Merit Review and Peer Evaluation of FY 2004 DOE Advanced Combustion Engine R&D

Argonne National Laboratory, Argonne, IL
May 18-20, 2004

Office of Energy Efficiency and Renewable Energy
FreedomCAR and Vehicle Technologies Program

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U.S. Department of Energy
Energy Efficiency and Renewable Energy

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

Department of Energy
Washington, DC 20585

December 13, 2004

Dear Colleague:

This document summarizes the comments provided by the Review Panel for the FY 2004 Department of Energy (DOE) Advanced Combustion Engine R&D Merit Review and Peer Evaluation Meeting, the "ACE Review," held on May 18-20, 2004 at Argonne National Laboratory (ANL). The raw evaluations and comments of the panel were provided (with reviewers' names deleted) to the presenters in early June and were used by national laboratory researchers in the development of Annual Operating Plans (AOPs) for fiscal year (FY) 2005. The panel's recommendations have been taken into consideration, along with laboratory AOPs, by DOE Technology Managers in the development of work plans for FY 2005.

The table below lists the projects discussed at the review and the major actions to be taken during the upcoming fiscal year. As in past years, the panel members have been identified in this document, but specific comments by panel members remain anonymous.

This review covers only national laboratory projects funded under the Combustion and Emission Control line of the federal budget. Industry R&D projects, funded competitively, are not reviewed at this annual meeting, but are reviewed semi-annually by DOE Technology Managers.

Topic Title and Organization	FY 2005 Major Actions
In-Cylinder Combustion	
Analysis of Low-Temperature, Non-Sooting Diesel Combustion (Salvador Aceves, Lawrence Livermore National Laboratory)	Continue project – add detail to mixing correlations for low-temperature diesel combustion model. Compare model results with experimental data collected by SNL and ORNL.
Automotive HCCI Combustion Research (Richard Steeper, Sandia National Laboratories)	Continue project – characterize fuel-air-residual gas mixing effects on gasoline HCCI combustion in an automotive engine using various fuel injectors.
Automotive Low Temperature Diesel Combustion Research (Paul Miles, Sandia National Laboratories)	Continue project – characterize early-injection LTC combustion in a light-duty engine using diesel fuel.
Exploring Low NOx Low PM Combustion Regimes (Robert Wagner, Oak Ridge National Laboratory)	Continue project – focus on broadening the useful speed/load envelope for efficient LTC regimes with upgraded electronic control package and low pressure loop EGR.
Fuel Spray Research using X-Rays at the Advanced Photon Source (Chris Powell, Argonne National Laboratory)	Continue project – investigate higher pressures and temperatures and increase efforts in modeling.
HCCI and Stratified-Charge CI Engine Combustion (John Dec, Sandia National Laboratories)	Continue project – determine the effectiveness of thermal stratification for extending the load range for HCCI operation and investigate fuel constituent effects on HCCI ignition.
High-Energy Pulsed-Laser Diagnostics for the Measurement of Diesel Particulate Matter (Peter Witze, Sandia National Laboratories)	Continue project – quantify and improve the accuracy of time-resolved PM volatile fraction measurement and develop PM mean-particle-size measurement capability.
In-Cylinder Processes under Early Direct-Injection Diesel HCCI Conditions (Chuck Mueller, Sandia National Laboratories)	Continue project – investigate use of fuel properties to expand the load range for LTC operation and determine why biodiesel produces higher levels of NOx.
Initiatives of Fuel Spray Research at Argonne's APS (Jin Wang, Argonne National Laboratory)	Continue project – phase-contrast imaging inside the injector nozzle will be developed.

