Next Generation Biofuels and Advanced Engines for Tomorrow's Transportation Needs

A HITEC Workshop • *November 17-18, 2009*

Sandia National Laboratories

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Next Generation Biofuels and Advanced Engines for Tomorrow's Transportation Needs

November 17 and 18, 2009
San Ramon Marriott
San Ramon, CA

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November 17–18, 2009 San Ramon Marriott, San Ramon, CA

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Keynote: *Engineering Microorganisms for Production of Advanced Biofuels*—Jay Keasling, CEO, Joint BioEnergy Institute, & Professor, UC/Berkeley
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Afternoon—

Luncheon speaker: *Testing & Certification Requirements for the Biofuels Infrastructure*—Dr. Thomas Fabian, Underwriters Laboratories
Report from Breakout Session 3
Summary of the Workshop & Proposed Next Steps—Bob Carling, Sandia

OVERVIEW

In November 2009, Sandia National Laboratories hosted the **Next Generation Biofuels and Advanced Engines for Tomorrow's Transportation Needs Workshop**. The event focused on the combined opportunities in biofuels and engines in the transportation sector. The workshop brought together the DOE Combustion Research Facility and the DOE Joint BioEnergy Institute along with oil companies, biofuel developers, engine manufacturers, suppliers, and experts from the university, regulatory, finance, and national laboratory communities. The intersection of biofuels and engines, if properly scaled, can meet a triad of national goals:

- Reduced climate impact
- Economic development
- Energy security through energy diversity

The workshop identified opportunities for co-development of biofuels and engines, it addressed roadblocks to success, and it outlined joint biofuel and engine R&D needs. Over two days, participants underscored a series of key attributes that the community must address to make introducing next generation biofuels a reality in the transportation sector. These attributes can be summarized as the need for:

Clean, Sustainable, Compatible, Liquid, Fuels

- **Clean.** Next generation biofuels might be oxygenates, blended constituents, or drop-in replacements. Their combustion, however, must not increase Environmental Protection Agency (EPA) designated criteria pollutants, nor can these biofuels introduce other air and water contaminants.
- **Sustainable.** Based on a thorough life cycle analysis, the CO_2 footprint of biofuels must be lower than the petroleum-based fuels that are being displaced.
- **Compatible.** The need for compatibility has multiple dimensions. First, the biofuel should be compatible with both current and future engine designs, including any aftertreatment and fuel storage components on board the vehicle. Second, the biofuel should be compatible with the current distribution infrastructure as well as future infrastructures that may evolve. Compatibility with the current fuel industry infrastructure will accelerate the introduction of alternatives.
- **Liquid.** The driving force for biofuels is to displace petroleum feedstocks. The goal is to both reduce the CO_2 footprint and allow for enhanced security through diversity and choice in fuel sources. Liquid petroleum products are attractive in internal combustion engines due to their energy density (volume and weight). Next generation biofuels must be of the same or higher energy density.
- **Fuels.** To make a significant impact on the transportation energy sector, a path to scale-up of next generation biofuels must be included in the research, development, and deployment planning. Business models that address scaling to significant quantities are critical.

General Observations

The workshop recognized three important issues surrounding the development of biofuels:

- The definition of fungible or drop-in fuels (DIF) needs to be clarified. The framework for fungible fuels development is not clear, nor have the fuel and engine communities fully vetted the options.
- Fuel specifications can become the bridge between engines and biofuels. Both gasoline and diesel engine designers need to provide greater specificity to the fuels development communities, both for near-term and for future engine concepts.
- An integrated biofuels and engines research program is key. Today two separate DOE program offices fund research on biofuels and advanced engine concepts. A consolidated research program would accelerate the transition to biofuels for the transportation sector.

Proposed Actions

The above observations drive the following recommended actions:

- **Action 1.** Modernize the testing, specification, and certification of all fuels.

- **Action 2.** Plan and integrate the research and development of next generation biofuels in conjunction with the development of advanced engines.
- **Action 3.** Develop specific guidelines, roadmaps, and objectives for co-development of next generation biofuels and advanced engines.
- **Action 4.** Convene an International Fuels and Engines Summit, sponsored by industry with government and university participation, to ratify a fuels/engines strategy and implementation framework.

WORKSHOP MOTIVATION AND KEY QUESTIONS

The Next Generation Biofuels and Advanced Engines Workshop fostered a dialog among researchers and experts from industry, academia, and government. Attendees developed consensus regarding workshop goals, roadblocks to success, and ways to accelerate the transition to biofuels. Participating companies and institutions are listed in Appendix A. An agenda for the two day event appears on page iv.

The following key questions were posed to guide the discussion:

Breakout session 1:

- How does a new fuel get introduced into the marketplace?
- Where does the "handshake" occur between fuel formulation and engine design, and is this optimal?
- What means can accelerate the introduction of next generation biofuels into the marketplace?

Breakout session 2:

- Optimally, how would regulations enable the introduction of advanced engines and biofuels?
- Are today's gasoline and diesel fuel specifications robust?
- How might biofuels and engines evolve and scale up?

Breakout session 3:

- What are the institutional barriers to the joint support of biofuel and engine R&D?
- What research structure will meet the needs of the biofuel and engine communities?
- What are key issues that need research focus to accelerate the efficient use of biofuels?

BACKGROUND MATERIALS AND CHARTS

A pre-workshop white paper was developed to provide guidance and background for the discussion. This paper is included in Appendix B. In summary the white paper:

- Suggests opportunities and motivation for co-development of biofuels and engines.
- Outlines development of next generation biofuels from an infrastructure and feedstock conversion perspective, including the following:
  - Microbial production
  - Thermo chemical production
  - Algal production.
- Summarizes the impact of biofuel properties on engine design, including the following:
  - Downsizing and down speeding
  - Combustion system
  - Impacts of biofuel property changes on performance and infrastructure.

To guide thinking about integration of next generation biofuels and advanced engines, we developed two figures. Figure 1 is an overview of the various development paths that internal combustion engines might take over the next 40 years. The projections to

2020 are robust because eight to 10 years are typically required for a new engine concept to fully penetrate the marketplace. The timeframe for 2020–2050 is more speculative, but is based on predictions of technological maturity as well as evolution of the internal combustion engine marketplace.

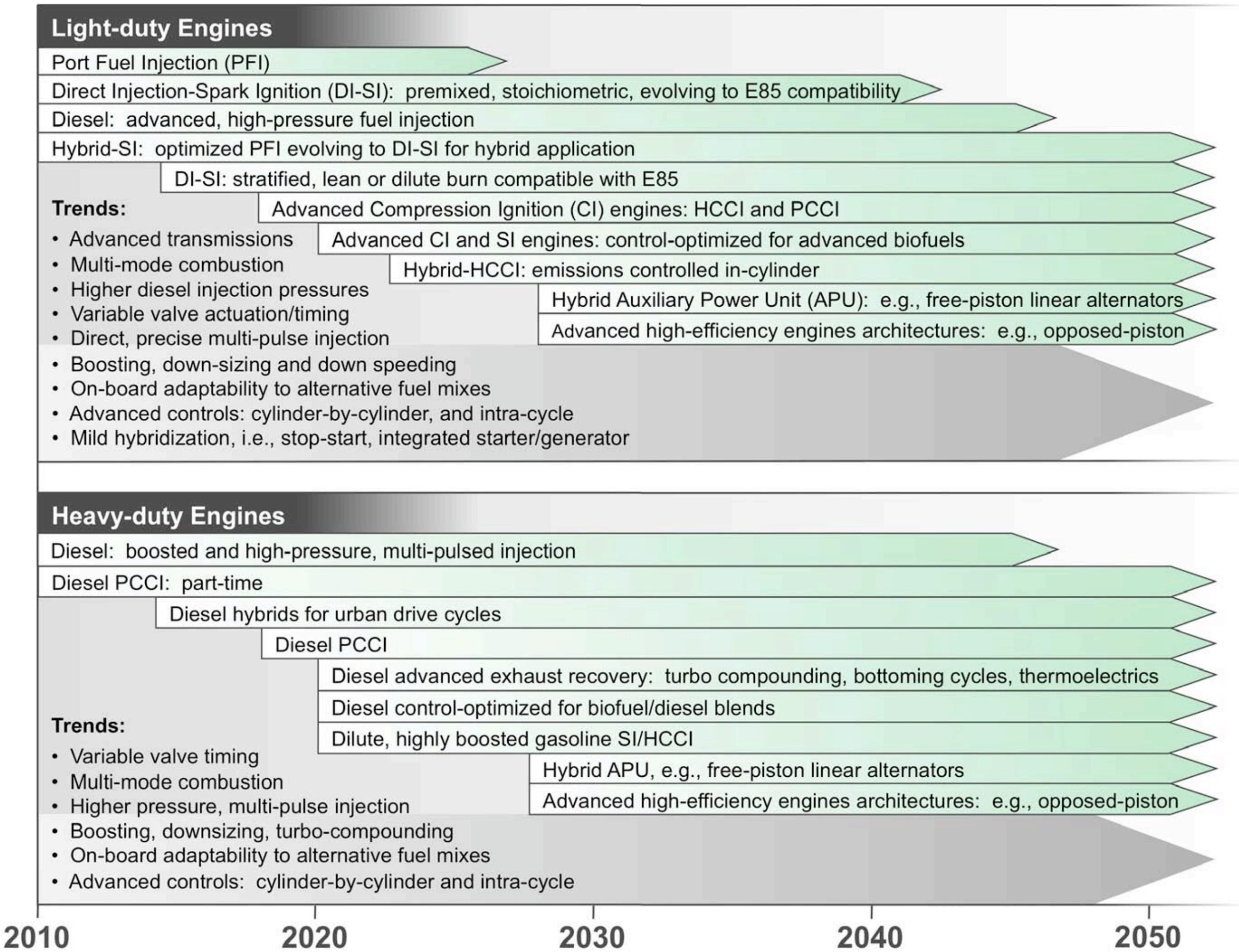

Figure 1: *An overview of internal combustion engine technologies, 2010-2050*. Actual and proposed technologies for internal combustion (IC) engines in both light duty and heavy duty applications. Information from Dennis Siebers, Sandia.

Figure 2 is a schematic of today's biofuels sector. The variety of feedstocks, conversion technologies, and end point fuels reflect the current opportunity driven nature of biofuels processing. Most new companies entering the field develop cooperative relationships with feedstock providers, oil companies, and in some cases specific engine companies. However, there is little market discipline or setting of standards, except in the case of ethanol. The level of biofuels in the total U.S. fuel mix in 2008 was 4%, mainly blended ethanol as an oxygenate. Projections by the Energy Information Administration (EIA) for 2035 envision a total of 12% biofuels in the future fuel mix for the United States.

