Invitational Workshop on Advanced Combustion and Fuels

June 16-17, 2003

Less dependence

on foreign oil, and

eventual transition

to an emissions-free,

petroleum-free vehicle

freedom CAR & vehicle technologies program

U.S. Department of Energy

Energy Efficiency and Renewable Energy

Bringing you a prosperous future where energy is clean, abundant, reliable and affordable

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Introduction

The U.S. Department of Energy's (DOE) Office of FreedomCAR and Vehicle Technologies conducted a workshop on Advanced Combustion and Fuels at Argonne National Laboratory on June 16–17, 2003. The purpose of the workshop was to identify research priorities for the DOE to pursue in the areas of advanced combustion and fuels. Attendees of the workshop were limited to managers of the DOE Advanced Combustion and Fuels Programs, representatives from the auto and heavy-duty engine manufacturers, energy suppliers, universities, national laboratory researchers, and selected individual experts. The workshop outcomes are being used to formulate multi-year research plans within the FreedomCAR and Vehicle Technologies Office in the areas of advanced combustion and fuels.

The workshop commenced with several presentations by representatives from industry, academia, government, and national laboratories. These presentations set the stage for the round-table discussions which followed. Each round-table was focused on a single topic and was led by a national laboratory representative having extensive expertise and experience in that topic area. The round-table topics included:

- Aftertreatment
- Engines (hardware, sensors, and controls)
- Combustion modeling
- In-cylinder combustion
- Base fuels
- Blending agents.

Each roundtable discussion was limited to one hour. A list of questions was presented for discussion (distributed to the participants before the beginning of the workshop) by the group. Significant comments were recorded (without attribution to the source) as the discussions proceeded. Each attendee was assigned to attend each round-table discussion in such a manner that the composition of each round-table was unique and contained representatives with a variety of interests. Each round-table was thus repeated six times, allowing everyone to attend each one during the course of the workshop. Comments from the attendees have been summarized and are presented in this report.

Executive Summary

The Advanced Combustion and Fuels Workshop was built around six separate round-table topics:

- Aftertreatment
- Engines (hardware, sensor, and controls)
- Combustion modeling
- In-cylinder combustion
- Base fuels
- Blending agents.

The purpose of the workshop was to identify research priorities for the DOE to pursue in the areas of advanced combustion and fuels to formulate multi-year research plans within the FreedomCAR and Vehicle Technologies Program. The following are highlights from each of the round-table sessions.

Aftertreatment

This session addressed the impacts of and synergies between new combustion regimes and aftertreatment, with strong consideration of fuels and lubricant interactions. The clear consensus view was that lower diesel engine-out NOx via expanded homogeneous charge compression ignition (HCCI) operating range may reduce the requirement for NOx conversion device efficiencies from >90% (very difficult to achieve with adequate durability) down to approximately 80%, seen as more achievable with reasonable energy penalty. There was no expectation that emissions regulations for 2010 could be met without aftertreatment devices, but as HCCI and related low-temperature combustion modes are further developed, the aftertreatment performance demands need to be continually evaluated. The expectation for HCCI and mixed mode engines is that they will still generate considerable NOx and PM at high loads and during startup and transient operation.

Engines (Hardware, Sensors, and Controls)

All workshop participants agreed that the diesel-powered vehicle of the future will be a sophisticated, high technology system. There was a nearly unanimous consensus that the "engine of the future" would have a multifaceted approach to emissions control, including elements of advanced combustion systems and advanced aftertreatment systems. A total systems approach was believed to be imperative, with most participants feeling that mixed-mode systems may be inevitable due to startability, power density, and off-cycle issues. Even with these new combustion system developments, the historic trends towards higher cylinder pressures, higher fuel injection pressures, flexible injection characteristics, smaller injector spray holes, and flexible air handling systems were generally predicted to continue. There was a nearly unanimous consensus that sensor technology was critical and in need of general development, especially NOx sensors.

Combustion Modeling

Workshop attendees noted that some degree of modeling was useful or essential to their R&D activities, and most would like to increase their use of modeling and to see improvement in the quality of the models in the future. Most agreed that simulations were generally cost-effective, reducing the time and effort for product development. Only the very largest companies did any appreciable amounts of formal or large-scale computer model development, although most relied heavily on science-based engineering models and correlations that could provide answers quickly using calculators or desktop computers. Existing combustion models need better submodels to describe processes of importance to industry problems, and existing models are hard to learn how to use, have poor user interfaces, and are difficult to modify to suit applications of particular interest. The most common complaint about more sophisticated computational models was that they needed much more time to provide useful answers than the time usually available due to computational intensity.

In-Cylinder Combustion

Discussions in the In-Cylinder Combustion Session focused on five topics: low-temperature combustion (LTC) strategies; advanced diesel combustion strategies, especially for use in a mixed-mode combustion system; alternative and advanced petroleum-based fuels; efficiency enhancement technologies (e.g., variable compression ratio, variable valve timing, improved exhaust heat recovery, etc.); and hydrogen-fueled engines. There was general agreement that LTC offers significant potential for enabling high efficiency, emissions compliant engines, but that the state-of-knowledge regarding LTC is insufficient. Discussions on advanced diesel combustion focused on advanced strategies for reducing emissions, thus reducing the burden on diesel aftertreatment systems. There was agreement that there is insufficient understanding about which fuel properties are critical and what the ideal fuel properties are for LTC. Such information would be helpful to suppliers providing fuels for LTC engines. More fundamental combustion research is needed to determine how fuel properties affect the various combustion modes from diesel to LTC and how to specify a fuel that will perform well under both HCCI and direct-injection diesel or spark ignition operation.

