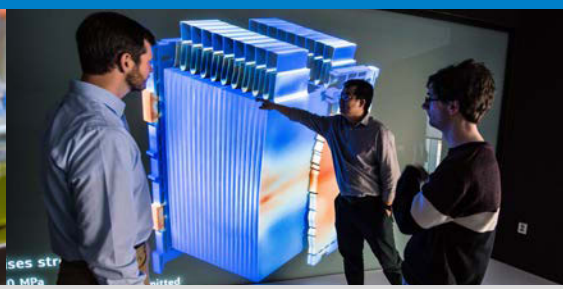
NREL
NATIONAL RENEWABLE ENERGY LABORATORY





FY17 Transportation and Hydrogen Systems Center Journal Publication Highlights

NREL's Transportation and Hydrogen Systems Center published more than 30 journal articles in the past year highlighting recent research in advanced vehicle technology, alternative fuels, and hydrogen systems.

Hydrogen and Fuel Cell Technologies Publications

Hydrogen Monitoring Requirements in the Global Technical Regulation on Hydrogen and Fuel Cell Vehicles, *International Journal of Hydrogen Energy*

NREL and the Joint Research Centre, Institute for Energy and Transport have been evaluating and developing analytical methods that can be used to verify compliance with the hydrogen release requirements as specified in the United Nations Economic Commission for Europe Global Technical Regulation Number 13—the defining document regulating safety requirements in hydrogen vehicles. The project identified the thermal conductivity sensor as a sensor platform that is sensitive to hydrogen as well as helium and is commercially available from numerous suppliers, including models configured in physically robust packages.

Optimizing Investments in Coupled Offshore Wind-Electrolytic Hydrogen Storage Systems in Denmark, *Journal of Power Sources*

In response to electricity markets with growing levels of wind energy production and varying electricity prices, this research examines incentives for investments in integrated renewable energy power systems by exploring a strategy for optimizing a power system consisting of wind turbines, electrolyzers, and hydrogen fuel cells. This research found that the most beneficial configuration is to produce hydrogen at a time that complements the wind farm and sell the hydrogen directly to end users.

Vehicle Technologies Publications

A Quantitative Model for the Prediction of Sooting Tendency from Molecular Structure, *Energy and Fuels*

This study developed a quantitative structure–activity relationship (QSAR) model of sooting tendency based on the experimental yield sooting index, which ranks molecules on a scale from n-hexane, 0, to benzene, 100. Through the development and application of a predictive QSAR model, this study demonstrated that the yield sooting index can be well-predicted by molecular structure.

Analysis of Long-Range Interaction in Lithium-Ion Battery Electrodes, *Journal of Electrochemical Energy Conversion and Storage*

This study proposes a mesoscale model to probe the effects of the cathode composition of lithium-ion batteries, e.g., the ratio of active material, conductive additive, and binder content, on the electrochemical properties and performance. The results reveal a complex nonmonotonic behavior in the effective electrical conductivity as the amount of conductive additive is increased. Insufficient electronic conductivity of the electrode limits the cell operation to lower currents. Once sufficient electron conduction (i.e., percolation) is achieved, the rate performance can be a strong function of ion-blockage effect and pore phase transport resistance.

Anisotropic Thermal Response of Packed Copper Wire, *Journal of Thermal Science and Engineering Applications*

The apparent thermal conductivity of packed copper wire test specimens was measured parallel and perpendicular to the axis of the wire using laser flash, transient plane source, and transmittance test methods. The Kanzaki model and a finite element analysis model were found to reasonably predict the apparent thermal conductivity perpendicular to the wires, but thermal conductivity percolation from nonideal wire-packing may result in their underestimation of it.

Anti-Knock Quality of Sugar Derived Levulinic Esters and Cyclic Ethers, *Fuel*

This paper investigated the anti-knock quality of sugar-derived levulinic esters (methyl levulinate [ML] and ethyl levulinate [EL]) and cyclic ethers (furfuryl ethyl ether [FEE] and ethyl tetrahydrofurfuryl ether [ETE]). The results from both apparatus demonstrate that ML, EL, and FEE have a higher anti-knock quality than the reference Euro95 gasoline, while ETE performed markedly worse than the reference fuel on both setups and might therefore be a more appropriate fuel for compression ignition engines.