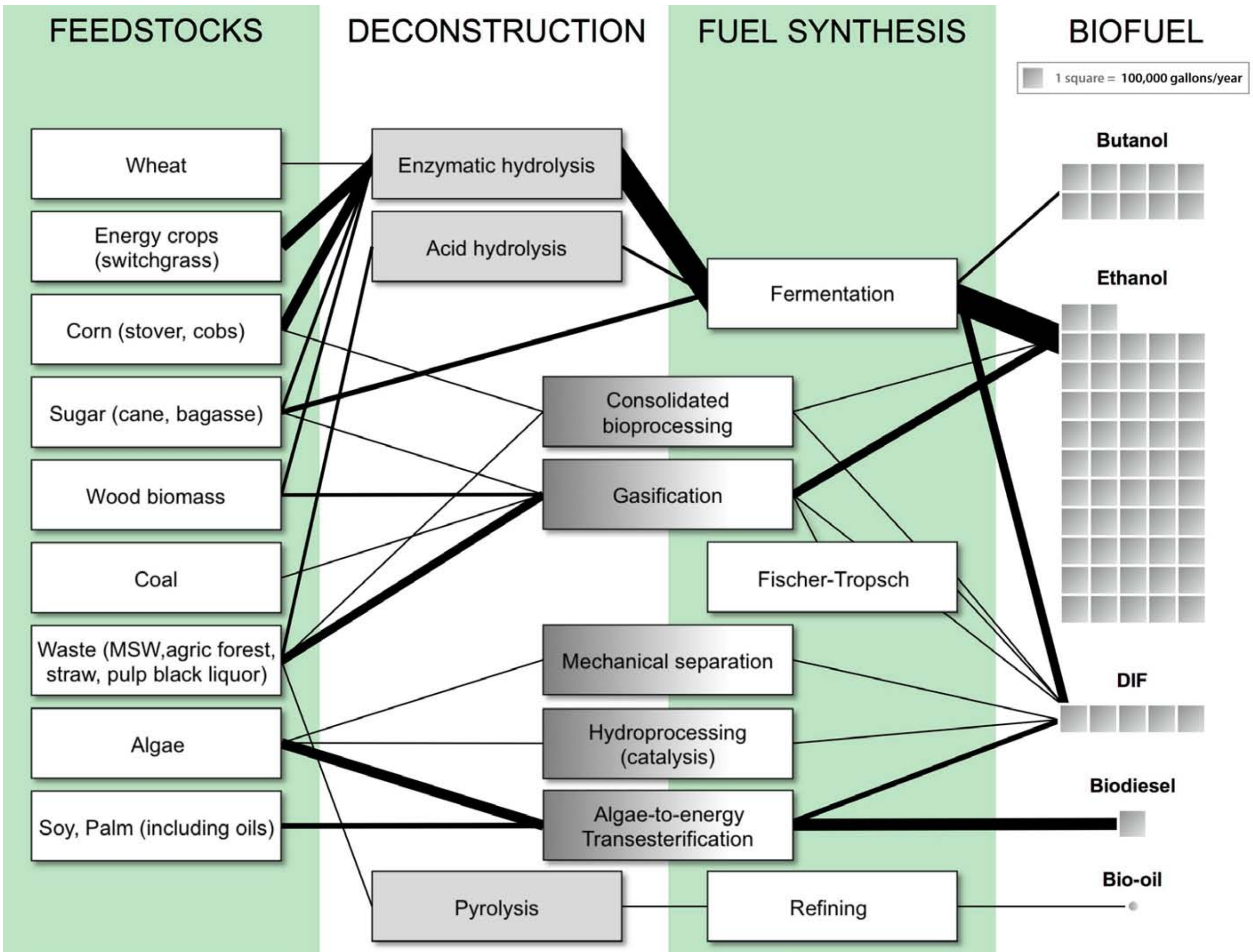

Figure 2: *Today's Biofuels Sector.* An overview of technologies used by the top 50 biofuel companies in 2009 in terms of feedstocks, conversion processes, and biofuels produced. Line thicknesses represent the relative number of these 50 companies using these processes in 2009. Quantities of biofuels produced are from 2009 company reports. Some companies produce fuels for markets outside of the United States. (DIF are drop-in fuels, mainly diesel type products.) Figure design from Nathan Hillson and Harry Beller, Berkeley Lab. Data from Jim Lane (ed.), Biofuels Digest: <biofuelsdigest.com>

MAJOR POINTS FROM KEYNOTE AND PANEL PRESENTATIONS

Keynote *Trends in the Transport Industry: New Vehicles, New Engines, New Fuel Sources.*

Kathryn Clay, Director of Research, Auto Alliance

Major Points

- Success in the future of the transport industry rests in three arenas: Vehicle technology, next generation fuels, and consumer acceptance.
- New vehicle/engine combinations over the next 20 years will include a mix of electric plug-ins, gasoline electric hybrids, and flex fuel (biofuels compatible) automobiles.
- Key to the near-term introduction of biofuels is the blending of new biofuels into the gasoline and diesel pool.
- A gasoline price floor would send firm price signals to the consumer and would encourage the development and sale of more fuel efficient vehicles.

Keynote *Engineering Microorganisms for Production of Advanced Biofuels.*

Jay Keasling, CEO Joint BioEnergy Institute and Professor, UC/Berkeley

Major Points

- To increase the amount of biofuels in the U.S. fuel mix, a bridge strategy is to tailor enzymes to more efficiently convert cellulose to ethanol.
- Synthetic biology allows scientists to alter the genetic makeup of bacteria and rewire their metabolism to synthesize desired molecules for drug, chemical, and fuel applications.
- As an example, isopentanol, a gasoline substitute, can be successfully produced through isopentanyl pyrophosphate metabolism in bacteria.
- Branched chain esters can be made from fatty acids and isoprenoids, as could biodiesel type fatty-acid esters through a synthetic biology pathway.
- Greater guidance from the engine and petroleum distribution sectors is needed to ensure that the next generation of biofuels is compatible with both engine combustion and fuel infrastructure.

Transportation Fuels, Emissions, and the Future of the Regulatory Regime in California.

Alberto Ayala, California Air Resources Board

Major Points

- Historical interests by the Air Resources Board were health effects and smog producing criteria pollutants: NO_x, CO, hydrocarbons, particulate matter, and toxics.
- Now GHGs (chiefly CO_2, but also N_2O, CH_4, HFCs, PFCs, and SF_6) have been added to the list of regulated exhaust components. Most recently, the State has been exploring the climate and air co-benefits of black carbon mitigation. In California 40% of GHGs come from transportation. Of that, 70% of GHGs come from passenger vehicles, 20% from heavy duty trucks, and 3% each from intrastate aviation, shipping, and locomotives.
- The State is taking a three pronged approach: cleaner vehicles through the Pavely I and Pavely II regulations on vehicle GHG emissions, lower carbon fuels through a Low Carbon Fuel Standard, and reduction in Vehicle Miles Traveled through zoning and land use planning.
- The new law, AB32 or the Global Warming Solutions Act of 2006, sets California's GHG reduction goals and timeframes.

  For motor vehicles

  - 2010–2016 focuses on GHG reduction improvements in conventional vehicles and the introduction of biofuels through ethanol blending.

  - **2016–2025** focuses on hybridization, lower vehicle weight, next generation biofuels.
  - **2025–2050** focuses on electric drive trains and ultra-low carbon fuels.
- Black carbon is becoming a greater concern to State regulators. Potential increases in black carbon may come from a new engine technology: direct injection of gasoline.

A Brief History of Fuels and Engines, circa 1900, and the Flow of Investments to Fuels and Transport Today.

Matt Trevithick, Partner, Venrock

Major Points

- Electric vehicles preceded the internal combustion (IC) engine, developing in parallel with the electrification of cities and towns.
- Internal combustion engines, championed by Henry Ford, were developed to provide extended range for touring the countryside.
- Initial IC engine fuels varied widely as did engine designs, but became more standardized over time. Octane number was identified as a standard for IC engines.
- Next generation fuels and advanced engine design concepts are a component of most venture capital investor portfolios. Issues of scale-up and broad applicability drive specific investment decisions.
- Most advances in automobile fuel and engine technology were first developed for the racing circuit, especially the long endurance 24-hour touring races. These venues and events are growing and becoming much more international in scope.

Testing and Certification Requirements for the Biofuels Infrastructure.

Thomas Fabian, Underwriters Laboratories (UL)

Major Points

- UL maintains a certified components and parts list for all equipment involved in the blending, storage, and distribution of fuels to the consumer.
- Not all equipment and storage facilities are compatible with ethanol blends. This problem will be made more severe as higher ethanol fractions are blended with conventional gasoline.
- Corrosion and compatibility with components outside the vehicle itself must be considered as new biofuels, both light duty gasoline replacements and heavier bio-diesels, are introduced into the fuel mix.
- The lack of standards and certification, ASTM, UL, or other, can limit the rate of penetration.

OBSERVATIONS FROM THE PANELS AND BREAKOUT SESSIONS

Historical Observations

In the 1970s, the United States undertook a major change in the available transportation fuels. The introduction of unleaded gasoline into the retail fuel mixture was accomplished within the existing petroleum refining and fuel distribution systems. Extensive consultation between fuel and engine/automobile companies preceded the introduction of this new fuel. The historical centralized structure of the supply chain was maintained. Standards and certification were developed before introducing unleaded formulations.

In the case of biodiesel, historical development followed a much more decentralized and entrepreneurial model, which persists today for all biofuels. The effort began as an underground market, assisted by the ability to avoid taxes from "backyard" production and sale of biodiesel. When utilization grew to a size that affected the performance of the vehicle fleet, standards were then proposed and developed with recognition of the biofuels market potential. Today, certification procedures and tests are being recast in an ongoing process. However, the fragmented and decentralized structure of the diesel industry remains, and to some extent it remains in the gasoline replacement industry as well. Ethanol is the exception, especially as a blended oxygenate. Increasingly, the centralized fuel and engine communities are capturing the ethanol market.

Conference participants brainstorm opportunities for biofuels and advanced engines.

The interface between next generation biofuels and advanced engine development also remains fragmented, with many of the entrepreneurial biofuel start-up producers following independent paths and partnerships with specific automobile and engine manufacturers. This fragmentation introduces a tension between incumbent oil and engine companies and those new companies seeking to introduce their process and product into the future fuel mix.

Today's State-of-Play

The workshop identified the following near-term considerations. First we must:

Anticipate need. Many workshop participants asserted that due to the current infrastructure and due to the 20-year turnover rate of the car park, any next generation fuel must look like gasoline and diesel. However, what this meant was cast in terms of today's engine requirements, today's specification, and the current distribution infrastructure. The future needs and opportunities were less strongly articulated.

Define fungible fuel. Participants raised the key point that uncertainty surrounds the definition of a fungible fuel. In particular, at what point do we assess and determine whether a fungible fuel is similar to today's fuel mix? When the fungible fuel is a:

- biocrude, compatible with the existing refining and upgrading infrastructure?
- fuel component that is readily blended with existing gasoline and diesel, such as the E5, E10, E15 and B10, B20 approach?
- drop-in-fuel compatible with both today's and future engine concepts?

Set clear objectives. Another observation was that the objectives for producing and introducing biofuels into the fuels mix must be clearly articulated. One participant observed that there is a regulatory restriction on co-processing or co-refining of biocrude with conventional petroleum-based crudes. This drives the greatest value added step in the supply chain (the development of final fuel products) away from the oil companies and refiners and toward new entrants to the marketplace. One rationale suggested for this restriction is that biofuel policies are driven by a desire to strengthen the agricultural sector and the economic vitality of the rural sections of the country.

Ensure security. Also noted was the need for energy security. This can be achieved through fuel diversity and competition, and by not importing significant portions of our transportation sector energy. An additional rationale was to reduce the carbon footprint through use of biofuels for transportation. During the workshop there was no discussion of the magnitude of the climate benefits from biofuels, although this remains a significant topic of debate among the technical and policy making communities.

Map out development. Workshop participants suggested that a) the market alone will not achieve the desired objective, once that objective it is articulated, and b) regulations are needed to drive changes. The new Renewable Fuel Standard and other regulatory regimes are beginning to affect the direction of the marketplace. However, close integration between fuels and engines is still lacking and not covered by regulation or a strategic framework to enable this integration. Essentially, no roadmap exists to guide future development.

Consider risks. Finally most attendees agreed that there is a great deal of risk in the system and that risk reduction efforts are needed to accelerate changes in the fuel mix. One risk arena was the conflicting regulatory requirements, especially in California, between biofuels and zero emission vehicle mandates. Another risk arena was the legal framework surrounding warranties and the burden on the vehicle companies to bear the predominant share of the liability.