Discussion on the topic of needs for efficiency enhancement technologies was very limited. A sentiment expressed was that the focus should be on getting the low-emission, high-efficiency LTC and advanced diesel combustion strategies to work prior to considering additional technologies for improving efficiency. There was agreement that hydrogen-fueled engines could play a role in the transition to a hydrogen economy. The primary advantage to using hydrogen as fuel in internal combustion engines is the low lower-flammability limit, which allows lean or dilute combustion for NOx control. There are issues that need to be investigated such as the pre-ignition phenomena, combustion stability, as well as fuel/air mixing for spark ignition, direct injection engines.

Base Fuels

There was a clear consensus that lower sulfur levels in gasoline as well as diesel fuel are desirable. Most felt that standardization with Japan and Europe at something less than 10 ppm should be implemented, mainly as an aftertreatment enabler. A recurring discussion was whether DOE should encourage the energy industry to try to maximize the amount of fuel produced by today's refineries. It was repeatedly suggested that well-to-wheels analyses be conducted when considering any base fuel changes. Many participants believed well-to-wheels analysis will show that the largest energy security impact can be attained by very large-scale market penetration of light-duty diesel vehicles. It was generally acknowledged that we need to better understand the combustion characteristics of fuel components before we can identify ways of improving the efficiency of gasoline and diesel base fuel combustion. This is especially true for advanced combustion concepts such as HCCI. A new rating method is needed for low-temperature/HCCI combustion, and the ignition quality tester (IQT) method was referred to as having promise. Most participants acknowledged the impracticality of having two diesel grades but pointed out that development and certification of new engines will be difficult until an ultra-low sulfur grade is widely available. Other fuel property themes included a strong desire by the engine OEMs for higher-cetane, lower-aromatic diesel fuel in the near term. These property changes were viewed as an enabler for light-duty diesels to penetrate the U.S. market. Canadian oil sands were typically viewed as a non-event: we are already importing ever-increasing quantities of these fuels that are refined and blended to provide a finished fuel that meets D975. Tax policies were a common topic of discussion. It was suggested many times that tax policies similar to what Europe has towards diesel vehicles and diesel fuel should be explored. Near-term R&D on the impact of sulfur, as well as cetane and aromatic content, on engine performance was viewed as a priority by many, but not all, participants.

Blending Agents

It was generally agreed that the use of renewable and/or synthetic blending components would likely be driven by legislation or regulation, not by economics. Thus, fuels utilization R&D should be directed at obtaining the data required for legislative or regulatory consensus. There was also broad agreement on the need to understand the "well-to-wheels" life cycle energy efficiency and emissions of blending components. For example, an analysis to determine the relative benefits of running all vehicles on a 5% blend, versus running 5% of the vehicles on a 100% biofuel, should be undertaken. In general, the consensus was that blending should not be done if increases in engine-out emissions occur. Because of the highly dispersed nature of biomass and the variation in biomass properties from region to region, it may make sense to have different bio-based blending components for different regions. Engine manufacturers pointed out that they make engines for sale worldwide. Thus, any fuel blend or blend specification must be applicable internationally. There was much discussion of blending components for advanced engines operating in advanced combustion regimes such as HCCI. It was generally agreed that fuel performance standards would have to be tightened considerably to meet the requirements of these advanced engines. The potential of blending agents to enable operation in advanced combustion regimes (to expand the operation range of HCCI, for example) was regarded as an open question and an appropriate topic for DOE-sponsored research. The participants would like to see continued DOE investment in understanding fuel-engine interactions for renewable and synthetic blending components. These studies will provide data necessary for understanding fuel quality, fuel performance, and fuel specification issues and requirements. The participants also indicated an interest in DOE-sponsored research relevant to handling and blending of these components, and in particular, integration with the current refinery and distribution infrastructure. The importance of performing credible life-cycle analyses for all new fuels was emphasized.

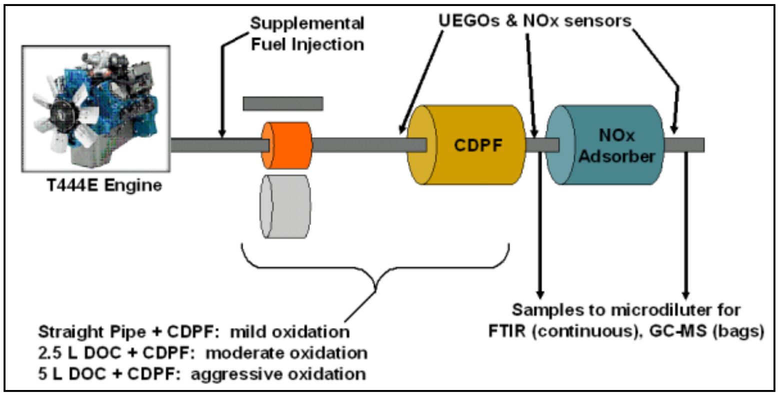
Summary of Roundtable Topic Discussions

Aftertreatment (Emission Control)

Ron Graves, Oak Ridge National Laboratory

This session addressed the impacts of and synergies between new combustion regimes and aftertreatment, with strong consideration of fuels and lubricant interactions. Hydrogen engines were included in the scope. The foremost question at hand was whether new combustion modes, such as HCCI or low-temperature combustion (LTC), would negate the need for NOx and PM aftertreatment, and if not entirely, to what degree would aftertreatment performance requirements be changed. The potential impact of fuel formulation was studied in the session because fuels can have significant effect on most types of emission controls as well as their fundamentally recognized impact on combustion and engine-out emissions. Throughout the session it was apparent that there were many unanswered questions. These questions were recorded as topics for research.