Topic Title and Organization	FY 2005 Major Actions
Investigate H_2 Spark-Ignited DI Engine Combustion using CFD and Detailed Chemical Kinetics (Salvador Aceves, Lawrence Livermore National Laboratory)	Continue project – develop and validate model for DI hydrogen ICE that is compatible with KIVA. Compare modeling results with experimental data.
Kinetic Modeling of Practical Hydrocarbon Fuels (Charles Westbrook, Lawrence Livermore National Laboratory)	Continue project – develop surrogate HCCI fuel mechanism. Use computational chemistry to compute the effects of sulfur poisoning and other exhaust species on NOx adsorption on trap surface (latter should become a separate project).
KIVA-4 Development (David Torres, Los Alamos National Laboratory)	Continue project – document KIVA-4, begin parallelization of KIVA-4, investigate methods of mesh construction to accommodate moving boundaries for KIVA-4. Funding will be increased.
LES Modeling Applied to LTC/Diesel/Hydrogen Engine Combustion Research (Joseph Oefelein, Sandia National Laboratories)	Continue project – perform baseline simulations of the optical hydrogen IC-engine configuration with emphasis on the H2 injection mixing processes.
Low Flame Temperature Diesel Combustion with Jet-Wall Interaction (Lyle Pickett, Sandia National Laboratories)	Continue project – determine limits for mixing-controlled LTC operation and how pilot and multiple injections affect diesel/LTC combustion and emissions.
Modeling of HCCI and PCCI Combustion Processes (Dan Flowers, Lawrence Livermore National Laboratory)	Continue project – extend PCCI model development to enable DI engine analysis.
Optimized Free Piston Engine Generator (Peter van Blarigan, Sandia National Laboratories)	Continue project – investigate and design a prototype free-piston engine configuration and optimize the two-stroke scavenging system. Increase level of interaction with industry.
Spark Stabilization of HCCI Combustion (Bruce Bunting, Oak Ridge National Laboratory)	Continue project – investigate higher loads with external EGR. Analyze and explain efficiency benefits seen in FY 2004.
Role of Radiative Heat Transfer on NOx Formation in a Heavy-Duty Diesel Engine (Mark Musculus, Sandia National Laboratories)	Continue project – investigate early and late injection LTC in diesel-fueled heavy-duty engine applications and develop conceptual model for these LTC modes.
Thermoelectrics (Larry Olsen, Pacific Northwest National Laboratory)	Continue project – performance measurements up to 800ºC; develop methods to integrate $Si/Si_{0.8}Ge_{0.2}$ and B_4C/B_9C multilayer structures into TEG modules. **This project will not be included in the ACE Review in the future. It will be reviewed in another forum.**
Emission Control Devices for NOx and PM Control	
Accelerated Catalyst Aging (Bruce Bunting, Oak Ridge National Laboratory)	Continue project – evaluate effects of phosphorous on exhaust chemistry, catalyst performance, and structure. Coordinate with catalyst and lube additive companies.
Advanced NOx Control for Locomotive Engines (Darryl Herling, Pacific Northwest National Laboratory)	Continue project – expand screening of multi-metal mixed oxides and perovskites with multiple oxygenate reductants, investigate additional oxygenates as reductants.
Bi-Functional Catalysts for the Selective Catalytic Reduction of NOx by Hydrocarbons (Chris Marshall, Argonne National Laboratory)	Continue project – use combinatorial chemistry software to analyze current results; sign CRADA with industry partner.
Characterizing NOx Adsorber Regeneration (Shean Huff, Oak Ridge National Laboratory)	Continue project – characterize H2, CO, and HC species interactions with fresh, aged, and sulfated LNTs. Work with industry partners through CLEERS to share data.
CLEERS DPF Modeling (George Muntean, Pacific Northwest National Laboratory)	Continue project – focus on quantitative studies of filter performance, incorporate oxidation mechanism(s); increase validation efforts.
CLEERS Kinetics: Lean NOx Traps (Stuart Daw, Oak Ridge National Laboratory)	Continue project – continue development and coordination of focus groups and increasing participation from emission control component suppliers. Add a careful definition of degreening as part of the standard CLEERS LNT protocol.
Dedicated Sulfur Trap for Diesel Emission Control (David King, Pacific Northwest National Laboratory	Continue project – continue studies with metal modified cryptomelane to further increase SO_2 uptake capacity at 200^{o}C and below, investigate on-board regeneration.