The biofuels conference brought together representatives from the oil industry, fuels developers, and engine manufacturers and suppliers to meet with experts from academia and the finance and research communities. They discussed timely solutions to problems that surround the transition to clean, sustainable fuels.

Tomorrow: Looking to the Future

Workshop participants suggested these broad actions as a means to accelerate next generation biofuels into future engine designs:

Finalize products. Set requirements for finished products, then let the market determine the most efficient and cost effective feedstocks. Don't dictate the feedstocks for biomass-derived fuels.

Work toward scale. Develop technologies and incentives with a scale of millions of gallons per year in mind.

Build flexibility into engine design. Take advantage of new on-board engine control systems to account for variability in fuel chemistries. Also, incorporate dual fuel tanks to increase fuel mix flexibility.

Account for carbon. Refine the methodology to better account for the life cycle carbon footprint from biofuels.

Reduce risk. Build more long-term certainty into the regulatory regime. Use previous models, like the Automobile Oil Program of the 1980s, to coordinate and conceptualize fuel and engine design strategies for the future. Share liability between fuel and engine/automobile companies.

Recognize differences. Refining fuels from crude oil is a separations process that still results in a complicated and diverse mixture of chemicals. Engines that run on gasoline and diesel are designed for and take advantage of this complexity. Processing biomass into liquid biofuels often results in a highly reduced set of chemical species. Except possibly for ethanol, engines have not yet been designed to take advantage of the benefits of biofuels' unique and more restricted chemistries.

Revise specifications. Introduction of bio-derived fuels and also of petroleum-based fuels from unconventional crude sources requires a review and modernization of fuel characteristics and specifications.

Scale up the demand and fleet testing. Utilize the market power of the federal government and its vehicle fleet purchases to provide additional demand and to provide a fleet for testing new engines and new fuels.

Shift the policy focus. The thrust of biofuels policy should shift from rural development to energy security. This would change the incentive framework and the potential evolution of the U.S. fuels industry.

PROPOSED ACTIONS TO MEET THE WORKSHOP GOALS

Action 1: Modernize the testing, specification, and certification of all fuels.

Test methods and specifications are the final link between the fuel producer and the engine manufacturer. After a fuel is considered fit for use, it enters the marketplace with a certification that it will meet all customer and performance requirements. A strong consensus among workshop participants was that new emission and performance requirements, new fuel chemistry opportunities, and new engine concepts will all need a modernized approach to testing and certification. Please see *Improving Test Methods for Emerging Fuels* for suggestions on what should be analyzed and what new test methods are now available.

IMPROVING TEST METHODS FOR EMERGING FUELS

Text and figures from Charles Mueller, Sandia National Laboratories

Fuel test methods are techniques by which fuel properties (such as ignition quality, volatility, and compositional characteristics) are measured. The properties of a given fuel determine how well it is suited to a given engine application. Standardized test methods are employed to demonstrate whether fuel properties fall within ranges that have been deemed acceptable for a given application. The acceptable range of measured values yielded by a given test method is called a *specification*. Today, each commercial fuel is required to meet specifications on a number of different properties, mainly to help ensure that the fuel satisfies all customer requirements (e.g., the fuel provides adequate engine performance and durability). When a fuel satisfies all agreed upon requirements, it is said to be *fit for use*.

With the introduction of advanced engine technologies, exhaust-gas aftertreatment systems, and nontraditional blend stocks, situations have arisen in which fuels have met all of the prevailing specifications but have caused substantial engine system degradation. One reason for this is that, although fuel test methods have evolved over time, many were developed between the 1920s and the 1950s for the petroleum-based fuels, engine technologies, and the analytical techniques available at the time. Many have remained substantially unchanged ever since. For example, the cetane number test method for diesel fuel ignition quality was developed in the 1930s. The distillation test method for diesel fuel volatility was introduced in 1921 and also remains largely unchanged.

The present environment of rapidly changing fuels, engines, and aftertreatment systems necessitates the re-evaluation of existing fuel test methods. This presents opportunities for the introduction of more accurate, science-based techniques to characterize all fuels and their suitability for use in advanced combustion engines. One opportunity is in development of an improved ignition quality test method because it has been shown that neither octane number nor cetane number adequately predicts the auto-ignition behavior of a fuel over a range of partially premixed charge conditions (see Figure A1). Advanced analytical techniques (e.g., nuclear magnetic resonance and advanced gas chromatography/mass spectrometry) could be standardized to give valuable insight into fuel chemical composition (see Figure A2). Precise knowledge of fuel composition, combined with highly advanced models and computer-based simulations, may be able to predict the in-cylinder performance of a fuel. An improved volatility test method could help elucidate the relationships between fuel composition and vaporization characteristics (see Figure A3). A test method to quantify the sooting propensity of a fuel also could be established. Progress is being made in all of these areas, but guidance from engine designers is needed regarding the desired parameter space for both current and future fuels. These ranges of values would need to be agreed upon and adjusted as new engine concepts are conceived and planned for introduction into the marketplace, usually an eight to 10 year process.

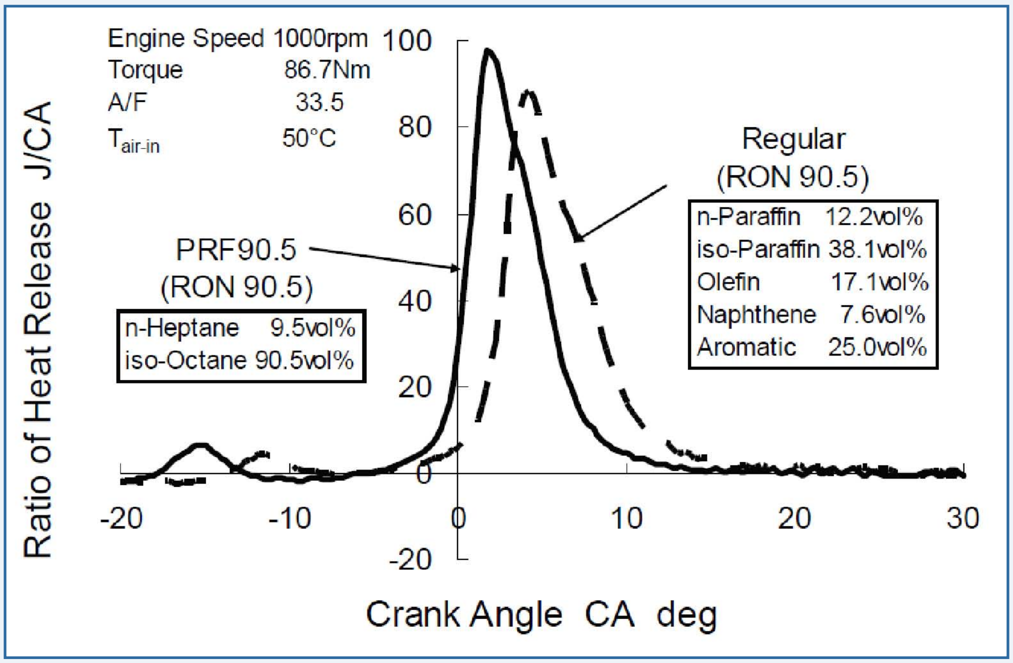

Figure A1. ***Failure of octane number to predict auto-ignition (knock) behavior.*** Two fuels with the same research octane number (RON) can exhibit significantly different heat release timings in a homogeneous charge compression ignition (HCCI) engine. The low and high temperature heat release peaks occur 4.0 and 2.5 crank-angle degrees later, respectively, for the gasoline that contains olefins, naphthenes, and aromatics in addition to n- and iso-paraffins[1]. This behavior indicates both the insufficiency of the RON test method to predict HCCI ignition delay and the potential impact of a fuel's chemical composition on its combustion characteristics.

[1] Shibata, G. and Urushihara, T., "Auto-Ignition Characteristics of Hydrocarbons and Development of HCCI Fuel Index," SAE Technical Paper 2007-01-0220 (2007).

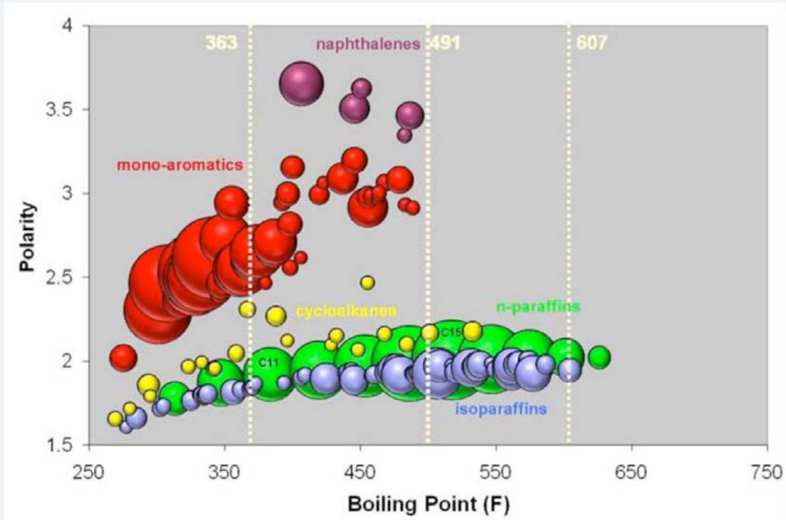

Figure A2. ***Advanced fuels chemistry characterization.*** Modern analytical approaches, such as two dimensional gas chromatography/mass spectrometry (2 D GC/MS), can provide detailed information about the chemical composition of a fuel. This plot uses "bubbles" to show the compositional characteristics of a #2 diesel fuel, where each bubble represents a collection of molecules containing a given number of carbon atoms and within a given hydrocarbon family. The size and color of each bubble indicate relative abundance in the fuel and hydrocarbon family, respectively, and the bubbles are distributed according to boiling point and polarity.[2]

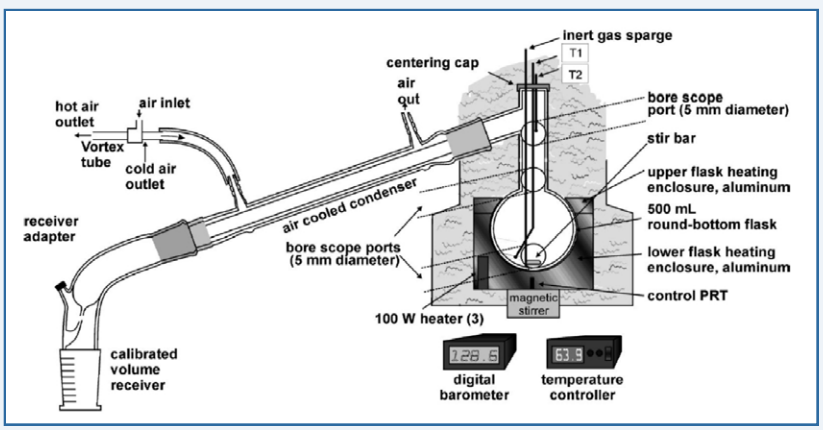

Figure A3. ***Technique for measuring fuel volatility.*** Apparatus for measuring the boiling point distribution of a fuel via the advanced distillation curve (ADC) method. The ADC method has a number of advantages over current techniques for measuring distillation curves, including the following: 1) temperature, volume, and pressure measurements that are true thermodynamic state points and useful for developing equations of state and 2) the potential to sample and quantitatively assess the composition of each distillate fraction as well as resultant characteristics such as energy content, corrosivity, and trace impurities.[3]

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[2] Gallant, T., Franz, J.A., Alnajjar, M.S., Storey, J.M.E., Lewis, S.A., Sluder, C.S., Cannella, W.J., Fairbridge, C., Hager, D., Dettman, H., Luecke, J., Ratcliff, M.A., and Zigler, B.T., "Fuels for Advanced Combustion Engines Research Diesel Fuels: Analysis of Physical and Chemical Properties," SAE Technical Paper 2009-01-2769 (2009).