The clear consensus view was that lower engine-out NOx via expanded HCCI operating range may reduce the requirement for NOx conversion efficiencies in aftertreatment devices from >90%, very difficult to achieve with adequate durability, down to approximately 80%, seen as more achievable with reasonable energy penalty. There was no expectation that emissions regulations for 2010 could be met without aftertreatment devices, but as HCCI modes are further developed, the aftertreatment performance demands need to be continually evaluated. The expectation for HCCI and mixed mode engines is that they will still generate considerable NOx and PM at high loads. The nature of the PM has been seen to be different than in normal diesel combustion, giving cause to rethink regeneration strategies and filter technology, especially whether filter cost could be reduced. Even hydrogen-fueled engines (lean-burn) will require NOx aftertreatment if power density and fuel efficiency expectations are to be met.



Example Diesel Engine Aftertreatment System

Aside from NOx and PM, LTC modes are known to generate high HC emissions that will require at least a simple oxidation catalyst, and the expected low exhaust temperatures may cause increased need for active temperature control for NOx and PM aftertreatment. With the relatively high HC/NOx ratio typically seen in LTC, passive lean-NOx catalysis was seen as deserving re-evaluation. Although future engines could be mixed-mode (part time HCCI/LTC) and have lower average engine-out NOx, the overall aftertreatment system and controls could possibly increase in complexity if each combustion mode requires a particular aftertreatment approach. This expectation reinforced the need for modeling to know what aftertreatment to use at what time, to resolve control issues, to optimize regeneration, and to combine the aftertreatment systems with the in-cylinder combustion.

Certain fuel and lubricant constituents (sulfur, phosphorous) can be strong inhibitors of aftertreatment performance, whereas other components can enhance aftertreatment performance. Fuel formulation, therefore, is a significant contributor to an optimal emission-control system. For NOx control, it is recognized that fuel composition can influence the HC reductant species in the exhaust, perhaps even H_2 and CO levels, thus impacting the effectiveness of both lean-NOx traps (LNTs) and lean-NOx catalysts. For PM filters, fuel additives are already in commercial use to aid regeneration. Overall, a message is that fuel formulation efforts should focus on boosting the effectiveness of expanded LTC operations without inhibiting the downstream emission control devices.

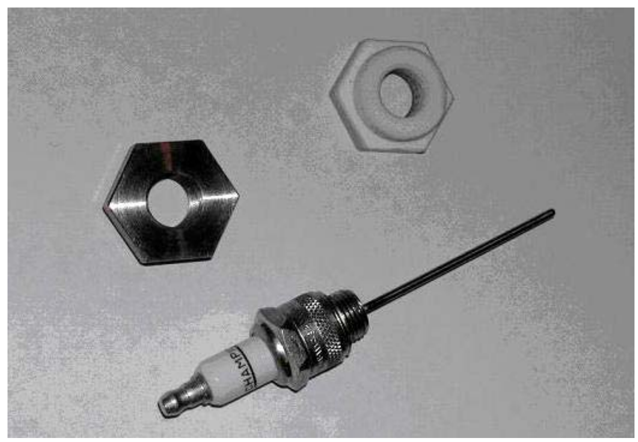
A partial list of the most-recommended research issues is as follows:

- Research and develop the strategies and technologies for integrating LTC modes, characterized by high HC, “wet” PM, and probable lower exhaust temperatures, with aftertreatment technologies for NOx, HC, and PM.
- Extend the strategies to mixed-mode engines and the transitions between modes.
- Develop and exercise models for the above.
- Research the mechanisms and processes of DPF regeneration in LTC modes, and consider whether lower-cost filter technology would be acceptable.
- Re-examine lean-NOx catalysis potential for LTC modes, characterized by much higher HC/NOx ratio in exhaust than with conventional combustion. Similarly, a HC trap may deserve re-evaluation.
- Develop an understanding of effects of fuel composition on aftertreatment devices and LTC modes, looking for advantageous fuel constituents yet keeping a well-to-wheels perspective as a guide for what constituents are reasonable. The auto, engine, and energy companies should work together on this. Include biofuels and synfuels in the research.
- Develop a better understanding of the lubricant constituent effects on the aftertreatment devices and develop corrective measures for poisoning phenomena. Consider special lube requirements for hydrogen-fueled engines.
- Fuel reforming to improve combustion or emission controls has some potential, but should be studied in a broad sense (e.g. reforming via post-injection or other relatively passive measures).
- Research how to make NOx catalysts or traps work in hydrogen engine exhaust (however, hydrogen combustion engines should not be a top priority for DOE).

Engines (Hardware, Sensors, and Controls)

George Muntean, Pacific Northwest National Laboratory

All the engineers participating in the workshop agreed that the diesel-powered vehicle of the future will be a sophisticated, high technology system. The engine in these vehicles may, in fact, be better described as something other than a "diesel" as novel combustion approaches are incorporated. Furthermore, these new engines will most likely have advanced electronics and aftertreatment systems which are highly integrated with one another and with the vehicle systems. These engines may operate in some form of low temperature combustion (LTC) mode, rich smokeless mode, or perhaps in a novel or mixed mode. They may have a variety of aftertreatment devices to control PM, NOx, HC and CO. In addition, the fuel formulation as well as the lubricating oil may be significantly different than today's standards. We may see bio-fuels, hydrogen blends, and reformulated diesel. Given these likely engine and fuel developments, a considerable amount of research and development on the base engine system will be required to achieve the vision of a reliable, highly efficient, and environmentally friendly power source.

