts that directly quantifies the energetics of the ammonia storage process, thereby avoiding the complications of transport and kinetics that hindered past measurement and modeling efforts. The methodology relies on experimental measurement of equilibrium ammonia storage isotherms and calculation of adsorption enthalpy as a function of coverage through the use of a standard thermodynamic relation (the Clausius-Clayperon equation). In addition to providing critical model parameters, a calculation of how the adsorption enthalpy changes as a function of coverage will help direct model structure formulation and will provide insights into the fundamental adsorption processes occurring on the catalyst surface. The improved models built with this technique will serve as an essential tool for the design of next generation SCR systems that meet emissions regulations and fuel economy targets in high efficiency lean burn engines.

FEERC Research Demonstrates Combustion Noise Challenges with Advanced Combustion

A recently published study by FEERC researchers Scott Curran, Jim Szybist, and Robert Wagner explored combustion noise with reactivity controlled compression ignition (RCCI) over a range of engine operating conditions on a multi-cylinder engine. The study published at the 2013 American Society of Mechanical Engineers (ASME) Internal Combustion Engine Fall (ICEF) Conference examined different combustion noise metrics over an RCCI map to help investigate potential noise vibration and harshness concerns with advanced combustion on production-viable engines.

FEERC Research Improves Understanding of Nature of Particulate Matter (PM) from Low Temperature Combustion

A recently completed RCCI PM investigation conducted with gasoline and diesel fuels at ORNL investigated the effect of a diesel oxidation catalyst on particle size distribution to better understand the nature of RCCI PM. The study took advantage of advanced combustion PM expertise at ORNL to investigate RCCI PM over a number of engine speeds and load conditions including exhaust temperatures well below the light-off temperature. Findings suggest that the PM is composed mostly of volatile and semivolatile organic species from unburned fuel. A paper detailing the study and findings was submitted for review for the 2014 Society of Automotive Engineers (SAE) World Congress meeting.

Gasoline-Alcohol Blends Reduce Soot Precursor Formation in Gasoline-Direct Injection (GDI) Engine Exhaust

Using a novel direct thermal desorption-pyrolysis gas chromatograph-mass spectrometer (GC-MS) method, Sam Lewis and John Storey identified over 20 individual polycyclic aromatic hydrocarbons (PAHs) in the PM collected from a GDI engine operating on gasoline and gasoline-alcohol blends. The engine was operated in a mode typical of transient loads like vehicle acceleration. The gasoline-alcohol blends reduced the quantity of PAHs on the PM, even when allowing for the lesser amount of gasoline

burned. This reduction in PAHs may indicate that fuel oxygen is interfering with PAH formation during combustion.

High Efficiency Ionic Liquid (IL) Lubricant Additive Evaluated for Catalyst Compatibility at ORNL

An IL, which is currently being considered as a high efficiency lubricant additive, recently passed a series of engine wear durability tests and has demonstrated a 2% fuel economy gain over the industry standard, Mobil 1. A team at ORNL further investigated the compatibility of the IL for catalyst compatibility for gasoline applications by employing an accelerated aging system using a gasoline genset equipped with a three-way catalyst (TWC). As a point of comparison, the industry standard lubricant additive, zinc dialkyldithiophosphate (ZDDP), was also evaluated. The genset was used to expose the catalysts to exhaust doped with the two additives. After exposing the catalysts, the catalytic performance of the IL- or ZDDP-aged TWCs was evaluated in our flow reactor. Evaluating the front of the TWC (which would be most impacted by the additive) showed that the IL has similar or less adverse impact on the TWC performance versus ZDDP. Comparison with a non-additive (base) case is forthcoming.

HIGH-LEVEL OR NOTEWORTHY VISITS

Vehicle Technologies Office (VTO) Visits the ORNL/FEERC for Advanced Combustion Engines Research and Development (R&D) Program Review

Gurpreet Singh, Steve Goguen, Ken Howden, and Leo Breton from the Department of Energy's (DOE's) VTO visited FEERC on October 29–30. The visit was a review of the Advanced Combustion Engines R&D Program at ORNL. Presentations included overviews of the advanced combustion and emissions controls research as well as more detailed presentations on ORNL PM research, neutron imaging of fuel injectors and particulate filters, and the use of DOE leadership computing at ORNL for accelerating the development of advanced combustion engines. In addition, staff presented overviews of the ORNL Sustainable Transportation Program, the FEERC Fuel and Lubricant Technologies Program, and ORNL research supported by the Bioenergy Technology Office. The visit also included detailed tours of the FEERC as well as the Vehicle Systems Integration (VSI) laboratory.

INVITED TALKS AND PRESENTATIONS

FEERC Staff Member Invited to Speak at Chemical Engineering World Congress

Dr. Jae-Soon Choi and Dr. William Partridge presented some of their DOE-funded research at the 9th World Congress of Chemical Engineering (WCCE9) in Seoul, Korea, August 18–23, 2013. Dr. Choi reported on new developments in reaction pathways for N_2O formation over automotive NO_x adsorber catalyst, which is part of the Cross-Cut Lean Exhaust Emissions Reduction Simulations (CLEERS) project and an ongoing collaboration with the Prague Institute of Chemical Technology. Dr. Partridge gave an invited presentation describing the spatially-distributed nature of NH_3 storage over an automotive SCR catalyst, which is part of the DOE-funded Cummins Cooperative Research and Development Agreement (CRADA).