[3] Ott, L.S. and Bruno, T.J., "Variability of Biodiesel Fuel and Comparison to Petroleum-Derived Diesel Fuel: Application of a Composition and Enthalpy Explicit Distillation Curve Method," Energy & Fuels 22:2861–2868 (2008).

Action 2: Plan and integrate the development of next generation biofuels in conjunction with the development of advanced engines.

While there was general agreement that "boutique" fuels should not be pursued, (i.e., specific fuels for specific engines), an alternate approach is to redefine *fungibility* and consider it from both the engine and the fuel perspective. The concept of fungible fuels (as currently construed among policy makers, biofuels entrepreneurs and engine developers) focuses on today's engine designs and today's biofuel production pathways (see Figures 1 and 2 in **Background Materials and Charts** section). Within the current broad spectrum of chemical species present in gasoline and diesel, there are likely specific molecules from tailored biofuels that can achieve even better performance from future engines. There is great leverage if these can be blended with petroleum-based products. At the same time, engine concepts described in Figure 1 could be developed with the anticipation of future fuel chemistries, if a sufficient lead time can be built into the development cycle. Please see ***Designing Spark Injection Engines to Take Advantage of Ethanol*** for a description of how engine downsizing, a currently available technology, could be optimized to take advantage of the higher octane of ethanol. Please see ***Designing Biofuels to Improve Performance in Advanced Diesel Engines*** for a description of how a new biomass feedstock, cuphea, can be tailored to produce a higher volatility biodiesel to enable an engine design scheme called low temperature, early injection diesel. This low temperature approach is being adopted today by some engine manufacturers.

DESIGNING SPARK INJECTION ENGINES TO TAKE ADVANTAGE OF ETHANOL

Text and figures from Magnus Sjoberg, Sandia National Laboratories

The United States and most industrialized countries are committed to substantial reductions of CO_2 emissions, in part through the use of bio-derived fuels. Ethanol is the most widely used biofuel today with a 4% contribution to the energy needs of gasoline type powered vehicles in the United States.

One effective technique for increasing the fuel mileage of vehicles powered by gasoline type spark ignition (SI) piston engines is to apply engine downsizing. The reduction can be achieved by reducing the number of cylinders and/or by reducing the swept volume of each cylinder. If no further measures are taken, increased fuel mileage will be attained at the expense of peak torque and power. In order to not comprise vehicle drivability, it is desirable to maintain both power and torque at the level of the standard engine. This can be achieved by applying intake pressure boost, either by the use of a turbocharger or a mechanical supercharger. With higher intake boost pressure, the engine can be downsized more for better fuel economy, while vehicle performance is maintained.

However, the maximum intake boost that can be applied will at some point become limited by the onset of knock. Engine knock is the manifestation of auto-ignition of the end-gas, which is being compressed and heated by the pressure rise caused by the flame that propagates from the spark plug. The resistance to auto-ignition, and, therefore, the resistance to engine knock, is typically measured in traditional research octane number (RON). To first order, a fuel with higher octane rating will resist auto-ignition better and, therefore, also be more suitable for boosted engines using downsizing and turbo charging. Premium gasoline may have RON = 91 whereas pure ethanol boasts a higher RON = 107. Auto-ignition data acquired for homogeneous charge compression ignition (HCCI) operation indicate that there are reasons to believe that ethanol has superior resistance to knock for highly boosted operation.

Ethanol maintains true single stage auto-ignition characteristics even for boosted operation. Figure B1 plots the early heat release rate (HRR) for ethanol auto-ignition for a range of intake pressure (P_{in}). As can be seen, essentially no exothermic heat releasing reactions occur until 355°CA (crank angle) (5°CA before TDC [top dead center]). Beyond this point, the HRR gradually increases until hot ignition occurs around 366°CA. The shape of the normalized HRR traces are very similar, and ethanol shows no tendency to develop low temperature heat release (LTHR) as P_{in} is increased. In sharp contrast, gasoline exhibits a marked increase of the HRR preceding the hot ignition point as P_{in} is increased (Figure B1). For the lowest P_{in} of 100 kPa, the HRR trace does not start to curve up until 355°CA, which is similar to ethanol. However, for the higher P_{in} it is clear that the heat release starts earlier and that the early HRR prior to hot ignition is substantially higher. At the highest P_{in} = 180 kPa, gasoline even starts to exhibit LTHR around 347°CA. These results indicate that boosted operation with regular gasoline can relatively quickly become limited by the onset of knock, whereas ethanol maintains its single stage ignition behavior and has the potential to tolerate much higher pressure levels. In summary, ethanol has a clear potential to enable increased engine efficiency through its good high pressure performance and true single stage auto-ignition characteristics, while simultaneously replacing petroleum by being a renewable fuel.

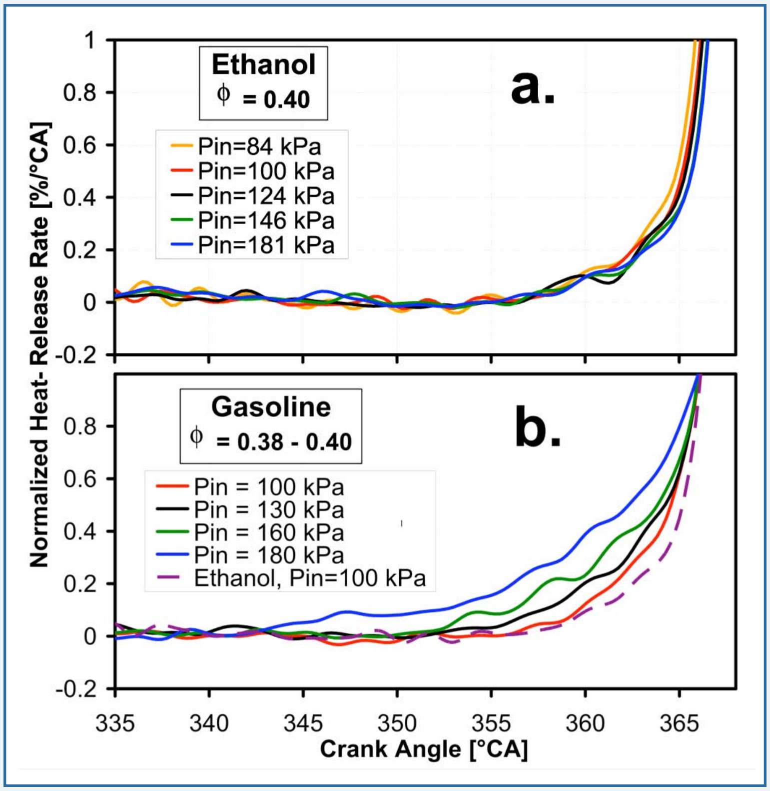

Figure B1. Experiments that indicate the benefit of ethanol over gasoline to resist knock in high pressure engines. Early auto-ignition HRR as the intake pressure, P_{in} is changed, using ethanol (a) and gasoline (b). Reproduced from SAE paper 2010-01-0338.

DESIGNING BIOFUELS TO IMPROVE PERFORMANCE IN ADVANCED DIESEL ENGINES

Text and figures Brian Fisher, Sandia National Laboratories

Low temperature combustion (LTC) strategies employing early direct injection (DI) of fuel offer the promise of lower emissions of nitrogen oxides (NO_x) and particulate matter from diesel engines. Early DI, intended to enhance pre-combustion mixing, unfortunately, can lead to impingement of liquid phase fuel on in-cylinder engine surfaces because of the low temperature and low density conditions in the cylinder during fuel injection. Liquid fuel impingement results in increased fuel consumption and higher emissions of unburned hydrocarbons and CO. Recent research has also shown that fuel films resulting from impingement can ignite to form in-cylinder pool fires that significantly raise soot and NO_x emissions[4,5,6,7,8,9,10]. The good news is that impingement and its negative potential consequences can be avoided by using higher volatility fuels.[11]

These observations have important implications for future alternative fuels. Biodiesel, which has been shown to be a viable compression ignition engine fuel, has lower volatility than conventional diesel and is, therefore, more prone to liquid fuel impingement.[12] Biodiesel fuels are comprised of mono-alkyl esters of long chain fatty acids typically containing at least sixteen carbon atoms. For example, soy-derived biodiesel is composed primarily of methyl oleate and methyl linoleate, both of which contain eighteen carbon atoms in their hydrocarbon chains. Next generation biodiesel fuels, however, might contain shorter chain molecules to promote higher volatility. For example, biodiesel-derived from cuphea oil is being considered because its primary constituent is methyl decanoate, a methyl ester that contains only ten carbon atoms in its hydrocarbon chain.[13] The chemical structures of methyl decanoate and methyl linoleate are shown in Figure C1, and the composition profiles of soy- and cuphea-derived biodiesel are shown in Figure C2.

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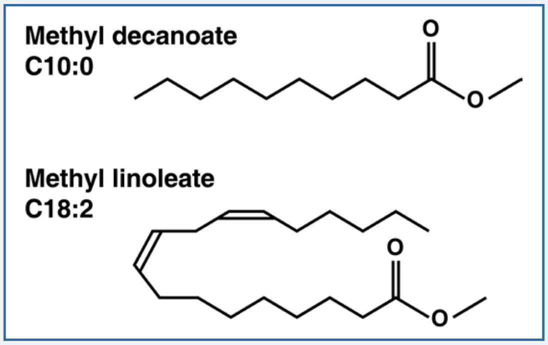


Figure C1. ***Variation in chemistry between soy and cuphea for biodiesel.*** Chemical structures of methyl decanoate (C10:0) and methyl linoleate (C18:2), the primary constituents of cuphea- and soy-derived biodiesel fuels, respectively. The Cx:y notation is commonly used to abbreviate fatty-acid methyl esters, where x and y denote the number of carbon atoms and the number of carbon-carbon double bonds, respectively, in the alkyl chain.

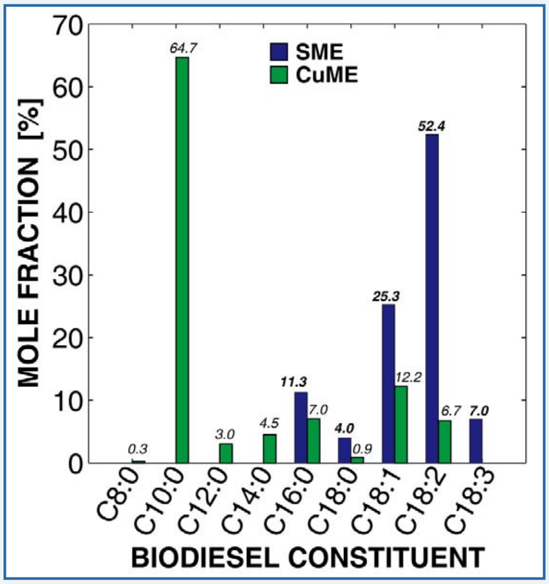
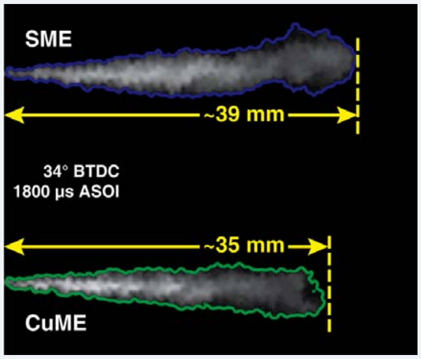


Figure C2. ***Carbon chain lengths for soy and cuphea biodiesel.*** Fatty-acid methyl ester compositions for neat soy- (SME = soy methyl esters) and cuphea-derived (CuME = cuphea methyl esters) biodiesel fuels.