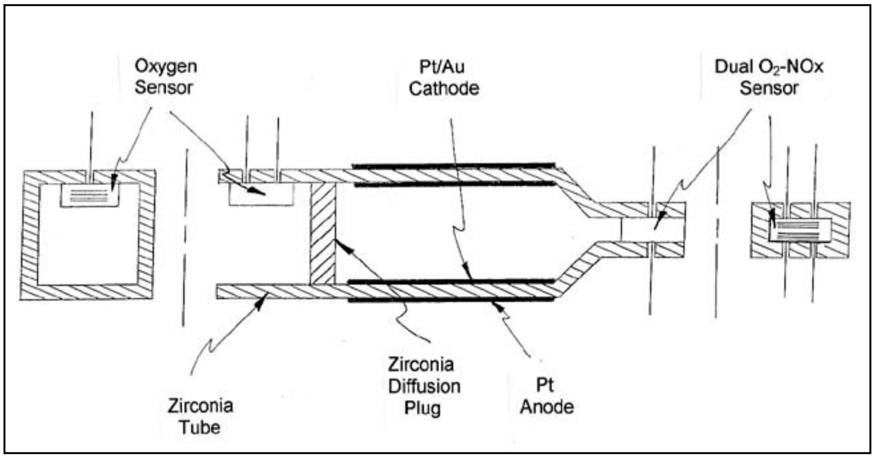


Prototype Honeywell PM Sensor

Amongst the workshop participants, there was a nearly unanimous consensus that the "engine of the future" would have a multifaceted approach to emissions control, including elements of advanced combustion systems and advanced aftertreatment systems. A total systems approach was believed to be imperative, with most participants feeling that mixed-mode systems may be inevitable due to startability, power density, and off-cycle issues. Even with these new combustion system developments, the historic trends towards higher cylinder pressures, higher fuel injection pressures, flexible injection characteristics, smaller injector spray holes, and flexible air handling systems were generally predicted to continue. In fact, some felt as if the new combustion regimes and aftertreatment devices would demand these advancements. Despite all the predicted advancements, there was a general consensus that the fundamental "slider-crank" configuration of IC engines would remain ubiquitous. Likewise, poppet valves, central vertical injectors, and turbomachinery will remain similar to current engines but with improved functionality across the board. There was a broad array of opinions as to the specifics concerning these functional improvements. The role of EGR was not universally agreed upon although nearly everyone felt it had a large role to play for the foreseeable future. The majority believed that EGR would remain a key technology and that better sensing, control, and durability will be required.

Turning to broader issues, there was a nearly unanimous consensus that sensor technology was critical and in need of general development, especially NOx sensors. However, there was a variety of opinions as to which combustion and/or exhaust gas characteristics need be sensed and in which specific configuration. Technology migration of automotive technologies to off-road and smaller bore engines was generally believed to be limited predominately by economic considerations.

When discussing specific research needs for the future, participants had a wide range of opinions. In the areas of increased cylinder pressure, boost, and EGR, they felt a great deal of work remained to be done but that these areas were not optimally within the domain of DOE-funded programs. On the other hand, several engineers expressed interest in variable valve timing technologies, specifically mentioning hydraulic valve actuation. A very small minority expressed interest in pursuing non-conventional engine configurations (e.g. opposed or free piston engines). When it came to fuel systems, a fair number indicated interest in research on variable injector spray and variable injection pressure systems. Likewise, some felt that fuel reformation would become significant, but there was no general consensus on the form it should take. The only issue which appeared to have unanimous consent was in the area of sensors. All the participants felt that sensors will play a critical role in the future. Once again, though, the specifics were not well agreed upon. Most felt that NOx sensors and combustion sensors will be important. Finally, modeling activities were not explicitly solicited in the original questions but were brought up fairly consistently throughout the groups as an area for research.



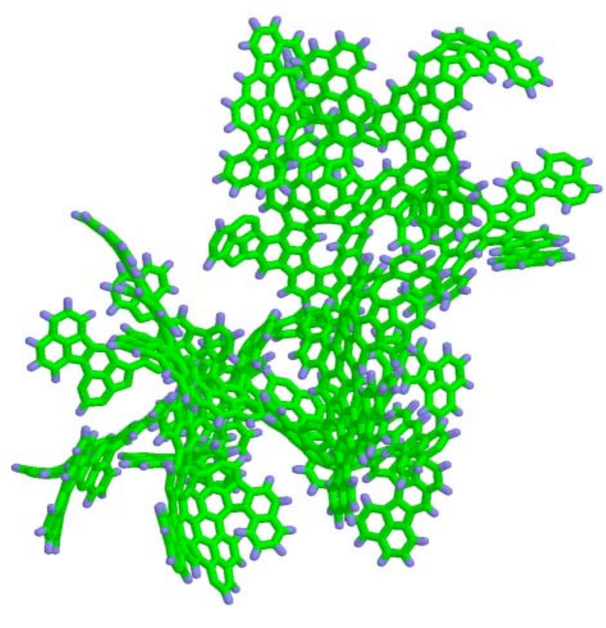
Prototype Combined Oxygen and NOx Sensor

Combustion Modeling

Charlie Westbrook, Lawrence Livermore National Laboratory

The discipline of computer modeling of combustion processes has existed for more than 35 years and is used virtually everywhere in the field of engine design and performance assessment. However, combustion modeling has evolved in a rather disorganized and fragmented way, with little overall planning or organization. Today there are dozens or hundreds of combustion submodels with all levels of complexity describing every possible type of system. Models that include computational fluid dynamics (CFD), turbulent mass and energy transport, combustion chemistry, radiation transport, and multiphase liquid spray and jet injection are used to simulate and/or predict flame/wall interactions, flame quenching, pollutant formation and destruction, exhaust catalyst performance, and many other combustion characteristics. Few of these submodels were ever intended to communicate with each other to provide a coherent overall model, and few are supported financially with enough continuity to become and remain effective "industry standards" in the sense of being used throughout the combustion field. Even in cases where combustion codes developed with DOE funding have become "industry standards," such as KIVA or Chemkin, the burden of continuing support for code development and maintenance, as well as support for code users in industry, has made it necessary to transfer them to private sector software companies to provide these services to code users.

