November 2014 Highlights

ORNL Fuels, Engines, and Emissions Research Center

TECHNICAL HIGHLIGHTS

ORNL Research Team Extends Validation of Single, Supported Platinum (Pt) Atom Catalytic Oxidation Activity to Nitrogen (NO) in their Recent Publication in Nature's Open Access Journal – *Scientific Report*

This Materials Science and Technology Division (MSTD)/Fuels, Engines, and Emissions Research Center (FEERC) research team has shown that single, supported Pt atoms are active for NO oxidation, defying the trend of decreasing activity as Pt particles size decreases. Previously, Chaitanya Narula and Malcolm Stocks had employed first principles modeling work to propose that single supported Pt atoms will be catalytically active. In this work, they propose a modified Langmuir-Hinshelwood pathway for NO oxidation on single supported Pt atoms on an inert alumina support. Experimental validation comes from work by Lawrence Allard and FEERC researcher, Melanie DeBusk, who found that alumina supported Pt atoms have comparable turn-over-frequency (TOF, a measure of catalytic activity) to larger, fully formed supported Pt particles and the Pt atoms do not sinter during NO oxidation. Fresh emission treatment catalysts contain small fractions of noble metal single atoms and this work shows that these can be contributors to the catalytic processes.

Citation: M. Moses-DeBusk et al., "Remarkable NO Oxidation on Single Supported Platinum Atoms," *Scientific Report,* **4**, 7238; DOI: 10.1038/srep07238, November 28, 2014.
http://www.nature.com/srep/2014/141128/srep07238/full/srep07238.html

Oil-Soluble Phosphonium-Based Ionic Liquids (ILs) Recently Reported as Potential Ashless Lubricant Additives

This study is to expand the IL chemistry envelope and to achieve fundamental correlations between the ion structures and ILs' physiochemical and tribological properties. Here we present eight ILs containing two different phosphonium cations and seven different anions from three groups: organophosphate, carboxylate, and sulfonate. The oil solubility of ILs seems largely governed by the IL molecule size and structure complexity. When used as oil additives, the ranking of effectiveness in wear protection for the anions are organophosphate > carboxylate > sulfonate. All selected ILs outperformed a commercial ashless antiwear additive. Surface characterization from the top and the cross-section revealed the nanostructures and compositions of the tribo-films formed by the ILs. Some fundamental insights were achieved: branched and long alkyls improve the IL's oil solubility, anions of a phosphonium-phosphate IL contribute most phosphorus in the tribo-film, and carboxylate anions, though free of P, S, N, or halogen, can promote the formation of an antiwear tribo-film.

Citation: Y. Zhou, J. Dyck, T. Graham, H. Luo, D. N. Leonard, and J. Qu, "Ionic Liquids Composed of Phosphonium Cations and Organophosphate, Carboxylate, and Sulfonate as Lubricant Antiwear Additives," pp. 13301–13311 in *Langmuir*, 30(44), November 2014.

ORNL Well-to-Wheel Analysis of Natural Gas for Light-Duty Vehicles Ranked Third in Number of Views/Downloads

A recent paper published in the journal *Energy* titled, "Well-to-Wheel Analysis of Direct and Indirect use of Natural Gas in Passenger Vehicles," has had over 1,500 views or downloads since its online publication on August 21, 2014. The open access paper, currently ranked number 3 in views/downloads in the last 90 days for the journal, was

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authored by FEERC researcher Scott Curran, FEERC director Robert Wagner, Sustainable Transportation Program Director Ron Graves, Energy and Transportation Science Division (ETSD) Director Johney Green Jr., and Associate Laboratory Director for Energy & Environmental Sciences Directorate (ESD) Martin Keller. The study investigated the well-to-wheels energy use and greenhouse gas emissions from natural gas vehicles running on compressed natural gas compared against electric vehicles charged with electricity produced solely from natural gas combustion in stationary power plants.

INVITED TALKS AND PRESENTATIONS

FEERC Director Organizes and Moderates Society of Automotive Engineers (SAE) Meeting in China
FEERC Director Robert Wagner organized a 2-day 2014 SAE Energy Saving and Emission Reduction (ESER) Forum in Shanghai, China. In addition to organizing, he participated in a panel session on the future of high efficiency engine technologies, presented during the high efficiency combustion systems session, and moderated a light-weighing session with ETSD Division Director Johney Green. The 2014 SAE ESER Forum included presentations on the latest breakthroughs in light-weight materials and cutting-edge adaptive applications of energy efficiency and emission reduction from original equipment manufacturers (OEMs), Tier 1 suppliers, universities, and research institutions. The presenters and audience represented an international mix spanning North America, Europe, and Asia.

FEERC Advanced Combustion Research Featured at Penn State Graduate Seminar
FEERC researcher Scott Curran presented an overview of ORNL advanced combustion and emissions control research and development as part of the Penn State Mechanical and Nuclear Engineering Department's graduate seminar series. The invited talk focused on dual-fuel reactivity controlled compression ignition and associated emissions control opportunities and challenges. FEERC has a long history of hosting graduate student researchers from Penn State as well as research collaborations on alternative fuels and combustion.

AWARDS

FEERC Researchers Honored at R&D 100 Award Ceremony in Conjunction with Two Transportation-Related Technological Innovations
In recognition for outstanding innovations, two technologies being developed in conjunction with FEERC researchers were honored at the R&D Award Ceremony in Las Vegas, Nevada on November 7, 2014. Jun Qu and Todd Toops received the R&D 100 Award for their efforts on the "Ionic Liquid Anti-wear Additives for Fuel-Efficient Engine Lubricants;" also attending from ORNL were Huimin Lu and Sheng Dai. The technology employs a group of ILs 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 a collaboration between ORNL, General Motors, Shell, and Lubrizol. Other ORNL team members on the DOE-sponsored activity (EERE-VTO) were Peter Blau, Brian West, and Bruce Bunting. The second honored technology, "The RF-DPF Diesel Particulate Filter Sensor," was received by FEERC researcher Vitaly Prikhodko and his industrial partner, Alex Sappok of Filter Sensing Technologies Inc. (FSTI); the Massachusetts Institute of Technology (MIT) was the other partner in the technology. The RF-DPF 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. Other FEERC team members on the FSTI and DOE-VTO funded activity were Jim Parks and John Storey.

ORNL Receives Award from Local Clean Cities for Leadership in Alternative Fuel Use, Sustainable Transportation Research, and Public Engagement
FEERC researcher Scott Curran accepted the 2014 Davy Crockett Volunteer Leadership award on behalf of ORNL from the local DOE Clean Cities program, the East Tennessee Clean Coalition presented as part of the coalition's special 10th anniversary celebration. The award citation recognized ORNL as a leader in alternative fuel use in the southeast and amongst national laboratories. ORNL has reduced petroleum energy consumption by 55% since 2005 and increased alternative fuel use by 136% since 2005 to be well ahead of government mandates on alternate fuel use. ORNL has an onsite B20 and two E85 pumps for fleet use and in 2014 all vehicle acquisitions were biofuel ready. ORNL is well known for continued innovation in sustainable transportation research and development for the U.S. Department of Energy. ORNL has been a strong partner in regional outreach and public education on advanced vehicle technologies and alternative fuels.