Technical Highlights
November 2012

Biodiesel Solubility to Common Elastomers Determined Using Hansen Solubility Parameters

A solubility analysis evaluating biodiesel fuels and blends to common elastomers and plastic materials was performed by Oak Ridge National Laboratory (ORNL) researcher Mike Kass. Hansen solubility parameters for soybean, rapeseed, palm, canola, beef tallow, and coconut biodiesels were determined from the literature and used to calculate the solubility distance for each biodiesel type and elastomer material as a function of blend level with diesel fuel. The results show that biodiesels derived from soybean, rapeseed, palm, canola, and beef tallow (SRPCB) oils all exhibited nearly identical compatibility behavior to polymers and generally show increased solubility (swell) with increasing bio-oil content. Coconut-derived biodiesel differed markedly from the other biodiesel types. For instance, a common o-ring material like nitrile rubber appears to be insoluble to coconut-based biodiesel but was highly soluble to the other types, especially at concentrations exceeding 50% by volume. Surprisingly, another common elastomer, silicone, showed more susceptibility to swell with exposure to coconut-derived biodiesels than the other types studied. The results suggest that material compatibility needs to be carefully considered for any components developed for general biodiesel use. Certain biodiesel types, such as coconut, may not be compatible with those systems developed for one (or more) of the SRPCB oils; likewise SRPCB oils may not be compatible with systems developed for use with coconut-derived biodiesel.

Fuels, Engines, and Emissions Research Centre (FEERC) Partners with Southwest Research Institute (SwRI) and the Environmental Protection Agency (EPA)

FEERC researchers, Teresa Barone and John Storey, will work with SwRI and EPA on the development of a soot generator used to mimic exhaust particles for the evaluation of instrument response to varying particle characteristics. The team will investigate soot generator conditions required to produce diesel-like particle morphologies. The EPA system will enable tailoring of soot characteristics for a wide range of instrument calibrations and assessments, particularly those instruments designed for on-road measurements of exhaust particulate matter (PM) in heavy-duty trucks. Other potential uses of the system include generating soot in locations where engines are not allowed and fundamental particulate filter studies. The ORNL particle morphology study enables a key developmental milestone for the EPA system.

Identifying Pathways to Control Nitrogen Oxide (NO_X) Emissions while Maintaining the High Fuel Efficiency of Lean Gasoline Engines through a Combination of Proven Three-Way Catalyst (TWC) and Selective Catalytic Reduction (SCR) Catalyst Technologies

Lean gasoline engines have the potential to significantly reduce petroleum consumption by light duty vehicles in the United States (U.S.), but vehicles based on this technology are currently unable to cost effectively meet U.S. NO_X emissions regulations. Researchers at ORNL's FEERC have partnered with General Motors (GM) and Umicore to investigate passive on-board ammonia (NH_3) SCR as a potential solution for controlling NO_X emissions from lean gasoline engines. This strategy uses periodic excursions to slightly rich engine operation to generate NH_3 from engine out NO_X over a close coupled catalyst. This NH_3 is stored on an underfloor SCR catalyst where it is used to reduce NO_X when the engine returns to lean operation. In this way, lean gasoline vehicles can take advantage of highly effective and durable commercial SCR catalysts without requiring an onboard urea storage and injection system or refueling infrastructure. A recently conducted series of detailed flow reactor studies on the key components of a passive SCR system have shown that commercially available TWC formulations are effective NH_3 generators that could selectively convert engine out NO_X to NH_3 under moderately rich conditions (AFR

of 14.0–14.3) over a wide temperature range. Results also indicate that a Pd-only formulation had a higher selectivity to NH_3 than more complex TWC or lean NO_X trap (LNT) formulations that contained Rh and Ce. The Pd-only TWC in combination with two Umicore zeolite SCR catalysts (one exchanged with Cu, the other with Fe) was tested in a unique dual furnace flow reactor to evaluate the performance of the TWC + SCR system while cycling between lean and rich exhaust conditions. The Cu zeolite achieved very high NO_X conversions (>99%) over a temperature window (200–350°C) consistent with underfloor catalyst operating conditions. However, due to its low NO_X conversion at low temperatures and low NH_3 storage capacity at high temperatures, the Fe zeolite was much less effective. Estimates indicate that a lean gasoline engine coupled with this type of emissions control system would still retain much of its fuel efficiency advantage over a comparable stoichiometrically operated engine. Future work will focus on demonstrating the system in engine exhaust and identifying catalyst formulations that can widen the operating window and reduce the fuel penalty and cost associated with the passive SCR system.