Dr. William Partridge Presents Three Invited Lectures at Korean Research Facilities

Dr. William Partridge presented invited lectures at two universities and one research institute in South Korea, August 26–28, following the WCCE9 conference. These presentations were at (1) the Department of Chemical Engineering, School of Environmental Science and Engineering, Pohang University of Science and Technology (POSTECH), hosted by Professor In-Sik Nam, (2) the Department of Applied Chemical Engineering, Chonnam National University (CNU), hosted by Professor Gon Seo, and

(3) the Honam Technology Application Division, Korea Institute of Industrial Technology (KITECH), hosted by Dr. Inchul Choi. The POSTECH and CNU lectures focused on spatially distributed NH_3 storage over SCR catalysts and the KITECH lecture applications of the spatially resolved capillary inlet mass spectrometer (SpaciMS), Fuel-in-Oil, and exhaust gas recirculation (EGR) Probe diagnostics developed in the DOE-funded Cummins CRADA.

FEERC Distinguished Staff Presents Invited Talk to American Institute of Chemical (AIChE) Engineering Group

Dr. William Partridge presented an invited talk to the Knoxville-Oak Ridge chapter of AIChE in Knoxville, Tennessee, October 10. The presentation highlighted ORNL's Sustainable Transportation Program and specifically applications of several DOE-funded diagnostics and studies for improving automotive efficiency, durability, emissions, and cost. There were very active interactions at the meeting, which provided a good and successful forum for communicating some of the DOE and ORNL efforts for practically benefiting society.

FEERC Post Docs, Visitors and Staff Present Research at Southeastern Catalysis Society (SECS) Meeting

Several FEERC researchers presented at SECS 12th Annual Fall Symposium in Asheville, North Carolina, September 29–30. The SECS is part of the North American Catalysis Society. Oral presentations were given by post-doctoral research associate Dr. Mi-Young Kim and visiting student researcher David Mráček, and poster presentations were given by FEERC research staff Dr. Maggie Connatser, Dr. Jae-Soon Choi, and Dr. Todd Toops; the presentations covered a wide range of DOE-sponsored research in the Advanced Combustion Engine, Biomass, and Fuels R&D areas. Mr. Mráček is visiting ORNL as part of an ongoing collaboration with Professor Miloš Marek and Dr. Petr Kočí at the Prague Institute of Chemical Technology focused on elucidating N_2O formation pathways in automotive catalysts and as part of the DOE-funded CLEERS program.

Internal Collaboration Highlighted in the United States Research and Innovation for Vehicle Efficiency (USDRIVE) Presentation

FEERC researcher Scott Curran presented results of current research featuring collaboration between FEERC and the VSI lab at ORNL in a recent presentation to the USDRIVE Vehicle Systems and Simulation Tech Team. The presentation was part of the ORNL deep dive presentations for the meeting and highlights how ORNL is leveraging research from different DOE program offices to deliver valuable R&D results.

Research from FEERC-Chalmers Partnership Presented at CLEERS Telecom

Xavier Auvray presented results from his research involving modeling the spatiotemporal reactions along an automotive SCR catalyst in the October CLEERS Telecom, October 17; the telecom was broadly attended by an international audience of industry, university, and national laboratory researchers and is part of the DOE-funded CLEERS coordination project. Mr. Auvray is a Ph.D. student at Chalmers Institute of Chemical Technology and the research is part of an ongoing ORNL-Chalmers collaboration led by Professor Louise Olsson at Chalmers and Dr. William Partridge at ORNL\FEERC in support of the DOE Cummins-ORNL CRADA and CLEERS projects. The talk was the first broadly public presentation of using SpaciMS intra-catalyst data to determine kinetic parameters for the various SCR reactions; this approach is unique in that it allows determining these parameters under realistic operating conditions, rather than at unrealistically low temperatures or space velocities as is often required to achieve differential conditions using conventional methodologies. This demonstrates another practical and significant benefit, strength, and contribution to the automotive research community via the DOE Cummins-ORNL CRADA.

AWARDS

FEERC Researcher Awarded Best Presentation at the ASME ICEF Conference

FEERC researcher, Scott Curran, was awarded "Best Presentation of a Paper" at the 2013 ASME ICEF. The presentation was awarded for an advanced combustion research paper presented at 2012 ASME ICEF.

Patent Granted for Diagnostic Developed in DOE ORNL-Cummins CRADA

A patent was granted to FEERC staff Dr. James Parks and Dr. William Partridge for a diagnostic developed in the DOE ORNL-Cummins Combustion CRADA for high-speed measurement of particulate in engine exhaust stream; the diagnostic was developed and applied to resolve cylinder-to-cylinder and cycle-to-cycle combustion variations in multi-cylinder engines. The U.S. Patent No. 8,451,444 was issued May 28, 2013, and is titled *Optical Backscatter Probe for Sensing Particulate in a Combustion Gas Stream*, with Dr. Parks and Dr. Partridge acknowledged as inventors.