Nearly all companies in the general field of combustion (e.g., engine design, fuels, safety equipment, emissions control, environmental monitoring, etc.) use or would like to use some sort of computer modeling capabilities, ranging from full 3D simulations of fluid mechanics to models of combustion chemistry, spray evolution, pollutant control in-cylinder or with aftertreatment, and many other characteristics. Few of these companies have originally developed any of these models due to the complexity of the models, the cost of developing and maintaining them, the lack of specialized skills in computing science, and other factors. Therefore, most industrial R&D groups use models developed outside their company.



Soot Particle During Molecular Growth Period
Based on Combustion Modeling Work

There are usually multiple simulation codes available for every type of combustion problem. Some are available free, while others are marketed commercially with a substantial license fee required. Most have been developed for a rather narrow range of experimental conditions, and their applicability to a new set of operating conditions is uncertain. In extreme cases, model parameters have been highly tuned for a particular problem, and there is no additional guidance on how relevant they might be for practical engine problems. In some subject areas such as chemical kinetics or turbulence modeling, there are multiple models in the literature with varying levels of complexity, and it may be very difficult for the non-expert to know what to use. In other situations, including both chemical kinetics and multidimensional fluid mechanics, the choice of approach may be limited by the costs of the computer time and the time required to get a solution to a given problem. Finally, in some cases the researchers know what they need as a model but have no easy way to get it; for example, one might need a simplified kinetic model for gasoline ignition, but without in-house expertise in kinetic modeling or in reaction mechanism reduction, such a model would usually be impossible to obtain. In this particular example, such a model for gasoline doesn't currently exist, so the challenge would be to convince someone they ought to work on it and provide it for you.

Although representatives of each company expressed it in different ways, usually depending on the specific technical focus of their company and the computing resources available to them, all of the industrial members of the panel in this session on combustion modeling expressed very similar views. Each noted that some degree of modeling was useful or essential to their R&D activities, and most or all would like to increase and improve their usage in the future. Most agreed that simulations were generally cost-effective, reducing the time and effort for product development. Only the very largest companies did any appreciable amounts of formal or large-scale computer model development, although most relied heavily on science-based engineering models and correlations that could provide answers quickly using calculators or desktop computers. In fact, the most common complaint about more sophisticated computational models was that they needed much more time to provide useful answers than the time usually available.

This tradeoff between short-term project needs and the time (and money) needed to carry out high science content computing represents the basic dilemma faced by all of these industry representatives, combined with the fact that the model experts and builders usually reside at universities, national labs, or other companies and are thus not readily available to work on specific problems as needed. Interestingly, this situation is rather analogous, at least on its surface, to the situation of access to sophisticated instrumentation and techniques such as advanced laser diagnostics for in-cylinder or other similar applications. However, two important factors have made a big difference. First, most of these diagnostics are essentially self-contained and can be purchased as a complete unit. Second, the combustion field has found effective methods of transferring the working expertise of using such tools to industry practitioners. The Sandia National Laboratories Combustion Research Facility is the prime example of this technology transfer function in the area of combustion diagnostics, and one important part of the Sandia CRF charter is to provide visitors with that technology transfer, educational function. In addition, many universities and other experts welcome opportunities to train newcomers in the skills required to use these advanced diagnostic tools on real industry problems.

The same function is much less organized and available in the field of combustion modeling. It is much more difficult to define a "complete system" in combustion modeling than in diagnostic hardware. The large CFD codes like KIVA or FLUENT contain many submodels that have been necessarily simplified, often drastically, to permit multidimensional simulations. They do not come supplied with the more detailed versions of submodels that are often needed, and the data and problem parameters for those more detailed submodels must either be obtained elsewhere or do not yet exist. Recent programs including the DOE Diesel Collaborative Project recognize the need for this type of activity, but their impact on the R&D environment at most companies has been quite small.

Equally important, the experience and skills of using the best models are not transferred to interested industry users as effectively as in the field of complex diagnostics. The LANL KIVA group has done a fine job in this area, but not everyone wants to use that specific code and similar training and help is not available except for the commercially marketed codes like Chemkin and the major CFD codes.

At the workshop, the most important feedback from industry involved frustration with these two major elements. Existing combustion models need better submodels to describe processes of importance to industry problems, and existing models are hard to learn how to use, have poor user interfaces, and are difficult to modify to suit applications of particular interest. The comments of "need better turbulence model", "need better spray model", "need kinetics for gasoline", and others really address the first factor above. The researchers who would be the natural providers of such improvements or new features are not supported to provide them and are funded or rewarded for doing other things, and the industry researchers do not then have the expertise to do it themselves. The practical result is that the industry researchers do not have a tool they can use conveniently.

If code developers were more closely coupled to the industry code users, the education functions would probably happen very naturally and effectively. There are difficulties associated with proprietary issues associated with specific products, but if industry code users became sufficiently expert at using available tools, they could then do the specific problems themselves. One solution often used at present by some companies is to hire subject matter experts as consultants to develop specific modeling capabilities they need, which can solve their problem but does not benefit the entire combustion community very well.