High-Level or Noteworthy Visits

ORNL-Shell Cooperative Research and Development Agreement (CRADA) Progress Meeting held on November 13, 2012, at Shell Houston Tech Center

ORNL staff Jun Qu and Brian West along with the Vehicle Technologies Program (VTP) program manager, Steve Przesmitzki, had a face-to-face project meeting with Shell engineers on November 13, 2012, at the Shell Houston Tech Center for a recently signed CRADA NFE-12-03876, ionic liquids as multi-functional lubricant additives to enhance engine efficiency. Supported by VTP through a FOA0000239 award, this joint project aims to develop next-generation, ionic liquids-based lubricant additives to improve the engine fuel economy. At this meeting, Shell's PI Brian Papke gave an overview of Shell and tours of their recently renovated, well-equipped tribology and rheology labs. Both parties reported recent technical results. Although this project only started three months ago, substantial progress has already been made. The team discussed the detailed technical plan and finalized the screening test matrix for the coming quarter.

Global President of DENSO Corporation visits ORNL

A high level delegation from DENSO Corporation recently visited the National Transportation Research Center (NTRC) at ORNL. Visitors included Nobuaki Katoh (Global President), Yasushi Yamanaka (Executive Director R&D), and several other high level executives from DENSO International America and DENSO Manufacturing Tennessee. Their visit included an overview of the ORNL Sustainable Transportation Program and tours of FEERC, Power Electronics and Electric Machinery Research, Vehicle Systems Integration Laboratory, Battery Manufacturing Facility, and the Manufacturing Demonstration Facility (MDF).

Local Scouts Tour the NTRC and MDF

Several boys and their parents from local Scout troops toured the NTRC and MDF this month. Tim Theiss of FEERC organized the tour which consisted of about 20 boys in middle and high school and several of their leaders. The group toured the analytical chemistry lab with Dr. Maggie Connatser and the Additive Manufacturing Lab with Dr. Lonnie Love, as well as the vehicle dynamometer lab and several engine dynamometer labs. The boys were given an appreciation for some of the technologies needed and complexity in increasing fuel economy and in the enabling power of additive manufacturing.

Awards

Science Communicator Award

Brian West of FEERC has been awarded the ORNL/UT-Battelle Science Communicator Award for his sustained commitment to sharing his research expertise and also for his passion to educate the general and non-automotive technical communities on the details of transportation energy use, especially with respect to the potential impact of biofuels. Mr. West has received four "Excellence in Oral Presentation" awards from the Society of Automotive Engineers (SAE) and the SAE Lloyd Withrow Distinguished Speaker award. He has been invited to speak at many venues and has frequently been interviewed by nontechnical media personnel on topics such as transportation energy and biofuel utilization.

Patent Granted to FEERC Researcher on Novel 6-Stroke Engine Cycle

Jim Szybist was granted US patent No. 8,291,872 entitled "Highly Efficient 6-Stroke Engine Cycle with Water Injection." The engine cycle is a methodology to perform in-cylinder waste heat recovery by essentially combining a 4-stroke Otto cycle with a 2-stroke steam cycle. The engine cycle has been investigated experimentally and did not meet expectations due to a number of factors. Variations of the engine cycle continue to be pursued, including using the 6-stroke experimental capability as a research tool to investigate thermochemical recuperation and to understand the chemistry occurring during the negative valve overlap relevant to homogeneous charge compression ignition (HCCI) research.

FEERC Researcher attended National Academies Keck Futures Initiative (NAKFI)

Dr. Andreas Malikopoulos attended the 10th Annual NAKFI conference, "The Informed Brain in a Digital World," and presented his recent research efforts on developing mathematical decision-making models that can reproduce intelligence in applications related to energy and transportation. NAKFI is a 15-year effort of the National Academy of Sciences (NAS), the National Academy of Engineering (NAE), and the Institute of Medicine to catalyze interdisciplinary inquiry and to enhance communication among researchers, funding organizations, universities, and the general public. The objective is to support the climate for conducting interdisciplinary research and to break down related institutional and systemic barriers. NAKFI worked towards these objectives by harnessing the intellectual horsepower of approximately 150 individuals from diverse backgrounds who were selected to attend its annual "think-tank" style conference and by awarding $1 million in seed grants – on a competitive basis – to conference participants to enable further pursuit of bold, new ideas and connections stimulated by the conference.