**NREL is a national laboratory of the U.S. Department of Energy,
Office of Energy Efficiency and Renewable Energy, operated by the Alliance for Sustainable Energy, LLC.**

BioCompoundML: A General Biofuel Property Screening Tool for Biological Molecules Using Random Forest Classifiers, *Energy and Fuels*

Screening a large number of biologically derived molecules for potential fuel compounds without recourse to experimental testing is important in identifying understudied yet valuable molecules. This paper discusses the development of BioCompoundML, a general-purpose fuel property tool, using machine learning, whose outcome is to screen molecules for desirable fuel properties. This article provides measures of the tool's success as it is demonstrated using three different fuel properties: research octane number, threshold soot index, and melting point.

Bleaching and Hydroprocessing of Algal Biomass-Derived Lipids to Produce Renewable Diesel Fuel, *Energy and Fuels*

Algal lipids represent a promising feedstock for production of renewable diesel, but there is little information available regarding the integration of pretreatment, extraction, and catalytic upgrading steps. This work examined oil bleaching by two methods and the effects of bleaching on oil deoxygenation and hydroisomerization. The bulk chemistry of the deoxygenation and isomerization was not strongly affected by bleaching, as post-isomerization products with cloud points less than −10°C and boiling ranges within or close to specification for No. 2 diesel fuel were obtained.

Characterising Thermal Runaway within Lithium-Ion Cells by Inducing and Monitoring Internal Short Circuits, *Energy and Environmental Science*

This study demonstrates the application of an internal short-circuiting device for controlled, on-demand, initiation of thermal runaway. By combining the use of a novel device (which generates an internal short circuit within commercial cell designs, on-demand and at a pre-determined location) with high-speed X-ray imaging at 2,000 frames per second, the study characterized for the first time the initiation and propagation of thermal runaway from a known location within a Li-ion cell.

Characterization of Upgraded Fast Pyrolysis Oak Oil Distillate Fractions from Sulfided and Non-Sulfided Catalytic Hydrotreating, *Fuel*

This paper presents the characterization of a group of five distillate fractions from each of two types of hydroprocessed oils from oak pyrolysis oil: a low oxygen content (LOC, 1.8% O, wet basis) oil and a medium oxygen content (MOC, 6.4% O, wet basis) oil. LOC fractions 1 and 2 have the potential to satisfy boiling point requirements for gasoline, which can also be true for the same MOC fractions, but the presence of acid will likely preclude these from being direct gasoline blendstock.

Comparison of Vehicle-Broadcasted Fuel Consumption Rates against Precise Fuel Measurements for Medium- and Heavy-Duty Vehicles and Engines, *SAE International Journal of Fuels and Lubricants*

To assess the accuracy of real-time fuel consumption estimates, controller area network-reported fuel consumption data are compared against fuel measurements from precise instrumentation. A drive cycle analysis revealed that while controller area network fueling estimate accuracy differs for individual vehicles, estimates capture the relative fuel consumption differences between drive cycles within 4% for all vehicles and even more accurately for some, so in situations where only controller area network-reported data are available, fueling estimates can provide relative fuel consumption trends but not precise fuel consumption rates.

Constitutive Behavior and Progressive Mechanical Failure of Electrodes in Lithium-Ion Batteries, *Journal of Power Sources*

This paper presents experimental and numerical studies on the constitutive behavior and progression of failure in lithium-ion battery electrodes, the understanding of which is critical for the safety of lithium-ion battery cells. The study identified the mechanism of complex failure behavior that involves both tensile and compression failure and shows sensitivities to the tensile strength of active materials; also, the yielding of the current collector results in a slope change for the global compressive stress-strain response and the global force-strain curve for the indentation tests. These suggest that it is essential to take into consideration the tensile properties of the active-material layer and plastic deformation of the current collectors.