Topic Title and Organization	FY 2005 Major Actions
Development of an Advanced Automotive NOx Sensor (Larry Pederson, Pacific Northwest National Laboratory)	Continue project – determine how sensor operation is affected by the presence of ammonia in exhaust gases. Investigate pulsed detection methods as a means of enhancing sensor sensitivity and accuracy.
Lean NOx Trap Chemical Behavior and Thermal Deactivation Effects (Todd Toops, Oak Ridge National Laboratory)	Continue project – continue defining deactivation mechanisms of LNT systems, using DRIFTS characterization of model catalysts that are representative of the technology.
Mechanisms of Sulfur Poisoning of NOx Adsorber Materials (Chuck Peden, Pacific Northwest National Laboratory)	Continue project – identify the mechanisms of sulfur poisoning by investigating the amount and type of sulfur deposited on the catalyst surface as a function of exposure time using the characterization techniques established in the first phase of the program. Investigate de-sulfation processes – effects on performance and materials properties. Identify the mechanisms of thermal degradation of Johnson/Matthey supplied materials by correlating performance measurements with changes in the material properties.

We are still considering the date and location for the FY 2005 ACE review and will follow-up with an email on this matter within the next few weeks. We would like to express our sincere appreciation to the researchers and reviewers who make this report possible and influence our decisions for the new fiscal year. Special thanks go to the staff at Argonne National Laboratory for hosting the 2004 meeting.

Thank you for participating in the FY 2004 DOE Advanced Combustion Engine R&D review meeting. Please feel free to provide suggestions for improving this annual meeting. We look forward to your participation in the FY 2005 review.

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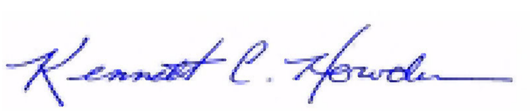

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Introduction

This report is a summary and analysis of comments from the Advisory Panel at the FY 2004 DOE National Laboratory Advanced Combustion Engine R&D Merit Review and Peer Evaluation, held May 18-20, 2004 at Argonne National Laboratory. The work evaluated in this document supports the FreedomCAR and Vehicle Technologies Program. The results of this merit review and peer evaluation are major inputs used by DOE in making its funding decisions for the upcoming fiscal year. The objectives of this meeting were to:

- Review and evaluate FY 2004 accomplishments and FY 2005 plans for DOE laboratory programs in advanced combustion engine R&D.
- Provide an opportunity for industry program participants (engine manufacturers, emission control manufacturers, vehicle manufacturers, etc.) to shape the DOE-sponsored R&D program so that the highest priority technical barriers are addressed. The meeting also serves to facilitate technology transfer.
- Foster interactions among the national laboratories conducting the R&D.

The Review Panel members, listed in Table 1, attended the meeting and provided comments on the projects presented. They are peer experts from a variety of related backgrounds including automobile and truck companies, engine manufacturers, emission control system manufacturers, fuels manufacturers, universities, and other U.S. Government agencies. A complete list of the meeting participants is presented as an appendix.

Table 1: Review Panel Members

Member Name	Affiliation
Moataz Ali	Volvo Powertrain Corporation
Richard Blint	General Motors Corporation
Andre Boehman	Penn State University
Phil Bohl	Robert Bosch Corporation
Brian Bolton	Detroit Diesel Corporation
Joseph Bonadies	Delphi Corporation
Hai-ying Chen	Johnson Matthey , Inc.
Russell Durrett	Cummins Inc.
Kenneth Erdman	Caterpillar, Inc.
Christoph Espey	DaimlerChrysler Corporation
John Farrell	ExxonMobil Research & Engineering
Xinqun Gui	International Truck & Engine Corporation
Craig Haberger	Caterpillar, Inc.
Nabil Hakim	Delphi Corporation
Carl-Anders Hergart	General Motors Corporation
John Hoard	Ford Motor Company
Bernd Krutzsch	DaimlerChrysler Corporation
John Lapetz	Ford Motor Company
Jonathan Male	General Electric Company
Richard Peterson	General Motors Corporation
Ramesh Poola	GM Electro-Motive Division
Giorgio Rizzoni	Ohio State University
Stan Roth	Engelhard Corporation
Peter Schihl	U.S. Army TARDEC
Richard Winsor	Deere & Company
Tom Yonushonis	Cummins Inc.