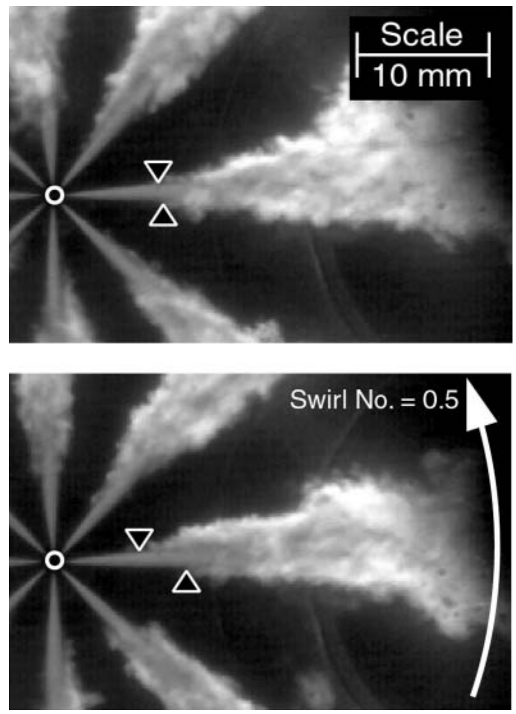
Interestingly, there was very little concern about computer power or access to supercomputing resources. Most companies indicated that they had or could obtain the level of computing power they needed. Collaborations with DOE labs or others with big computing resources seem to work when raw computing power is essential, and otherwise the capabilities of desktop computing seem to be sufficient.

In-Cylinder Combustion

Dennis Siebers, Sandia National Laboratories

Discussions in the In-Cylinder Combustion Session focused on identifying the critical in-cylinder combustion and emissions research needs for enabling advanced high efficiency, emission compliant internal combustion engines for transportation. The discussions addressed research needs related to five topics: low-temperature combustion (LTC) strategies; advanced diesel combustion strategies, especially for use in a mixed-mode combustion system; alternative and advanced petroleum-based fuels; efficiency enhancement technologies (e.g., variable compression ratio, variable valve timing, improved exhaust heat recovery, etc.); and hydrogen-fueled engines.

The LTC topic generated the most discussion. LTC refers to combustion strategies such as Homogeneous Charge Compression Ignition (HCCI) or the various forms of stratified charge compression ignition that have been proposed. LTC strategies offer the potential for enabling engines with high diesel-like thermal efficiencies and very low NOx and PM emissions. Mixed-mode combustion systems would use LTC at light to moderate loads to take advantage of the low emission, high efficiency potential of LTC at part loads and either diesel or spark ignition at high loads to enable higher power density than may be possible with LTC alone.



Laser Image Showing the Effect of In-Cylinder Swirl on Combustion

There was general agreement that LTC offers significant potential for enabling high efficiency, emissions compliant engines, but that the state-of-knowledge regarding LTC is insufficient. A fundamental knowledge-base on in-cylinder LTC processes must be established to aid the development of "real world" engines using LTC. The improvements in understanding are needed in all aspects of fuel injection, fuel-air mixing, combustion, emissions formation, and engine-out emissions. Some of the specific in-cylinder issues that were discussed included:

- Limits of Operation.
  - low and high load, combustion rate, and emissions formation.
- Ignition Process, Start and Phasing of Combustion.
- Mixed–Mode Operation, Optimal Chamber and Fuel Injection System Design.
- Fuel Injection and Mixing Strategies.
- Control of Combustion during Transients and Mode Switching.
- Heat Transfer (to cylinder walls) during LTC Modes.
- Fuel Characteristics for Optimal LTC.
- Cold Start and Light Load Operation (HCCI or LTC).
- Combustion System Optimization.

Discussions on diesel combustion focused on advanced strategies for reducing emissions, thus reducing the burden on diesel aftertreatment systems. Reductions in emissions will also be critical for enabling the application of diesel combustion at higher loads in mixed-mode applications. Areas suggested for continued research included:

- Multiple injection strategies, including multiple injection strategies that result in LTC combustion of a portion of the fuel during a given engine cycle.
- Fuel jet structure and the impact of engine and fuel parameters on fuel injection, especially during multiple injections.
- Combustion system optimization over the full load range when using diesel/LTC mixed-mode operation:
  - bowl design/geometry
  - fuel spray characteristics
- Variable fuel injector orifice geometry.
- Application of high levels of EGR for NOx control, especially in mixed-mode combustion applications.

The fuels topic also generated significant discussion. There was agreement that there is insufficient understanding about which fuel properties are critical and what the ideal fuel properties are for LTC. Such information would be helpful to suppliers providing fuels for LTC engines. More fundamental combustion research is needed to determine how fuel properties affect the various combustion modes from diesel to LTC and how to specify a fuel that will perform well under both HCCI and diesel or spark ignition operation. The likelihood of different fuel property requirements for each mode makes use of mixed-mode combustion very challenging. A multi-grade fuel may be needed for LTC and mixed-mode combustion engines. Some participants in the discussions called for research on a relatively large matrix of fuels to develop a better understanding of fuel effects on LTC. A more strongly expressed opinion, however, was that since diesel fuel and gasoline are the fuels for the near term, they should be the focus of research in the near future. It was also recognized that a new parameter (besides the cetane and octane numbers) may be necessary for specifying fuels for operation in LTC regimes. In addition, a suggestion was made that gas-to-liquid (GTL) fuels may enable tailoring of fuel properties.

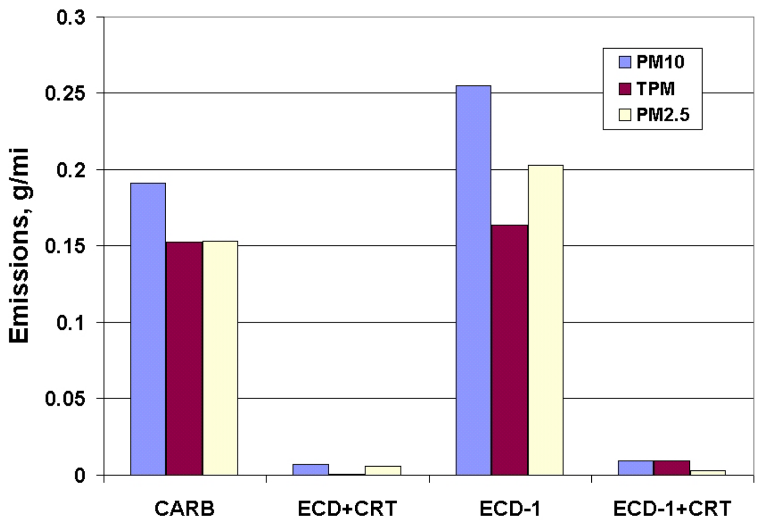
Discussion on the topic of in-cylinder research needs for efficiency improvement technologies was very limited. A sentiment expressed was that the focus should be on getting the low-emission, high-efficiency LTC and advanced diesel combustion strategies to work, then consider additional technologies for improving efficiency. Moreover, it was suggested that there may be little opportunity for waste heat recovery on high-efficiency, light-duty engine technology and that friction losses with variable compression ratio technology could outweigh potential efficiency gains depending on the duty cycle.