Data-Driven Fuel Consumption Estimation: A Multivariate Adaptive Regression Spline Approach, *Transportation Research Part C: Emerging Technologies*

This paper developed a mesoscopic fuel consumption estimation model that can be implemented into an eco-routing system. Compared with similar macroscopic and mesoscopic fuel estimation models, this model can achieve higher accuracy due to the added features in the model, which shows its potential for implementation into an eco-routing system for rapidly estimating fuel consumption of routes.

Development of Algae Biorefinery Concepts for Biofuels and Bioproducts; A Perspective on Process-Compatible Products and Their Impact on Cost-Reduction, *Energy and Environmental Science*

The concept of developing a biorefinery approach to maximize the value derived from algal biomass is placed in the context needed to address the pressing technical, economic, and sustainability challenges for ultimate commercial realization of a bioeconomy. This review placed bioproducts in the context of a defined conversion pathway based on a recently demonstrated fractionation approach, leaving lipids, solubilized carbohydrates, and proteins accessible for respective bioproduct routes.

Distillation-Based Droplet Modeling of Non-Ideal Oxygenated Gasoline Blends: Investigating the Role of Droplet Evaporation on PM Emissions, *SAE International Journal of Fuels and Lubricants*

A droplet vaporization model was developed to explore ethanol's effect on the evaporation of aromatic compounds known to be particulate matter precursors. Results predict that the presence of ethanol causes enrichment of the higher boiling fractions in the aromatic components as well as lengthens the droplet lifetime. A simulation of the evaporation process in a transient environment as experienced within an engine cylinder predicts a decrease in mixing time of the heaviest fractions of the fuel prior to spark initiation, possibly explaining observations linking ethanol to particulate matter.

Effects of iso-Octane/Ethanol Blend Ratios on the Observance of Negative Temperature Coefficient Behavior Within the Ignition Quality Tester, *Fuel*

An ignition delay study investigating the reduction in low temperature heat release and negative temperature coefficient region with increasing ethanol concentration in binary blends of ethanol/iso-octane was conducted in the Ignition Quality Tester. Significant observations include: (1) Negative temperature coefficient behavior was observed for ethanol/iso-octane fuel blends up to 20% ethanol. (2) Ethanol produced shorter ignition delay times than iso-octane in the high temperature region. (3) The initial increase in ethanol from 0% to 10% had a lesser impact on ignition delay than increasing ethanol from 10% to 20%. (4) The 0-D model predicts that at 0.5 and 1.0 MPa, ethanol produces the shortest ignition time in the high-temperature regime, as seen experimentally.

Efficient and Extensible Quasi-Explicit Modular Nonlinear Multiscale Battery Model: GH-MSMD, *Journal of the Electrochemical Society*

This paper enhances the computational efficiency of the multiscale multidomain model—which aids the scale-up of Li-ion material and electrode designs to complete cell and pack designs, capturing electrochemical interplay with 3-D electronic current pathways and thermal response—using a separation of time-scales principle to decompose model field variables. Simulations demonstrate that the model retains accuracy while substantially reducing computational time, opening an opportunity to use a high-fidelity physics model for design optimization, system parameter identification, and real-time control.

EPA GHG Certification of Medium- and Heavy-Duty Vehicles: Development of Road Grade Profiles Representative of US Controlled Access Highways, *SAE International Journal of Commercial Vehicles*

NREL conducted a national analysis of road grade characteristics experienced by U.S. medium- and heavy-duty trucks on controlled access highways. National statistics on road grade and hill distances were generated and weighted for activity of medium- and heavy-duty trucks. This information was used to develop sample grade profiles potentially to be used in the U.S. Environmental Protection Agency's Greenhouse Gas Emissions Model certification tool as well as in dynamometer testing of medium- and heavy-duty vehicles and their powertrains.