Analysis Method

As shown in Table 1, a total of twenty-six advisory panel members participated in the merit review. A total of 29 project presentations were given at the meeting, and a total of 431 review sheets were received from the review panel members (not every panel member reviewed every project). To determine the scores for these projects, the projects were placed into two categories that were established in consultation with DOE program managers. These two categories were:

- In-Cylinder Combustion and Modeling Studies, and
- Emission Control Devices for NOx and PM Control.

Review panel members were asked to provide numeric scores (on a scale of one to four, with four being the highest) for five aspects of the research on their review form, a sample of which can be found as an appendix to this report. The five aspects were:

- Relevance to overall DOE objectives;
- Approach to performing the research and development;
- Technical accomplishments and progress toward achieving the project and DOE goals;
- Technology transfer and collaborations with industries, universities, and other laboratories; and
- Approach to and relevance of proposed future research.

The numeric scores given to each project by the reviewers were averaged to provide the overall score for that project for each of the five criteria. An average score for the five criteria was also calculated within each of the two project categories for all projects in that category. In this manner, a project's overall score can be compared to other projects in that category.

Reviewers were also asked to provide qualitative comments on the five research aspects, as well as on the specific strengths and weaknesses of the project and any recommendations for additions or deletions to the work scope. These comments, along with the quantitative scores, were placed into a database for easy retrieval and analysis. These comments are summarized in the following sections, with an indication of how many reviewers provided written comments for that project and that question. All reviewers of a given project provided a numeric score for each of the five criteria, but did not necessarily provide qualitative comments.

Organization of the Report

This report is organized in two main sections, one section for each of the two main R&D categories. The first page of each section presents a summary of the average scores for the projects in that category, highlighting the highest scores for each of the five scoring aspects and the category average for those aspects. A brief description of the general type of research being performed in each category is also presented.

The remaining pages of each section present the results of the analysis for each of the projects discussed at the merit review. Graphs showing how the particular project compared with other projects in its category are presented, as well as a discussion of these results. A summary of the qualitative comments is also provided.

This category includes projects to examine, through the use of optically accessible laboratory test engines and other tools, how diesel combustion occurs in a diesel engine cylinder. Research focuses on how particulates are formed in the cylinder, and how particulate formation might be related to fuel injection pressure and other engine parameters. Studies are also underway to relate experimental data obtained from these engines to thermophysical models of engine operation. This category also includes projects involving the homogeneous-charge compression-ignition engine (HCCI), which combines the high thermal efficiency of a diesel engine with the ability to use fuels other than diesel fuel. HCCI engines can produce lower emissions of NOx and PM than conventional diesel engines. Research is currently being done to combine laboratory HCCI engine experiments with detailed modeling to build a more complete understanding of HCCI combustion and facilitate design of engine control systems. Research is also beginning in this area on hydrogen combustion in internal combustion engines.

Below is a summary of average scores for 2004 for the nineteen projects in this category, along with the average, minimum, and maximum score for all projects in this report. The highest score in this category for each question is highlighted.