Researchers have developed a method to measure in-cylinder liquid phase fuel penetration length during injection in an optical diesel engine using high speed laser light scattering.[14] The method has been applied to soy- and cuphea-derived biodiesel fuels under identical early DI conditions, with sample results shown in Figure C3. Under the conditions studied, with the same injection timing and thermodynamic history during the engine cycle, the liquid length is ~10% shorter for cuphea-derived biodiesel than for soy-derived biodiesel. This behavior suggests that fuel volatility is an important consideration in designing next generation biofuels for advanced diesel engines. Future biodiesel fuels may be even more attractive, particularly for LTC strategies, if they are engineered to consist of relatively short hydrocarbon chains and have higher volatility.

Figure C3. ***Liquid fuel penetration.*** Images of elastically scattered light from soy- (SME) and cuphea-derived (CuME) biodiesel fuel droplets at 1800 μs after start of injection (ASOI). Liquid penetration is 10% less for cuphea, indicating higher volatility and improved performance.



[14] Fisher, B.T. and Mueller, C.J., "Liquid Penetration Length of Heptamethylnonane and Trimethylpentane under Unsteady In-Cylinder Conditions," *Fuel*, 2010 (in press, doi 10.1016/j.fuel.2010.04.024).

Action 3: Develop specific guidelines, roadmaps, and objectives for co-development of next generation biofuels and advanced engines.

The developments in future petroleum-based fuels, advanced engines, and next generation biofuels are proceeding without a clear view of the future beyond their local sector domains. This is in part due to the fragmented nature of the biofuels development sector (see Figure 2), combined with the more centralized business model of the oil and automobile industries. While some agreements have been made between biofuel startups and specific oil and automobile companies, there is no industry wide approach to accelerate introducing biofuels into the future fuel mix along with future engine concepts.

This lack of an integrated approach is exacerbated by the following: 1) the organizational separation of federal R&D into separate offices within DOE, and 2) the separate definition for success in next generation biofuels program vs. the definition for success in the advanced engines program. At worst, this creates uncertainty and tension, especially between the incumbent players and the new entrants to the marketplace. At best, this slows the potential scale-up that the global marketplace will eventually expect and demand.

Research roadmaps are often called for in situations where uncertainty exists regarding future development. However, the fuels/engines interface calls for more specific guidance. It falls under three areas, all of which can be combined into a dynamic framework:

- Development guidelines agreed upon by the incumbents and new entrants into the biofuels and transportation sectors.
- An agreed upon set of objectives (such as specific molecules of interest, and new methods for testing and certification) that will leverage co-development of fuels and engines for the future.
- A strategic planning framework that allows the guidelines and objectives to be reviewed on a regular basis as new information becomes available, new regulations are imposed, and/or new economic conditions arise.

These efforts should be directed by industry and commercial leaders and by the investment community that underwrites the new entrants in the biofuels sector. Otherwise the momentum will not be sustained.

At the same time there is an important role for government: in research and development, in policy, and in promulgating regulations. These include the following:

- Risk reduction through new R&D initiatives in predictive simulation. This would include research in the conversion of feedstocks to fuels and understanding the combustion processes in new engines with different fuel chemistries.
- Pre-competitive research that provides the foundation for analysis, experimentation, and certification needed at the interface between fuels and engines.
- Regular review of the effects of the policy and regulatory frameworks (such as the Low Carbon Fuel Standard and the Renewable Fuel Standard) to assess whether those regulations imposed separately on the fuel suppliers and the engine manufacturers are in fact well integrated and working to common purposes.
- A review of the policy drivers for biofuels (such as rural development, climate mitigation, and energy security) as well as the impact of the already significant investment in producing ethanol from corn. As next generation biofuels develop, their progress may not follow an agricultural economic development pathway. Also, potential competition with ethanol may arise, which must be considered as next generation fuels are scaled up.

Action 4: Convene an International Fuels and Engines Summit, sponsored by industry with government and university participation, to ratify a fuels/engines strategy and implementation framework.

Because the engine, automobile, and petroleum sectors are global in scope, there are compelling reasons to consider a fuels and engines framework in an international context. Two organizations have the reach and industry trust to move the three previous actions forward: BIO, the Biotechnology Industry Organization, led out of Washington, D.C.; and OICA, the International Organization of Automobile Manufacturers, headquartered in Paris, France. We propose that these organizations, with help from various national research agencies and universities, organize an **International Fuels and Engines Summit**. Prior to this summit, a set of working groups should consider and propose concrete efforts and actions in the areas outlined above: guidelines, objectives, frameworks, risk reduction, and foundational research needs. Once these issues are agreed upon, a summit could be held to review the output of the working groups and to sponsor specific actions.

APPENDIX A
PARTICIPATING INSTITUTIONS

Achates Power	Lawrence Livermore National Laboratory
Amyris Biotechnologies	Logos Technologies
Argonne National Laboratory	Oak Ridge National Laboratory
Aurora Biofuels	Pacific Northwest National Laboratory
Auto Alliance	Ricardo
British Petroleum	Sandia National Laboratories
CA Energy Commission	Toyota
CA Air Resources Board	Transonic Combustion
Chevron	Tufts University
Cummins	UC/Berkeley
Department of Energy, EERE	Underwriters Laboratories, Inc.
The Energy Biosciences Institute (EBI)	University of Michigan
General Motors	University of Wisconsin
Imperial College	U.S. Dept. of Agriculture (USDA)
Joint BioEnergy Institute (JBEI)	Vantage Point Venture Partners
John Deere	Venrock
Lawrence Berkeley National Laboratory	Virent

APPENDIX B

ADVANCED FUELS AND ENGINES WORKSHOP BACKGROUND DOCUMENT

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Harry Beller
Joint BioEnergy Institute, Lawrence Berkeley National Laboratory

Over the last century, the United States and much of the rest of the world have come to rely on fossil-fuel-based petroleum for our transportation energy needs. The consequences of this choice are many and varied. On the positive side, never before in human history have we been able to move goods and people so quickly and cheaply across great distances. Steadily advancing technological improvements combined with inexpensive fuel drove these achievements. These have not been attained without costs.

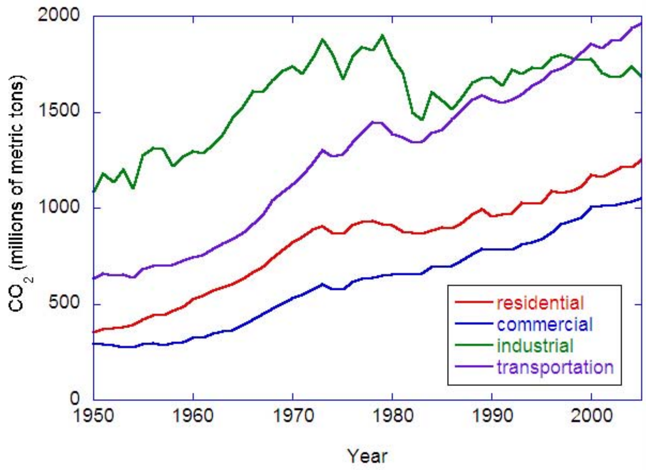

Figure 1: US CO2 emission by sector (Energy Information Administration, Annual Energy Review 2005, Report No. DOE/EIA-0384(2005)

The environmental consequences of wide spread, combustion driven transportation are manifest. So-called criteria pollutants, principally NO_x, unburned hydrocarbons and particulates have adversely affected human health and the environment, principally in urban areas. With policy adjustments and advancing technology, the impact of criteria pollutants has been drastically reduced over the last several decades. More recently, growing concern has arisen regarding the global climate change role of CO_2 emitted from combustion of hydrocarbons, the source of energy for >95% of our transportation infrastructure. Indeed, the US EPA is expected to deliver a positive finding of endangerment due to the climate change effects of CO_2 before the end of 2009, following the draft finding published in April 2009. Such a finding provides the basis for EPA regulation of CO_{2-} as a pollutant. This creates a fundamental challenge for hydrocarbon-based transportation. Improvements in engine efficiency and the development of alternative, low net-CO_2 fuels hold the promise of addressing these issues.

The geographic distribution of fuel resources creates additional issues. The dependence of much of the world on a few nations for crucial energy resources yields imbalances that create economic, political and military dislocations. As we look toward a future with more diverse fuel sources, driven by the need to reduce CO_2 emissions, we also gain the opportunity to develop a wider base of fuel resources that is less sensitive to singular international events, enhancing the energy security for all.

With the advent of an industrial-scale biofuels industry, currently composed principally of corn-based ethanol production, we are experiencing the first steps along this new energy path. The widespread use of ethanol as an oxygenate in so-called E10 fuels has created a market that has nearly expanded up to its full potential of 10% of fuel use. Waivers are currently under consideration that would allow the use of E15, and possibly E20, further expanding the role of domestic ethanol in transportation. Greater penetration of ethanol into the U.S. fuelstream is already beginning in the Midwest through the use of E85. To utilize E85 requires new, fuel flexible engines, which are now gaining greater market share. Indeed in many places, these flex-fuel engines are more common than the E85 fuel. Ethanol is only the beginning of the biofuel revolution. New biological and thermochemical routes are opening the door to a tremendous range of biofeedstock derived fuels.

In this environment, engine makers continue to innovate, producing new engine concepts with steadily increasing fuel efficiency. Indeed in the last 30 years, fuel efficiency has increased steadily, when the increase in vehicle weight is factored in to the analysis. Further advances through new engine concepts, including direct fuel injection (DI) with turbo charging, low-temperature combustion (LTC) and homogeneous-charge-compression ignition (HCCI), provide the opportunity for continued fuel efficiency increases for at least the next several decades.

As we move further down this path toward an alternative fuel future, the interplay of engines and fuels will become increasingly important. For example, ethanol-based fuels such as E85 face the criticism that they provide lower energy density than gasoline. However, an ethanol optimized engine that makes use of the high octane rating of ethanol could be operated at substantially higher compression ratios than a standard gasoline engine, likely recapturing all of the lost energy density through increased efficiency, thus preserving vehicle range and minimizing operating costs. New engine concepts such as HCCI show increased sensitivity to fuel chemistry. With biofuels, as well as other synthesized fuels, the opportunity presents itself to tailor the fuel to meet the needs of HCCI both through fuel customization and consistency.

Opportunities in Co-developing Fuels and Engines

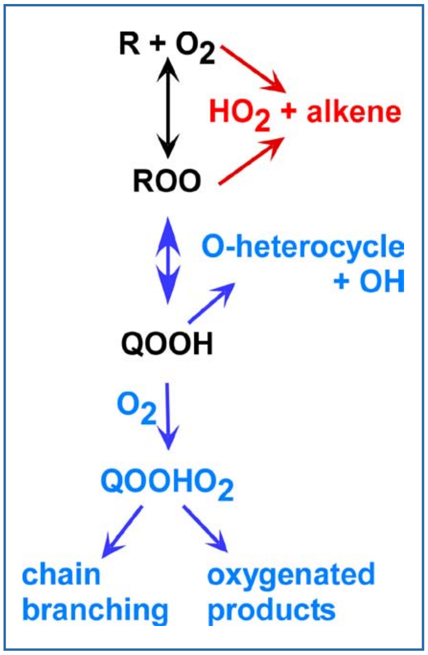

Figure 2: Simplified diagram of the low-temperature oxidation chemistry that leads to autoignition. Radical species R are formed by H atom removal from a fuel molecule. The details of subsequent reactions with oxygen are critical for autoignition and depend sensitively on the nature of the fuel.