Evaluation of Fuel-Borne Sodium Effects on a DOC-DPF-SCR Heavy-Duty Engine Emission Control System: Simulation of Full-Useful Life, *SAE International Journal of Fuels and Lubricants*

This study addresses the concerns related to the potential for pure biodiesel to degrade diesel emissions control systems, identifies deactivation mechanisms, and determines if a lower limit is needed. The study determined that the primary effect of higher levels of sodium in pure biodiesel resulted in an estimated 50% increase in ash in the diesel particulate filter, while a small amount of precious group metals contamination resulted in degradation of the selective catalytic reduction device.

Features of Resilience, *Environment Systems and Decisions*

The National Academy of Sciences' definition of resilience was used to organize common concepts and synthesize a set of key features of resilience that can be used across diverse application domains. The report proposes a framework for linking features of resilience—critical functions (services), thresholds, cross-scale (both space and time) interactions, and memory and adaptive management—to the planning, absorbing, recovering, and adapting phases identified in the National Academy of Sciences definition.

High-Resolution Mass Spectrometric Analysis of Biomass Pyrolysis Vapors, *Journal of Analytical and Applied Pyrolysis*

In this study, we analyzed the pyrolysis vapors of several biomass sources using a high-resolution double focusing mass spectrometer, allowing for speciation of several compounds that would be detected as a single ion with unit mass resolution. These data not only provide greater detail into the composition of pyrolysis vapors, but also highlight differences between vapors generated from multiple biomass feedstocks.

Investigation of iso-Octane Ignition and Validation of a Multizone Modeling Method in an Ignition Quality Tester, *Energy and Fuels*

An ignition quality tester was used to characterize the autoignition delay times of iso-octane. This work characterized the effectiveness of three modeling methods: a single-zone homogeneous batch reactor, a multizone engine model, and a three-dimensional computational fluid dynamics model. Results suggest using a combined modeling approach wherein the computational fluid dynamics calculations can be used to examine the sensitivity of various model inputs to in-cylinder temperature and equivalence ratios. These values can be used as inputs to the multizone model to examine the impact on ignition delay.

Metal-Organic-Inorganic Nanocomposite Thermal Interface Materials with Ultralow Thermal Resistances, *ACS Applied Materials and Interfaces*

This paper reports a new class of high-performance thermal interface materials—involving the chemical integration of boron nitride nanosheets, soft organic linkers, and a copper matrix—to facilitate the removal of heat dissipated during the operation of electronic, electrochemical, and mechanical devices. The synergistic combination of these properties led to the ultralow total thermal resistivity values in the range of 0.38–0.56 mm^2 K/W for a typical bond-line thickness of 30–50 µm, advancing the current state-of-art transformatively. Moreover, its coefficient of thermal expansion (CTE) is 11 ppm/K, forming a mediation zone with a low thermally induced axial stress due to its proximity to the CTE of most coupling surfaces needing thermal management.

On-Road Validation of a Simplified Model for Estimating Real-World Fuel Economy, *SAE International Journal of Fuels and Lubricants*

This work introduces a methodology for rapidly simulating a specific vehicle's fuel economy over the wide range of real-world conditions experienced across the country. Application of the simplified model to on-road data produced a root-mean-square error of 5.6%, and increase from the 2.4% observed for the model in a controlled laboratory environment. The increase in model error observed in the on-road data demonstrates the difficulty in accurately predicting real-world fuel economy and necessitates appropriate treatment of real-world driving conditions including ambient temperature, road grade, air density, cabin climate control loads, and wind speed and direction.

Performance of Lignin Derived Compounds as Octane Boosters, *Fuel*

The performance of spark ignition engines is highly dependent on fuel anti-knock quality, which in turn is governed by autoignition chemistry. This study explores this chemistry for various aromatic oxygenates—with distinct oxygen functionalities and degrees of alkylation—that can be produced from lignin, to ascertain what the impact is of side groups on anti-knock quality. The results demonstrate that alkylation has a negligible impact on anti-knock quality.

Prediction of Individual Social-Demographic Role Based on Travel Behavior Variability Using Long-Term GPS Data, Journal of Advanced Transportation

This study investigates the pattern of individual travel behavior and its correlation with social-demographic features. The analysis shows that as the number of home-based tour thresholds increases, the variability of most travel behavior features converges, while the prediction performance may not change for the fixed test data.