Summary of Scores for Projects in this Section

Page Number for Project Summary	Research Project Title	Q1 Relevance Score	Q2 Approach Score	Q3 Technical Accomplish -ments Score	Q4 Tech Transfer Score	Q5 Future Research Score
5	*Analysis of Low-Temperature, Non-Sooting Diesel Combustion*: Salvador Aceves (Lawrence Livermore National Laboratory	3.23	3.31	2.92	3.08	3.23
8	*Automotive HCCI Combustion Research*: Dick Steeper (Sandia National Laboratories)	3.56	3.63	3.13	3.25	3.44
11	*Automotive Low-Temperature Diesel Combustion Research:* Paul Miles (Sandia National Laboratories)	3.79	3.74	3.42	3.68	3.42
14	*Exploring Low-NOx,Low-PM Combustion Regimes:* Robert Wagner (Oak Ridge National Laboratory)	3.39	3.31	3.39	3.08	3.31
17	*Fuel Spray Research using X-Rays at the Advanced Photon Source:* Chris Powell (Argonne National Laboratory)	3.06	3.06	2.89	3.44	2.94
22	*HCCI and Stratified-Charge CI Engine Combustion Research:* John Dec (Sandia National Laboratories)	**3.88**	3.81	**3.69**	3.69	**3.69**
25	*High-Energy Pulsed Laser Diagnostics for the Measurement of Diesel Particulate Matter:* Peter Witze (Sandia National Laboratories)	3.79	**3.84**	3.68	**3.84**	3.56
28	*In-Cylinder Processes under Early Direct-Injection Diesel HCCI Conditions:* Charles Mueller (Sandia National Laboratories)	3.60	3.67	3.40	3.73	3.60
31	*Initiatives of Fuel Spray Research at Argonne's APS:* Jin Wang (Argonne National Laboratory)	2.80	3.07	2.80	3.07	2.73
35	*Investigate Hydrogen Spark Ignited Direct Injected Engine Combustion Using CFD & Detailed Chemical Kinetics:* Salvador Aceves (Lawrence Livermore National Laboratory)	2.82	3.00	2.50	3.00	2.91
37	*Kinetic Modeling of Practical Hydrocarbon Fuels:* Charles Westbrook (Lawrence Livermore National Laboratory)	3.41	3.47	3.47	3.24	3.25
41	*KIVA-4 Development:* David Torres (Los Alamos National Laboratory)	3.28	3.33	3.11	3.28	3.22
45	*LES Modeling Applied to LTC/Diesel/Hydrogen Engine Combustion Research:* Joseph Oefelein (Sandia National Laboratories)	3.27	3.30	3.09	2.70	3.36
47	*Low Flame Temperature Diesel Combustion with Jet-Wall Interaction:* Lyle Pickett (Sandia National Laboratories)	3.80	3.53	3.67	3.47	3.47
50	*Modeling of HCCI and PCCI Combustion Processes:* Dan Flowers (Lawrence Livermore National Laboratory)	3.21	3.13	3.00	3.53	3.13
54	*Optimized Free Piston Engine Generator:* Peter van Blarigan (Sandia National Laboratories)	3.07	3.29	2.71	2.71	2.79
57	*Spark Stabilization of HCCI Combustion:* Bruce Bunting (Oak Ridge National Laboratory)	3.12	3.00	2.94	2.65	2.82

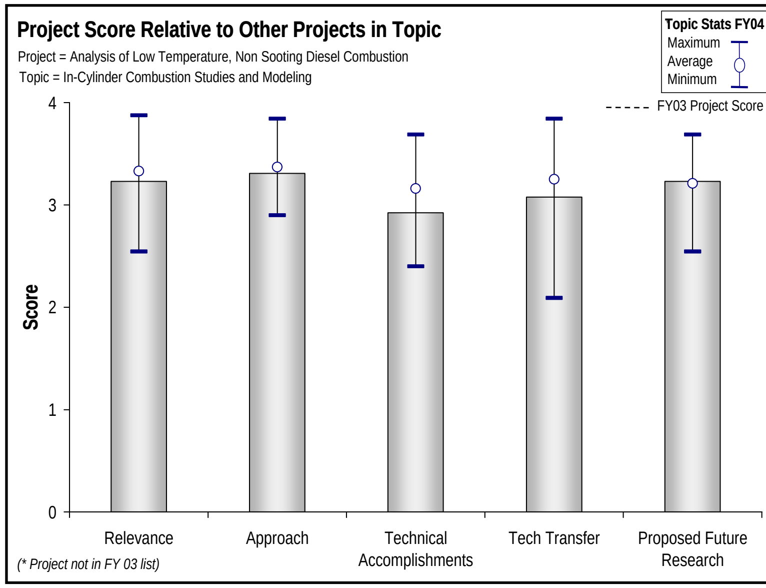
Page Number for Project Summary	Research Project Title	Q1 Relevance Score	Q2 Approach Score	Q3 Technical Accomplish-ments Score	Q4 Tech Transfer Score	Q5 Future Research Score
61	*The Role of Radiative Heat Transfer on NOx Formation in a HD Diesel Engine:* Mark Musculus (Sandia National Laboratories)	3.13	3.27	3.20	3.33	3.33
64	*Thermoelectrics:* Larry Olsen (Pacific Northwest National Laboratory)	2.55	2.90	2.40	2.09	2.55
	Average Score for This Category	**3.30**	**3.35**	**3.13**	**3.20**	**3.20**