As a consequence of the drivers discussed above, the fuel stream has already begun to change. At the same time, engine manufacturers are increasingly turning to new combustion concepts in the drive towards higher efficiency and low emissions. Historically, energy companies refined crude petroleum to meet specifications that were devised for performance in traditional diesel and spark ignition engines, and engine manufacturers made engines that would perform well with a range of distillate fuels that met those specifications. This resulted in a hundred-year truce between the conflicting interests of fuel producers and combustion engineers. Now the situation is changing on both sides, which offers an historic challenge and opportunity.

Rather than pursue energy-intensive refining of qualitatively different emerging fuels to match current fuel formulations, it may be possible to achieve a "dual revolution" by interdependently advancing both fuel and engine technologies. Spark-ignited gasoline engines equipped with catalytic after-treatment operate cleanly but well below optimal efficiency due to low compression ratios and throttle-plate losses used to control air intake. Diesel engines operate more efficiently at higher compression ratios but sample broad realms of fuel/air ratio, thereby producing soot and NO_x for which burnout and/or removal can prove problematic. A number of new engine technologies are attempting to overcome these efficiency and emissions compromises. Direct injection, stratified charge gasoline engines operate with reduced throttling, increasing efficiency, while retaining the use of a catalytic converter. Ultra-dilute, high-pressure, low temperature diesel combustion seeks to avoid the conditions that form pollutants, while maintaining very high efficiency. A new form of combustion, HCCI, attempts to combine the best of diesel and gasoline engines by operating unthrottled and employing a more thermodynamically advantageous heat release process. HCCI employs a premixed fuel-air charge that is ignited by compression, with the ignition timing controlled by in-cylinder fuel chemistry. Each of these advanced combustion strategies must permit and even exploit fuel flexibility as the 21st century fuel stream matures. The opportunity presented by new fuel sources and advanced engine concepts offers such an overwhelming design and operation parameter space that only those technologies that build upon a predictive science capability will likely mature to a product within a useful timeframe.

Changes in fuel chemistry can dramatically alter compression ignition behavior. As new engine technologies are developed, the availability of new fuels becomes an opportunity to optimize the fuel stream for new engines and potentially to develop fuels substantially different from current gasoline and diesel fuels. It is possible that new fuels may be *required* for some new engines to function within existing or even more stringent future environmental regulations. Many engine parameters can be varied to change combustion conditions, e.g., valve timing, fuel injection, boost, intake temperature, EGR, equivalence ratio, and these strategies can conceivably be designed to respond to changes in fuel properties. On the other hand, it may be that the choice of fuel can make a new combustion strategy succeed. For example, HCCI operation may demand ready volatilization for mixture preparation and specific autoignition properties to set combustion phasing and to control heat release rates. The present distillate fuels are not the ideal fuels for HCCI; it may be that the ideal properties lie somewhere between diesel and gasoline. The targets for development of a new biofuel should therefore not be limited to the current diesel and gasoline specifications, but should explore possible use in advanced engine technologies.

These advanced engines will likely demand new fuel specifications, although it is not yet clear what form these specifications may take. New understanding of which physical, chemical, and molecular properties of fuels govern their stability and combustion performance characteristics is required so that fuel performance can be predicted or designed. In this context the development of new biofuels may permit physical (e.g., viscosity, volatility) and chemical properties (e.g., ignition quality or emissions) to be combined in ways that are not easily accessible in traditional fuels. Blending of components will also affect performance – it is conceivable that some compounds may be enablers of novel clean, high-efficiency combustion methods even as minor components! Even strategies such as multiple fuel tanks on board a vehicle, with on-the-fly blending in response to driving conditions, may be feasible.

Finally, the increasing stringency of pollutant regulations and the requirements for reduction of emissions will continue to constrain the development of engines and the fuels that are used in them. The nature of unburned fuel or products of partial oxidation that are emitted from an engine will depend on the fuel chemistry as well as on the combustion strategy. After-treatment systems also place demands on fuel chemistry (e.g., low or zero sulfur to prevent catalyst poisoning), and the presence of some emissions (e.g., increased aldehyde emission from certain biofuels) may affect strategies to remove other pollutants. Optimization of the full combustion system should consider aftertreatment as well as engine/powertrain operation, although fuel effects on aftertreatment effectiveness have not yet been studied to any great extent. For example, low-temperature combustion strategies may require the use of a low-temperature oxidation catalyst that may nevertheless need to survive high-temperature excursions, e.g., if the engine reverts to spark-ignition operation at high load. The different partial oxidation products of biofuel combustion might in fact change oxidation catalyst requirements or alter the toxicity of particulate emissions. In addition, regulation of particulates may soon move to a number-density rather than a simple gravimetric requirement, which could change the aftertreatment landscape for all combustion strategies. In general, breakthroughs in aftertreatment technologies have the potential to completely change the calculus for emissions reduction by making a previously problematic pollutant irrelevant or by placing new restrictions on a previously ignored pollutant.

To prepare participants for the Advanced Fuels and Engines Workshop, below we highlight the current state of the biofuels and engines research and development communities. The goal is to provide common background information for participants and spark ideas regarding the opportunities of considering fuels and engines as a system, rather than separable components.

Development of Advanced Biofuels: An Infrastructure and Conversion Perspective

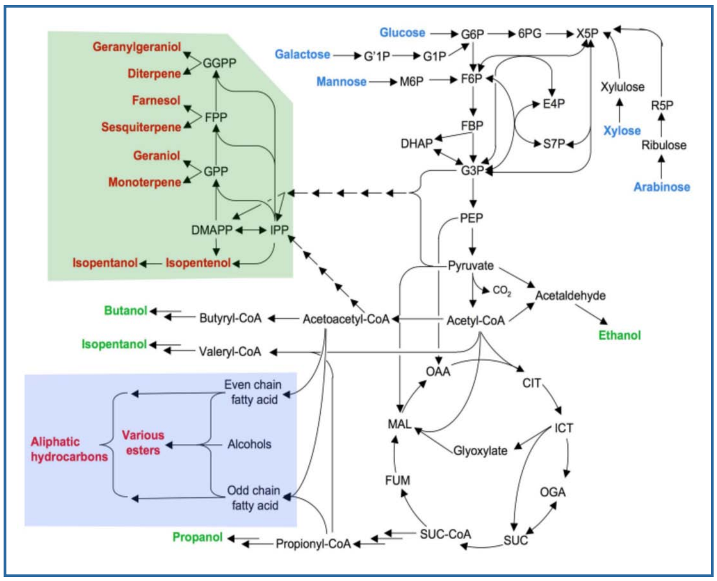

Figure 3: Central metabolic pathways and candidate fuel molecules that can be derived from them. The green box represents isoprenoid pathways and the blue box represents fatty acid pathways. Short-chain alcohols are in green text and lignocellulose-derived sugars are in blue text. Figure adapted from Fortman et al.[1]

A number of potentially viable strategies for converting renewable feedstocks into domestically produced, renewable replacements for petroleum gasoline, diesel, and jet fuel exist. These replacement fuels must be suitable for their applications in order to enjoy widespread use. When a fuel meets all customer requirements, it is referred to as "fit for purpose." While a successful fuel-conversion strategy will address the full range of desired fit-for-purpose properties (e.g., distillation range, ignition characteristics, energy density), the required fuel characteristics are driven primarily by a few industry standards. Several guiding truths became evident in addressing the conversion of renewable feedstocks to fuels, and these are noted here to help establish a reasonable framework for extension into practice of the most promising concepts presented below. First, the feedstock, conversion process, final fuel specifications, and the engines envisioned for transportation are highly interdependent and must be considered as a system if an optimal process is to be identified. As a result, accurate feedstock characterization (including both composition and variability) is essential, since this is an upstream boundary condition for the entire subsequent fuel-conversion process. Second, lifecycle analysis of energy and carbon will be a key tool in selecting the winning technologies from those discussed below. Third, the greatest challenge in biofuel conversion is not likely to be how to convert singular components within the feedstocks (e.g, monomeric sugars) into fuels most efficiently, but rather how to best use all of the components (cellulose, hemicelluloses, lignin, pectin, lipids) within the feedstock after desirable molecules have been liberated. Ideally, all of the petroleum feedstock that enters a conventional petroleum refinery should leave as marketable products, and this conservation law also must hold for the biorefineries of the future if their products are to achieve significant market penetration and displace fossil fuels.

Microbial Production of Advanced Biofuels

Recent revolutionary advances in biotechnology (including new techniques in metabolic engineering and synthetic biology) have greatly enhanced opportunities for microbial production of chemically diverse biofuel molecules from the saccharification products of lignocellulosic biomass (primarily glucose and xylose).

[1] Fortman, J. L., S. Chhabra, A. Mukhopadhyay, H. Chou, T. S. Lee, E. Steen, and J. D. Keasling. 2008. Biofuel alternatives to ethanol: pumping the microbial well. *Trends Biotechnol* **26**(7): 375-81.

Biosynthesis of a vast array of potential fuel molecules is being pursued. Known metabolic pathways provide a biochemical foundation, which can be incorporated (if non native) into industrially important and genetically tractable microbes (such as the bacterium *Escherichia coli* and the yeast *Saccharomyces cerevisiae*). These can be further optimized for higher production of target metabolites, and amended with genes from other organisms to provide additional or enhanced metabolic capabilities. The potential fuel molecules include:

- *short-chain alcohols* (such as *n*-butanol)
- *fatty acid-based fuels* [such as fatty acid ethyl esters (similar to current "biodiesel"), fatty alcohols, and aliphatic hydrocarbons (alkanes and alkenes), which are prominent components of petroleum-based gasoline and diesel fuel]
- *isoprenoid-based fuels* [such as the C_5 alcohols isopentenol and isopentanol, farnesene (an acyclic, unsaturated C_{15} isoprenoid that can be a precursor to the saturated, more desirable fuel molecule farnesane), and cyclic monoterpenes (C_{10}) and sesquiterpenes (C_{15})].

A broad overview showing biochemical pathways linking metabolism of sugars derived from lignocellulosic biomass (e.g., glucose and xylose) to the biosynthesis of a variety of potential biofuels (including fatty acid- and isoprenoid-based compounds) is shown in Figure 3. Depending on their physicochemical properties, advanced (i.e., non-ethanol) biofuels may be appropriate alternatives for gasoline or diesel fuels, or serve as ideal fuel alternatives for new engines. Examples of gasoline replacements or blends include short-chain alcohols (such as *n*-butanol, isobutanol, isopentanol, 2-methyl- or 3-methyl-1-butanol) and short-chain alkanes and alkenes. Examples of diesel replacements or blends include fatty acid ethyl esters, medium-chain alkanes and alkenes, various sesquiterpenes (preferably reduced to saturated hydrocarbons), and fatty alcohols. More information on microbial production of advanced biofuels is provided in recent reviews [1, 2, 3, 4]. Critical factors that will need to be addressed are the overall yields, toxicity of the fuel to the microorganisms producing them, process economics, and scalability of these advanced biofuel conversion technologies.