The last topic of discussion was on hydrogen-fueled IC engines. There was agreement that hydrogen-fueled engines could play a role in the transition to a hydrogen economy. The primary advantage to using hydrogen as fuel in internal combustion engines is the low lower-flammability limit, which allows lean or dilute combustion for NOx control. There are issues that need to be investigated such as the pre-ignition phenomena, combustion stability, as well as fuel/air mixing for spark ignition, direct injection engines. Research to explore methods such as boosting to increase power density when operating under lean or dilute conditions on hydrogen was suggested. However, little is known about combustion of hydrogen at the high pressures that will occur with boosting. It was also noted that use of stoichiometric hydrogen combustion to achieve high power density produces NOx, requiring aftertreatment systems effective in a hydrogen engine exhaust stream. Regarding on-board fuel reforming to generate a high hydrogen content fuel stream, there was doubt expressed as to its benefit as a transition strategy to hydrogen, since no benefit has been shown by studies to date. Reforming incurs a penalty of about 30 percent of the energy content of the fuel. However, on-board fuel reformation may be useful in generating small amounts of hydrogen for enhancing LTC or for supplying reductants for regenerating aftertreatment devices.

Base Fuels

Wendy Clark, National Renewable Energy Laboratory

Base fuels are conventional, commercial petroleum products that we expect to dominate the market for the forseeable future. A major objective is to identify technology barriers to the development and implementation of advanced base fuels. Advanced base fuels may be reformulated in some way, have altered physical or chemical properties, or be the major constituent of a finished fuel that is blended with other "blending agents" such as renewables and synthetics. Discussion included predictions of what fuel properties advanced engines might require, whether or not there was work still to be done to commercialize Canadian oil sands diesel, if more than one grade of diesel fuel is necessary or desirable, and what changes to gasoline may be required.



Emissions of Two Low-Emission Base Fuels With and Without Catalyzed Particulate Traps

There was a clear consensus that lower sulfur levels in gasoline as well as diesel fuel are desirable. Most felt that standardization with Japan and Europe at something less than 10 ppm should be implemented, mainly as an aftertreatment enabler. Beyond sulfur reduction, a frequent comment heard was that collaborative research (such as the APBF-DEC organization) on fuel properties would result in the most efficient solution. Such a coordinated effort between hardware manufacturers and energy suppliers could work to identify the optimum mix of engines and fuels. A near-term opportunity for this collaboration would be development of HCCI engines and fuels.

A recurring discussion was whether DOE should encourage the energy industry to try to maximize the amount of fuel produced by today's refineries. A related question worthy of analysis is whether it makes sense to change the gasoline to diesel ratio of our refineries to maximize use of crude oil given that (1) our refineries are optimized for gasoline production, (2) we need large amounts of gasoline, and (3) European refineries over-produce gasoline and are willing to sell it to us relatively cheaply.

It was repeatedly suggested that well-to-wheels analyses be conducted when considering any base fuel changes. Many participants believed well-to-wheels analysis will show that the largest energy security impact can be attained by very large-scale market penetration of light-duty diesel vehicles. There was consensus that more effort should be devoted to well-to-wheels analysis to choose fuels and combustion systems (e.g., should HCCI engines be designed for gasoline-like fuels or diesel fuels?).

It was generally acknowledged that we need to better understand the combustion characteristics of fuel components before we can identify ways of making base gasoline and diesel fuels combust more efficiently. This is especially true for advanced combustion concepts such as HCCI. A new rating method is needed for low-temperature/HCCI combustion, and the ignition quality tester (IQT) method was referred to as having promise. There was polarity around the discussion of tightening fuel specifications to reduce variability, as might be expected. Several comments about the fuel requirements converging for light- and heavy-duty applications were based upon speculation regarding fuel property requirements for low temperature, mixed-mode operation. It was noted that any changes in fuel physical and chemical properties would have to be backward-compatible with existing engines.

Most participants acknowledged the impracticality of having two diesel grades but pointed out that development and certification of new engines will be difficult until an ultra-low sulfur grade is widely available.

Other fuel property themes included a strong desire by the OEMs for higher cetane, lower aromatic diesel fuel in the near term. These property changes were viewed as an enabler for light-duty diesels to penetrate the US market. Lower sulfur versions of naphtha, JP-8 and kerosene were mentioned frequently as potential narrow-cuts that might serve as a near-term starting point for collaborative research projects. Alternately, a wider boiling range material was proposed as more amenable to HCCI operation. Although there was a wide consensus that petroleum-based fuels will be the base fuels for many more years, oxygenates, Fischer-Tropsch diesel and biodiesel were all seen as potentially favorable blending agents.

Canadian oil sands were typically viewed as a non-event: we are already importing ever-increasing quantities of these fuels that are refined and blended to provide a finished fuel that meets D975. The challenges remaining include lowering the cost of extraction even further and improving process efficiency to lower carbon emissions, which are higher than for conventional crude refining.

