December 2014 Highlights

ORNL Fuels, Engines, and Emissions Research Center

TECHNICAL HIGHLIGHTS

Exhaust Gas Recirculation (EGR) Limit Extended Through Localized Oxygen Enrichment at the Flame Kernel

Researchers at the Oak Ridge National Laboratory (ORNL) and the University of Tennessee (UT) have demonstrated that stable combustion in a static chamber can be extended from 15–22% simulated EGR by metering a minute quantity of oxygen at the spark plug gap during ignition. EGR is used on spark-ignition (SI) engines to lower nitrogen oxide (NOx) emissions and improve efficiency. The upper limit of EGR content in the test chamber was measured at 15% for a starting pressure of 100 psi. This limit was extended to 22% by metering a minute quantity of oxygen to the spark plug during the early stages of kernel formation. The added oxygen increases the reactivity of the flame kernel to promote stable propagation.

New ORNL-Shell Joint Journal Publication in *American Chemical Society (ACS) Applied Materials & Interfaces* (Impact Factor: 5.9)

Our previous work suggested great potential for a phosphonium-organophosphate ionic liquid (IL) as an anti-wear lubricant additive. In this study, a set of five ILs were carefully designed and synthesized with identical organophosphate anions but dissimilar phosphonium cations to allow systematic investigation of the effects of cation alkyl chain length and symmetry on physicochemical and tribological properties. Symmetric cations with shorter alkyl chains seem to increase the density and thermal stability due to closer packing. On the other hand, either higher cation symmetry or longer alkyl moieties induces a higher viscosity, though the viscosity index is dependent more on molecular mass than on symmetry. While a larger cation size generally increases an IL's solubility in non-polar hydrocarbon oils, six-carbon seems to be the critical minimum alkyl chain length for high oil miscibility. Both of the ILs that are mutually oil miscible have demonstrated promising lubricating performance at 1.04% treat rate, though the symmetric-cation IL moderately outperformed the asymmetric-cation IL. Characterizations on the tribofilm formed by the best-performing symmetric-cation IL revealed the film thickness, nanostructure, and chemical composition. Results provide fundamental insights for future molecular design in developing oil-soluble ILs as lubricant additives.

Reference: W. C. Barnhill, J. Qu, H. Luo, H. M. Meyer III, C. Ma, M. Chi, and B. L. Papke, "Phosphonium-Organophosphate Ionic Liquids as Lubricant Additives: Effects of Cation Structure on Physicochemical and Tribological Characteristics," pp. 22585–22593 in *ACS Applied Materials & Interfaces*, 6, 2014.

New Sequence VIE Engine Dynamometer Tests Demonstrated Improved Fuel Economy for a Combination of IL and Zinc Dithiophosphate (ZDDP)

In FY2014, the ORNL-Shell Cooperative Research and Development Agreement (CRADA) team had observed synergistic effects between phosphonium-organophosphate ILs and ZDDP in reducing both wear and friction in tribological bench tests. In FY2015-Q1, the team produced the first prototype fully-formulated Society of Automotive Engineers (SAE) 0W-16 GTL-based engine oil using a combination of IL and ZDDP (1:1 molecular ratio, total P content of 800 ppm meeting GF5/GF6 regulations). In December, this IL+ZDDP additized prototype engine oil was evaluated using the short (fuel economy improvement (FEI)1 only) Sequence VIE (upcoming new American Society of Mechanical Engineers (ASTM)

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standard, replacing VID) multi-cylinder engine dynamometer test. Results showed a 2.12% higher FEI over the standard baseline oil. Further comparison was done with another test oil having the same 0W-16 viscosity grade and almost identical formulation package except no IL (ZDDP only, but the same total P content of 800 ppm). This allowed separating the FEI contributions: 1.87% from the reduced viscosity and 0.25% from the lower boundary/mixed friction. The synergistic IL+ZDDP combination offers unique opportunity in mitigating the challenges of increased wear and boundary friction when using lower-viscosity engine oils.

ORNL FEERC Researchers Visit Argonne National Laboratory to Discuss Collaboration

Robert Wagner, Scott Curran and Jim Szybist from ORNL's FEERC visited the Center for Transportation Research at Argonne National Laboratory, hosted by Thomas Wallner who is the Section Leader for Fuels, Engine and Aftertreatment Research. The purpose of the visit was to discuss existing projects and identify areas that would be conducive to collaboration. A number of areas were identified where the two laboratories had complementary facilities and expertise, where working in alignment could be beneficial to both organizations to meet the Department of Energy (DOE) programmatic goals. Follow-up interactions between researchers at the two laboratories are ongoing. ORNL also delivered two technical presentations that were well received and spurred discussion.

High-Level or Noteworthy Visits

Manufacturers of Emission Controls Association (MECA) visits ORNL

Dr. Joseph Kubsh, Executive Director of MECA visited ORNL on December 1, 2014. During the visit, Dr. Kubsh gave a seminar on current emission rules and technologies of interest to control emissions to meet the upcoming regulations. The visit also included a tour and discussion of ORNL's emission control research activities. MECA represents industrial companies that manufacture emission control equipment for automotive and other engine emission control applications.

Invited Talks and Presentations

ORNL Presents Emissions Research at SAE Symposium

ORNL presented emissions research for fuel efficient vehicles at SAE 2014 Light Duty Emissions Control Symposium in Troy, Michigan, on December 9–10, 2014. Scott Curran, Vitaly Prikhodko, and Jim Parks presented research on advanced combustion emissions, lean gasoline emission control, and low temperature oxidation catalysts highlighting a wide range of research at ORNL relative to the industry challenges to meet fuel economy and emission regulations.

Awards

Fuels, Engines, and Emissions Research Center (FEERC) Researchers Receive Awards for Contributions to the SAE International Engineering Meetings Board

FEERC researchers Derek Splitter and Scott Curran received the 2014 McFarland Award from SAE International. This award recognizes individuals for their outstanding contributions toward the work of the SAE Engineering Meetings Board in the planning, development, and dissemination of technical information. Dr. Splitter's award was for distinguished contributions to the organization of the combustion track at the 2014 SAE World Congress including exemplary leadership and organizational skills in developing strong technical content, securing outstanding reviewers, and maintaining schedule. The award noted the demonstration the high potential of early career committee members to make valuable lasting contributions to SAE and Powertrain, Fuels, and Lubricants committees. Dr. Curran's award was for innovation in the development of a new SAE young professional initiative to improve the interaction of young SAE members with leading SAE professionals. Scott Curran spearheaded this initiative and facilitated the interaction of several younger members with senior SAE leadership. The award noted the success of this interaction could serve as a future model for networking and inspiring young professionals to be future SAE leaders. The awards will be presented at the 2015 SAE World Congress and Expo in April 2015.