Thermochemical Production of Advanced Biofuels

There are two major routes for the thermochemical conversion of biomass into biofuels: gasification and pyrolysis. Pyrolysis is the chemical decomposition of a condensed substance by heating. It does not involve reactions with oxygen or any other reagents but can frequently take place in their presence. The thermochemical treatment of lignocellulosic biomass can result in a wide range of products, depending on the reaction parameters. Liquid product yield tends to favor short residence times, fast heating rates, and moderate temperatures[5]. Pyrolysis has one major advantage over other conversion methods, in that it is extremely fast, with reaction times on the order of seconds to minutes. Although synthetic diesel fuel cannot yet be produced directly by pyrolysis of algae, one can produce an alternative liquid (bio-oil) that may be further upgraded in a conventional refinery. The bio-oil has an advantage in that it can enter directly into the refinery stream and, with some hydrotreating and hydrocracking, produce a suitable feedstock for generating standard diesel fuel and other fuel targets. Also, higher efficiency can be achieved by the so-called "flash pyrolysis" technology, where finely divided feedstock is quickly heated to between 350 and 500 ºC for less than 2 seconds.

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[2] Lee, S. K., H. Chou, T. S. Ham, T. S. Lee, and J. D. Keasling. 2008. Metabolic engineering of microorganisms for biofuels production: from bugs to synthetic biology to fuels. *Curr Opin Biotechnol* **19**(6): 556-63.

[3] Rude, M. A. and A. Schirmer. 2009. New microbial fuels: a biotech perspective. *Curr Opin Microbiol* **12**(3): 274-81.

[4] Yan, Y. and J. C. Liao. 2009. Engineering metabolic systems for production of advanced fuels. *J Ind Microbiol Biotechnol* **36**(4): 471-9.

[5] Carlson, Torren R.,Vispute, Tushar P., and Huber, George W. 2008. Green gasoline by catalytic fast pyrolysis of solid biomass derived compounds. *ChemSusChem* **1**(5), 397-400

Gasification provides an extremely flexible way to produce different liquid fuels, primarily through Fischer-Tropsch Synthesis (FTS) or alcohol synthesis of the resulting syngas. FTS is a mature technology where the syngas components (CO, CO_2, H_2O, H_2, and impurities) are cleaned and upgraded to usable liquid fuels through a water-gas shift and CO hydrogenation[6]. Conversion of bio-syngas has several advantages to other methods. First and foremost, it is possible to create a wide variety of fuels and alcohols with acceptable and known properties to downstream customers. Additionally, it is possible to make several products at once, making the process more flexible. Another advantage is the possibility to integrate an algal feedstock into an already existing gasification infrastructure. For example, it may be possible to feed biomass into a coal gasification plant to reduce the capital investment required, address the issue of availability for dedicated biomass plants, and improve the process efficiency through economy of scale.

Algal Production of Advanced Biofuels

Algae remain one of the most intriguing biological systems that are potentially capable of generating a large amount of next-generation biofuels. The conversion of extracts derived from algal sources is the typical mode of biofuel production from algae. There is an obvious and critical link between the type of extraction process used and the product composition, and as such a fundamental and exhaustive understanding of the different types of inputs to the conversion technologies must be in place. The most common type of algal extracts under consideration are lipid-based[7], e.g. triacylglycerides, which can be converted into biodiesel and green diesel through relatively mature conversion technologies – transesterification and hydrotreating, respectively.

In contrast, the direct production of biofuels from algal biomass has certain theoretical advantages in terms of process cost because it eliminates several upstream process steps (e.g., extraction) and their associated costs in the overall fuel production process. These approaches are quite different from the usual algal biofuel processes that use algae to produce biological oils that are subsequently extracted and used as a feedstock for liquid fuel production, typically biodiesel. There are several biofuels that can be produced directly from algae, including alcohols, alkanes, and hydrogen. In addition to the direct production of biofuels from algae, it is also possible to process whole algae into fuels instead of first extracting oils and post-processing. These approaches benefit from reduced costs associated with the extraction process, but still require some degree of dewatering. There are two major categories of conversion technologies that are capable of processing whole algae: thermochemical and supercritical processing.

Impact of Fuel Properties on Engine Design and Development Trends

Current light- and heavy-duty power trains, composed of engines, fuels, and after-treatment devices, are highly optimized systems. These systems must simultaneously meet many requirements. The customer demands performance, fuel economy and affordability. The engine manufacturers need to manufacture and sell engines at a competitive yet profitable cost, to provide for long service intervals, and to guarantee reliability. The energy companies must deliver uniform, fungible fuels. Finally the criteria emissions requirements of regulatory agencies must be met.

[6] Plass, Ludolf and Reimelt, Stephan. 2007. Second generation biofuels. *Hydrocarbon Engineering* **12**(6), 71-74.
[7] Griffiths, Melinda J. and Harrison, Susan T. L. 2009. Lipid productivity as a key characteristic for choosing algal species for biodiesel production. *Journal of Applied Phycology* **21**(5), 493-507.

Trends in engine design

In the light-duty arena, both diesel- and gasoline-fueled engines are following the same broad trends toward lower engines speeds (down-speeding) and smaller engines (down-sizing). The objective is an increase in vehicle efficiency through both increased engine efficiency and reduced vehicle mass. By running at lower engine speeds, frictional losses are significantly reduced. Moreover, with lower speed, the engine must be run at higher loads to maintain equal output power. Similarly, reducing engine displacement also requires that the engine run at higher loads. At high loads, parasitic frictional and heat transfer losses consume a smaller fraction of the total energy released. In addition, pumping losses are reduced as low-load, throttled operation is less frequent. A challenge imposed by the down-speeding and down-sizing trends is the high peak power density required to provide acceptable full-load performance. Hybridization schemes can help mitigate this difficulty, however.

Table 1 The requirements and concerns of the customer, the vehicle manufacturer, and the fuel supplier

Customer Demands	OEM Demands	Fuel Supplier Demands
• Performance • Fuel economy • Fuel and vehicle cost • Reliability • Fuel availability • Fuel odor • Convenience	• Competitive yet profitable cost • Criteria emissions • Fuel economy standards • Customer satisfaction • Service intervals • Warrantee issues	• Fungibility • Feedstock availability • End product stability • Transportation and pipeline issues

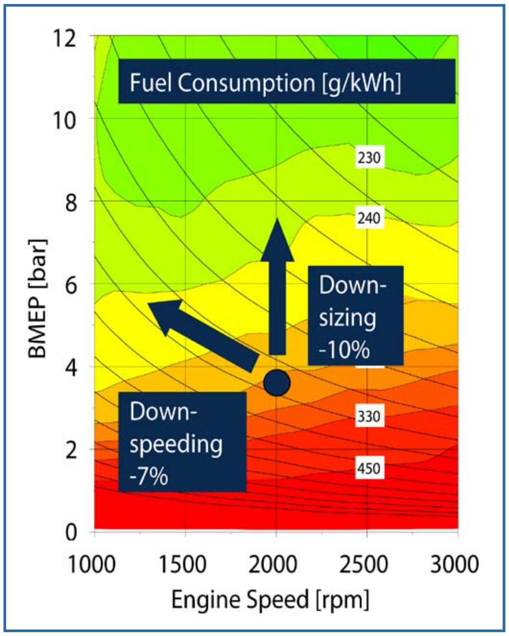

Figure 4: Engine down-speeding and down-sizing are both effective paths towards reduced fuel consumption. Source: Rueger J-J. 2008. Clean diesel– real life fuel economy and environmental performance, SAE Government and Industry Meeting, Washington DC, May 13, 2008.

Apart from the demands on the gas exchange process (supercharging or turbocharging) imposed by the higher power densities, the trends mentioned above have additional implications for the combustion system design and desirable fuel properties. Smaller displacement engines will result in a proportionately larger impact of boundary layer regions, charge mass (and fuel) trapped in crevices, and the relative importance of displacement independent sources of emissions and inefficiency—such as the injector nozzle sac volume. Liquid fuel impingement on combustion chamber surfaces may also be impacted due to the reduced combustion chamber dimensions. Tailoring fuels to have appropriate vaporization qualities could therefore maximize the benefits achieved by down-sizing. Likewise, the degree of down-sizing achievable is often limited by pre-ignition. The auto-ignition behavior of new fuels is thus a crucial consideration in how their use will impact down-sizing efforts, and ultimately engine efficiency.

Down-speeding also impacts the combustion process, as it works with the increased cylinder pressures associated with down-sizing efforts to change the relative time scales of the various physical processes impacting combustion. While higher pressures are decreasing chemical time scales, lower engine speeds are increasing mixing time scales. Consequently, achieving the desired level of mixing prior to ignition in compression ignition engines will be impacted, as will amelioration of overly rapid pressure rise rates by volume expansion due to piston motion. As with down-sizing, a detailed understanding of the oxidation kinetics of new fuels, potentially allowing tailoring of the ignition behavior at high pressures, could enhance the benefits achieved through down-speeding.

With its long-time emphasis on fuel efficiency, lower lifetime capital-to-operating cost ratio, and differing customer expectations for drivability, the heavy-duty industry has always embraced the down-sizing and down-speeding strategies currently being pursued in the light-duty sector. Accordingly, one might anticipate that the development of light- and heavy-duty engines could follow a consolidated path. Indeed, detailed engine scaling relationships have recently been developed[8] and explored to assess this possibility. Despite the fact that it is not possible to simultaneously satisfy all the requirements to obtain both exact geometric scaling as well as scaling of the time and length scales characterizing the fuel injection and combustion processes, good correspondence between the combustion behavior of small and large-bore engines has been observed. However, there is still a distinct difference in the typical load-speed map over which these engines operate, and an engine optimized for a light-duty application would be unlikely to perform optimally in a heavy-duty application. The need to limit initial cost for light-duty vehicles (10-speed transmissions aren't currently envisioned) and different customer expectations for drivability preserves these load-speed map differences. Nevertheless, advances in continuously variable transmissions and economical, modular hybridization schemes may eventually enable a consolidated development strategy to be pursued.

Apart from down-sizing and down-speeding trends, there has been a steady trend toward greater versatility (and complexity) in engines, including: flexible, multiple-injection capable common-rail fuel injection systems; electronic engine control; dual-stage turbochargers providing widely variable intake boost levels; combustion sensors; and variable valve timing and lift capabilities. These features enable a broad range of combustion strategies to be employed within a single engine architecture. Tailoring of the thermodynamic cycle to have variable (and differing) compression and expansion ratios is also possible, as are such advanced concepts as exhaust gas re-breathing, fuel reforming during recompression, and cycle-to-cycle control.

Trends in combustion system development

Both the increased versatility discussed above and increasing societal emphasis on fuel efficiency have enabled a number of combustion strategies to be investigated and deployed in production vehicles that were previously impractical due to either technical or economic barriers. In both gasoline and diesel-fueled platforms, direct in-cylinder fuel injection is now becoming the norm and stoichiometric combustion is not always possible or desirable. As a result, cost-effective, three-way catalysts cannot always provide effective NOx control. Consequently, low temperature combustion strategies (including HCCI) have been heavily emphasized in recent years due to their ability to control NO_x at the source. These strategies can also substantially reduce fuel consumption, as will be discussed below.

[8] Staples, L.R., R.D. Reitz, and C. Hergart. 2009. An experimental investigation into diesel engine size-scaling parameters. *SAE Technical Paper* 2009-01-1124.

In gasoline engines, HCCI (also called controlled auto-ignition, or CAI) is the principal low-temperature combustion strategy being pursued. In addition to providing very low levels of NO_x, the more nearly constant volume heat release of HCCI combustion is thermodynamically advantageous, and un-throttled low-load operation greatly reduces pumping losses. Consequently, a 15-25% fuel consumption reduction is realized over a typical drive cycle. Current state-of-the-art engine prototypes can run in HCCI for roughly 75% of the time, switching to conventional spark-ignition operation at idle and at high loads. One OEM has recently demonstrated un-throttled, spark-assisted "HCCI" operation even under idle[9] conditions, where a 25% fuel consumption benefit is observed. The remaining challenge is primarily to extend HCCI to high-load operation.