Tax policies were a common topic of discussion. It was suggested many times that tax policies similar to what Europe has towards diesel vehicles and diesel fuel should be explored. The current “loop-hole” for small businesses to purchase large SUVs used for personal transportation was cited as a policy that should be changed.

The participants indicated a desire for continued DOE involvement in broad collaborations with the hardware and energy industries to address base fuel issues. Near-term R&D on the impact of sulfur, as well as cetane and aromatic content, on engine performance was viewed as a priority. A harmonization of regulations and standards for base fuels with those in Europe and Japan was viewed as desirable. There was consensus that well-to-wheels analysis is critical for understanding the impacts of research investments, and that this should be applied to fossil energy production/utilization scenarios as well as to renewable and synthetic fuels. Research to improve fundamental understanding of combustion in different regimes and to develop fuels and engines for low-temperature/HCCI operation was viewed as the longer-term priority.

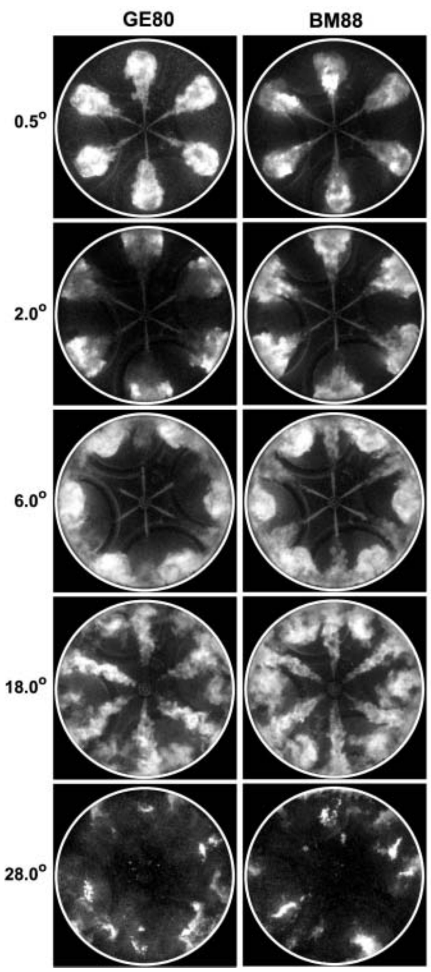
Blending Components

Robert McCormick, National Renewable Energy Laboratory

DOE views blending components as renewable or synthetic fuel components that can be blended with conventional components to accomplish the following goals:

1. Displace petroleum
2. Enable the development of more efficient and less polluting advanced engines

Biodiesel and Fischer-Tropsch diesel are examples of currently-available blending components. The discussion of blending components covered issues driving their use, life-cycle analysis, the need for standard specifications, fungibility, blending strategies, and the potential of blending to enable advanced combustion engines.



Laser Images Showing the Effects of Oxygenates on Diesel Fuel Combustion

It was generally agreed that the use of renewable blending components would likely be driven by legislation or regulation, not by economics. Thus, R&D should be directed at obtaining the data required for legislative or regulatory consensus. However, some participants were of the opinion that a business case could be made for certain blending components produced from biomass. And there was general agreement that cost of blending components is very important, even if required by legislation. Additionally, there was consensus that blending components must be available in very large quantities to be practical and to ever have a chance of being economical.

There was also broad agreement on the need to understand the "well-to-wheels" life cycle energy efficiency and emissions of blending components. Along with the "well-to-wheels" analysis, an analysis to determine the relative benefits of running all vehicles on a 5% blend, versus running 5% of the vehicles on a 100% biofuel, should be undertaken. In general, the consensus was that blending should not be done if increases in engine-out pollutant emissions occur.

Because of the highly dispersed nature of biomass and the variation in biomass properties from region to region, it may make sense to have different bio-based blending components for different regions. However, blends must meet the standard specification for diesel fuel, or a new standard specification must be developed for each blend. Blending agents may introduce various specification issues that do not currently apply to diesel fuel. Furthermore, current fuel specifications assume that the fuel is petroleum–based, and because of this assumption, there are a number of properties that do not have to be specified. This will not be the case for renewable blends. In general, a blend component cannot cause a reduction in quality based on any of the currently specified properties and must result in an adequately stable fuel. There was some interest in the idea of having one fuel specification nationwide for long haul trucks and separate, regional specifications for local use vehicles.

Engine manufacturers pointed out that they make engines for sale worldwide. Thus, any fuel blend or blend specification must be applicable internationally. Engine manufacturers also stated that given a consistent fuel specification, they could likely design an engine to operate on the fuel.

The issue of refinery blending as opposed to splash blending at the terminal was discussed. Refinery blending is lower cost and therefore preferred, but the blending component must be compatible with the pipeline system infrastructure and there must be adequate standard specifications for fungibility. Another option discussed was blending at the dispensing pump. If the blend component was required for an advanced engine but not appropriate for older engines, blending at the pump would allow the appropriate fuel for each to be dispensed.

There was much discussion of blending components for advanced engines operating in advanced combustion regimes such as HCCI. It was generally agreed that fuel performance standards would have to be tightened considerably to meet the requirements of these advanced engines. The potential of blending agents to enable operation in advanced combustion regimes (to expand the operation range of HCCI, for example) was regarded as an open question and an appropriate topic for DOE-sponsored research.

The participants would like to see continued DOE investment in understanding fuel-engine interactions for renewable and synthetic blending components. These studies will provide data necessary for understanding fuel quality, fuel performance, and fuel specification issues and requirements. The participants also indicated an interest in DOE-sponsored research relevant to handling and blending of these components, and in particular, integration with the current refinery and distribution infrastructure. The importance of performing credible life-cycle analyses for all new fuels was emphasized. The potential for blending components to enable advanced combustion engines was, by broad agreement, an appropriate area for DOE research.