Overall Program Scores

	Q1 Relevance Score	Q2 Approach Score	Q3 Technical Accomplishments Score	Q4 Tech Transfer Score	Q5 Future Research Score
Overall Program Average	3.30	3.29	3.08	3.17	3.14
Overall Program Maximum	3.88	3.84	3.69	3.84	3.69
Overall Program Minimum	2.47	2.47	2.40	2.09	2.55

In-Cylinder Combustion Studies and Modeling

Analysis of Low-Temperature, Non-Sooting Diesel Combustion, Salvador Aceves of Lawrence Livermore National Laboratory



Brief Summary of Project

The objective of the project is to develop an understanding of low-temperature, non-sooting diesel combustion through detailed modeling of the processes including smokeless, rich combustion and modulated kinetics. The detailed models will be based on chemical kinetics and on mixing, and will be used to optimize and extend operating regimes for these engines.

Question 1: Relevance to overall DOE Objectives (Written responses from 9 of 13 reviewers)

The majority of the reviewers felt that non-sooting, low-temperature, and/or stoichiometric diesel projects (including modeling a potential high-efficiency, clean combustion engine) are indeed relevant to DOE goals, in particular for light-duty diesels at part load. One reviewer stated that this work is at the forefront of ACE efforts. Another reviewer commented that the hydrogen work highlights the fact that a hydrogen-burning ICE is a better alternative in many ways than a fuel cell, and also said that the analysis of low-temperature combustion is a relevant and interesting problem. Another person said that the in-cylinder techniques work to improve fuel efficiency through examination of the combustion events while reducing emissions, and this is central to DOE's primary thrust. Another reviewer agreed with these comments, but suggested that a clearer statement of the objective was needed. One reviewer had questions regarding the modeling approach, and felt that it was not explained in sufficient detail to allow a complete assessment.

Question 2: Approach to performing the research and development (Written responses from 8 of 13 reviewers)

Several reviewers commented that this project is in an early stage, making it hard to assess and that the approach needs more substance. One person commented that while a combination of KIVA and kinetics modeling has been used to provide multi-zone information, a three-dimensional approach for HCCI combustion was needed to carry out realistic calculations. Another person felt that the approach involves sufficient depth in understanding of the fundamental characteristics of the HCCI combustion. Another reviewer felt the researchers have used outside data well, but wanted to see more detail on the proposed plan and expected results. Another person was concerned that they did not see a well-defined technical approach to this problem and felt that the project needs a better focus in identifying the technical challenges and a comprehensive method for overcoming them.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 12 of 13 reviewers)

Reviewers acknowledged that the project has just begun, but declared their interest in developing an understanding of soot precursor creation in the low-temperature regime. One person noted that not many accomplishments were shown but this being a new project may partly explain this. Another reviewer commented that the tools developed can be highly useful, considering their limitations. Several reviewers commented that the results showing low soot precursor formation in low-temperature combustion (LTC) were interesting. One reviewer stated that before the approach will be a viable modeling candidate for optimizing low-temperature diesel combustion systems, a lot needs to be shown. One person felt the finding that the jet temperature is the key parameter is an important result, but wondered whether there are any experimental validations of this conclusion.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 7 of 13 reviewers)

Reviewers acknowledged planned interactions with Sandia and Oak Ridge to get combustion and exhaust speciation data. A reviewer felt that the researchers had effective collaborations with domestic and international universities, along with industrial partners. Others backed this up, noting good collaboration with industry partners to get data for the analysis. One person felt the collaboration with national labs could be better (specifically Sandia experimental work as a source of data). One reviewer encouraged further university involvement and a clearer plan for dissemination at conferences and in publications. He went on to suggest that the group needs to develop a stronger association with at least one of the engine manufacturers. The final comment was that the results should be shared at crosscut team meetings if this has not already been done.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 7 of 13 reviewers)

The reviewers generally endorsed the approach and its relevance to future research. Several reviewers felt the use of experimental data from other national labs to validate the numerical model made a lot of sense, and one added that the validated model could be used to demonstrate how to optimize low-temperature combustion. One reviewer said the researchers need to ensure collaboration with the Sandia (Paul Miles) work. Another felt that understanding soot formation will be very important. One person thought the plans that were shown are good overall, but somewhat lacking in detail, and felt that it would be good to see more about how the work is to be performed, what the expected results are, and how the results will be useful. The final reviewer acknowledged the researchers' plan to use their expertise in chemical kinetics modeling, and that much of the input will come from other labs or OEMs in defining the technical tasks and guiding the goals of the program.