Role of the Freight Sector in Future Climate Change Mitigation Scenarios, *Environmental Science and Technology*

The freight sector's role is examined using the Global Change Assessment Model for a range of climate change mitigation scenarios and future freight demand assumptions. In climate change mitigation scenarios that apply a price to greenhouse gas emissions, mitigation of freight emissions (including the effects of demand elasticity, mode and technology shifting, and fuel substitution) is more limited than for other demand sectors. In such scenarios, shifting to less-emitting transportation modes and technologies is projected to play a relatively small role in reducing freight emissions in the Global Change Assessment Model.

Selection Criteria and Screening of Potential Biomass-Derived Streams as Fuel Blendstocks for Advanced Spark-Ignition Engines, *SAE International Journal of Fuels and Lubricants*

This article describes a study that identified potential biofuels that enable advanced spark-ignition engine efficiency strategies to be pursued more aggressively. The study produced a list of 40 bioblendstocks with promising qualities by screening an online database of properties and characteristics created through the study to determine which met the requirements for advanced spark ignition engines.

Simulated Impedance of Diffusion in Porous Media, *Electrochimica Acta*

A frequency domain, finite-difference scheme simulates the impedance spectra of diffusion in porous microstructures. In many cases, the spectra deviate significantly from the conventional Warburg-type elements typically used to represent diffusion in equivalent circuit analysis. Certain microstructures show multiple peaks in the complex plane, which may be misinterpreted as separate electrochemical processes in real impedance data. This is relevant to battery electrode design as the techniques for nano-scale fabrication become more widespread.

Socially Optimal Replacement of Conventional with Electric Vehicles for the U.S. Household Fleet, *International Journal of Sustainable Transportation*

In this study, a framework is proposed for minimizing the societal cost of replacing gas-powered household passenger cars with battery electric ones. Sensitivity analysis reveals that the timeframe for the socially optimal conversion of 80% of the sample varies from six to 12 years. The optimal decision variables are sensitive to battery pack and vehicle body cost, gasoline cost, the discount rate, and conventional vehicles' fuel economy.

Technological Growth of Fuel Efficiency in European Automobile Market 1975–2015, *Energy Policy*

This paper looks at the technological growth of new car fleet fuel efficiency in the European Union between 1975 and 2015. To meet the European Union's 2021 fuel consumption target, downsizing of cars, as well as at least maintaining the fuel efficiency technology growth trend observed between 2005 and 2015, is needed. Government policies on controlling improvement in acceleration performance or promoting alternative fuel vehicles are also important to achieve the European Union's 2021 target.

Understanding Trends in Autoignition of Biofuels: Homologous Series of Oxygenated C5 Molecules, *Journal of Physical Chemistry A*

This study used quantum mechanical modeling to systematically compare the effects of oxygen functionalities on potential energy surfaces of oxygenated biofuel reaction and associated kinetics to understand how they affect experimental trends in autoignition and cetane number. The quantum mechanical results in this work show that aldehydes and ethers have high cetane numbers because of low barriers to form hydroperoxy radicals, QOOH, from peroxy radicals, ROO•, and because of favorable energetics for hydrogen atom abstraction from pentanal. Alkyl groups adjacent to carbonyl groups have a low C–H bond dissociation energy because of resonance stabilization of the resulting radical. However, this also leads to a low energy barrier for dissociation of the peroxy radical, ROO•, which competes with formation of QOOH, an important reaction in chain branching. Thus, the cetane number for these molecules is typically low. Alcohols have low cetane numbers because reaction of the peroxy radical to give aldehydes or ketones is fast and reduces the formation of QOOH.

Urban Nexus Science for Future Cities: Focus on the Energy-Water-Food-X Nexus, *Current Sustainable/Renewable Energy Reports*

Rapid urban expansion of the world's cities is placing unprecedented demands on the energy, water, food, and other (X) systems (e.g., mobility) that each offer multiple life-supporting services. This paper proposes an applied "urban nexus science" framework to identify integrated and synergistic pathways toward achieving urban sustainability.

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