HCCI combustion strategies are strongly dependent on the details of the fuel oxidation process. Auto-ignition behavior of the fuel is of clear importance. However, fuel reforming and partial combustion during recompression is an enabler of some low-load HCCI strategies. Like auto-ignition, these processes can also be expected to be strongly dependent on the fuel type. Flame propagation characteristics of lean or dilute fuel/air mixtures, also impacted by fuel type, are important for idle operation, as they are for more mainstream, stratified charge SI technologies.

Despite the clear advantages of HCCI operation, it should be noted that there is not universal acceptance that it will dominate engines of the future. HCCI-based combustion systems will require sophisticated control strategies and the associated sensors can be costly. Moreover, due to the over-all lean or dilute operation, achieving high power densities is difficult, and the full benefits of engine down-sizing or down-speeding are not readily achieved. There are some synergies between down-sizing trends and HCCI combustion, however. The boosted intake pressures of the down-sized engine will allow HCCI operation to be pursued at higher loads than in a naturally aspirated engine, and the higher load at idle required due to lower speed or reduced displacement could facilitate the use of HCCI combustion. Which path, or combination of paths, will ultimately dominate future engine development remains to be seen; however, fuel properties will play an important part in any future engine technology.

In diesel engines, the main challenge engine developers face is to retain the high inherent efficiency of the diesel engine while reducing emissions. This challenge is not restricted just to the combustion process. Most aftertreatment devices also incur a fuel economy penalty in the regeneration process or in the warm-up/heating of a selective catalytic reduction (SCR) catalyst for NOx control. There is also additional cost for the urea needed for SCR systems.

For light-duty engines, the adoption of advanced low-temperature combustion strategies for in-cylinder NO_x control is central to the strategy of many OEM's for meeting criteria emissions. Indeed, Tier II, bin 5 emissions levels have been demonstrated without any NO_x aftertreatment, and Tier II, Bin 2 levels are being aggressively pursued[10]. Even if these levels are not met through in-cylinder control alone, low-temperature combustion processes can enable the use of lower cost aftertreatment solutions, such as lean NO_x traps (LNTs) as an alternative to SCR. Moreover, employing in-cylinder NO_x control at low loads can also reduce precious metal loading requirements for LNTs, further increasing their economic advantage.

The effectiveness of low-temperature combustion systems in reducing emissions without sacrificing fuel economy can be strongly impacted by fuel properties. Highly volatile fuels, which can be effective in minimizing the impact of wall-wetting when early injections are used to enhance premixing, can negatively impact combustion efficiency

[9]Yun, H., N. Wermuth, and P. Najt. 2009. Development of robust gasoline HCCI idle operation using multiple injection and multiple ignition (MIMI) strategy. *SAE Technical Paper* 2009-01-0499.
[10]Crosse, J. 2008. Near-zero emission diesels. *Ricardo Quarterly Review*, Q4.

and the concomitant unburned hydrocarbon and CO emissions. As with gasoline HCCI combustion schemes, the auto-ignition quality of the fuel is critical, and inappropriate ignition behavior can lead to both misfire and excessive noise. Particulate emissions are also highly dependent on specific fuel properties.

For heavy-duty diesel engines, many of the technology trends seen with down-sized light-duty engines will be followed: increased boost with two-stage turbocharging, correspondingly greater peak-cylinder pressures, higher EGR rates (even at full-load), and high (2500 bar) injection pressures. Although 2010 NO_x levels can be achieved using advanced, low-temperature combustion techniques, there is a widely-held view that relying on in-cylinder NO_x control alone will result in a fuel economy penalty. Thus, NO_x aftertreatment, while not required, may be desirable[11]. Nevertheless, low-temperature combustion techniques will likely play a role at low loads where aftertreatment efficiency is poor. As in the light-duty sector, fuel properties such as auto-ignition behavior, volatility, and atomization characteristics will be important.

Potential impacts of fuel property changes

Even seemingly innocuous changes to one of the components of power-train systems can have costly, unforeseen consequences. The most recent example is the introduction of ultra-low sulfur diesel (ULSD) fuel, phased in starting in 2006 to support aftertreatment technologies. Although some fuel property changes were anticipated as a consequence of the desulfurization process (e.g. a reduction in aromatics and lubricity), others were not. Most notably, chemical changes in the fuel are thought to have resulted in reduced oxidative stability. While this change did not cause problems in vehicles employing older fuel injection technology, it wreaked havoc on modern engines employing high-pressure common rail equipment. In these engines, the combination of reduced fuel stability and higher fuel temperatures and pressures caused rapid formation of difficult to remove internal injector deposits, resulting in both increased emissions and a loss of power. Notably, current industry bench and engine deposit tests were not able to predict ULSD's propensity for forming these deposits.

When a more significant change in fuels occurs, a myriad of difficulties can arise. An example is provided by the recent introduction of first generation biodiesel blends. While many of these difficulties have been overcome or significantly mitigated, it is nonetheless instructive to catalog them:

- Biodiesels are subject to far more oxidative degradation than even ULSD. Formation of peroxides can damage or degrade plastics and elastomers, and low molecular weight acids (e.g., formic acid) attack metal components. Increases in corrosion of metallic parts by an order of magnitude have been observed for a B10 blend (10% biodiesel blended with conventional diesel). Polymerization products also promote deposits, lacquer formation, and filter clogging.
- Biodiesel has a strong tendency to absorb moisture. Water accelerates fuel oxidation, dramatically increases corrosivity, and promotes microbial growth and the formation of precipitates. Precipitates and sedimentation issues are found to be even more pronounced in mixtures of biofuels with conventional fuels than in neat biodiesel fuels. These difficulties lead to increased maintenance requirements, including the need for tank cleaning. Farm machinery, that may undergo extended periods of non-operation, is especially vulnerable.
- Cold temperatures can also impact the performance of biodiesel blends. Filter clogging with "butterscotch pudding" has been observed in biodiesel blends as low as 2%[12] in cold climates, and cold temperatures can aggravate problems with precipitates. High mono-glyceride content has also been linked to solid deposits in fuel tanks when B5 blends are stored under winter conditions.

[11] Johnson, T.V. 2009. Diesel emission control in review. *SAE Technical Paper* 2009-01-0121

[12] Taracha, J. 2006. Technology issues and trends: biodiesel, ASPA spring meeting, June 2006, Lubrizol Corp.

- Trace metals in the fuel can lead to numerous problems. Ash formed from these metals clogs diesel particulate filters, and increased injector deposits that are not prevented or removed by conventional detergents are thought to be associated with metal content. Phosphorous is naturally present in plant oils, and alkali metals (Na, K) can be introduced by catalysts used in the biodiesel production process. Alkaline metals used as absorbents can likewise cause difficulties, as can the calcium and magnesium found in hard water. Substantial injector deposit formation, leading to a 24% decrease in power in only 48 hours of operation, has been observed[13] for a B10 blend.
- Residual methanol from the esterification process can lower the fuel flash point, decrease lubricity, and cause additional corrosion and material degradation.
- Changes in fuel properties, including kinematic viscosity, volatility, specific heat and latent heat of vaporization can impact injector operation fuel atomization and liquid penetration, impacting the fuel preparation and subsequent combustion process. At low temperatures, kinematic viscosity increases can also create potentially damaging loads on fuel pump drive components.
- Over-penetration of liquid fuel can result in increased piston top deposits, which are permeable to fresh fuel and can lead to increased emissions and fuel consumption. During particulate trap regeneration over-penetration can wash lubricant from cylinder walls and cause severe oil dilution. With B5 blends, oil dilution of 45% has been measured in light-duty engines after only 10,000 miles[14]. Apart from reduced lubricant effectiveness, such severe oil dilution can raise the sump level to a point where the engine runs on its sump oil and cannot be stopped unless stalled against the brakes.
- Fuel ignition properties can vary significantly when biofuels are used, further affecting the pre-combustion mixing and the subsequent combustion process, as well as overall combustion phasing. Moreover, ignition quality changes among different biofuel blends can also be significant. Engine calibrations optimized for conventional fuels can lead to significantly sub-optimal performance when biofuel blends are employed.
- The specific chemical composition can dramatically impact emissions performance of biodiesel blends. For some operating conditions, a B20 blend of a palm-based biodiesel has been observed to result in a 3-fold increase in soot emissions, while little change is observed with a soy-based blend.

For all of the above reasons, manufacturers have been reluctant to endorse operation with high biodiesel blend fractions, in some cases even restricting operation with blend fractions less than 20%. One manufacturer requires that operators a) obtain a Certificate of Analysis certifying that the bio-portion of the fuel meets either ASTM D6751 or EN14214 (at a minimum) and b) use the fuel within 3 months of the date the bio-portion was produced. For blends above B20, the bio-portion must meet EN14214, be used within 45 days, and be treated with a manufacturer approved fuel conditioner with a detergent/dispersant additive.

Even relatively minor changes in fuels can create significant problems, ranging well beyond the impact of the fuel on the combustion process alone. These problems have prompted one leading fuel additive and lubricant manufacturer to observe that "every time we have changed our fungible fuels, there have been supply disruptions and unintended consequences." In this light, it is not surprising that there is broad support for 2nd generation biofuels (e.g. NExBTL™) that can be nearly indistinguishable from conventional fossil-derived fuels.

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[13] Caprotti, R., A. Breakspear, T. Klaua, P. Weiland, O. Graupner, and M. Bittner. 2007. RME behavior in current and future diesel fuel FIE's, *SAE Technical Paper 2007-02-3982*.
[14] Kotrba, R. 2008. Understanding the post-injection problem, *Biodiesel Magazine*, Vol. 5, No. 5.

Background Document Summary

As the high level summary provided in this background document demonstrates, the current environment contains both a rich landscape of alternatives and a daunting set of challenges for the research, development and manufacturing communities. The HITEC Workshop on Advanced Fuels and Engines for the 21st Century will provide a forum to explore the opportunities and challenges of considering the full fuel and engine system in the context of the rapidly evolving transportation energy sector.

HUB FOR INNOVATION IN THE TRANSPORTATION ENERGY COMMUNITY

The mission of the Hub for Innovation in the Transportation Energy Community (HITEC) is to accelerate and increase the effectiveness of innovative research in low-carbon transportation energy solutions, creating global partnerships between DOE, industry, and academia to meet future energy needs, increase energy security, mitigate climate change, and ensure economic vitality. Multidisciplinary efforts focus on a research portfolio to reduce carbon emissions and increase energy security through fuel efficiency, vehicle electrification, and sustainable alternative fuels within a systems analysis framework.

COMBUSTION RESEARCH FACILITY

The Combustion Research Facility is the Department of Energy's premiere center for combustion science and technology. Founded by the Office of Science and funded principally by the Office of Science and the Office of Energy Efficiency and Renewable Energy, the CRF leads the nation and the world in the revealing the complex scientific underpinnings of combustion and linking this scientific understanding to technology development. Chemical imaging, based primarily on laser diagnostics, and high performance computer modeling and simulation provide the primary tools for revealing the intricate interplay of fluid dynamics and chemistry in combustion.

Joint BioEnergy Institute

The Joint BioEnergy Institute (JBEI), funded by the DOE Office of Science as one of three Bioenergy Research Centers, seeks to advance the development of next-generation biofuels—liquid fuels derived from the solar energy stored in plant biomass. JBEI is focused on converting lignocellulosic biomass into renewable transportation fuels using cost-effective, scalable development processes designed for rapid deployment to the commercial sector.

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