Specific Strengths and Weaknesses (Written responses from 10 of 13 reviewers)

- Specific Strengths
  - Generally, the group produces very good analytical work.
  - Understanding in this area is critical.
  - An additional advantage in the context of HCCI-modeling/ low-temperature combustion is their ability to incorporate very detailed chemical kinetics.
  - Further development and application of detailed chemical kinetics modeling shall benefit our understanding on rich combustion and low-temperature combustion regimes.
  - Focus on modeling, especially addressing kinetics and low-temperature soot formation.
  - Building on existing programs and models. Collaboration with other national laboratories.
  - Computational tools and approach and teaming arrangement.
  - The computationally efficient technique developed.
  - Low-cost computational work can be very useful when appropriately validated by experimental data from other programs at National Labs or from industry partner.
  - Description of low-temperature non-sooting regime to enable a new solution to the reduction of soot.
  - Development of new techniques for analyzing and modeling lo- temperature combustion. It remains to be seen how well the technique will work and how useful it will be for predictions.
- Specific Weaknesses
  - Too early to determine.
  - Reliance on H_2 as the primary fuel - limits potential near-term impact.
  - I am worried that the chemical reactions included in the heptane mechanism are insufficient to allow a "deep understanding of low T, non-sooting diesel combustion." I am also concerned that a more detailed treatment of CFD is required to actually capture the relevant dynamics (for example, the post processing approach used by Akihaunra, et al. SAE 2001 or 2001) Basically, I am not sure the success realized using this approach for HCCI will translate over to LTC. This is especially because of the high sensitivity of smokeless rich combustion to injection/fuel-air distribution.
  - Modeling approach appears based on Dec's conceptual picture for diesel combustion valid under heavy-duty, quasi-steady conditions. The modeling approach is not described in sufficient detail to be subject for rigorous evaluation. How will 3D-and transient effects be handled? Indicates the use of unrealistic EGR-rates (90%). Fuel economy implications?
  - Need to explain BMW results more thoroughly. Would be helpful to have more data available for the analysis which is being done here.

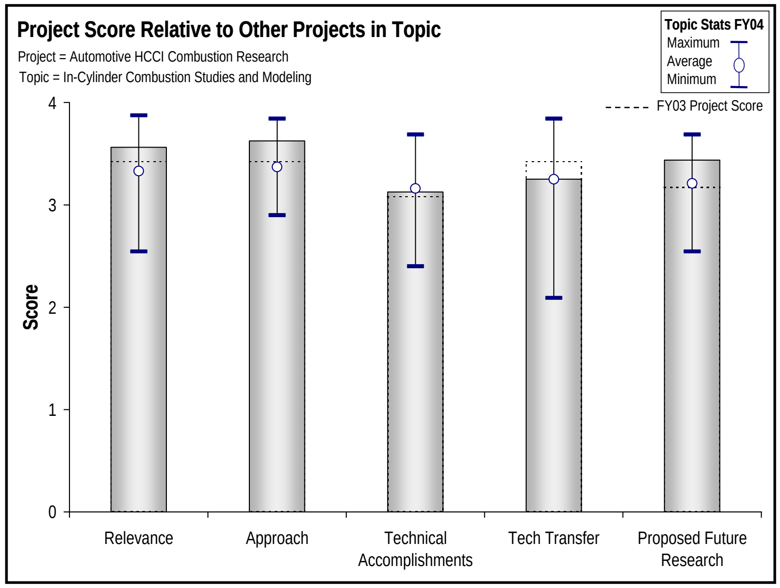
- If the investigators have already developed a detailed multi-zone chemical kinetics (the presenters claim that it predicted soot emissions identical to Toyota's measured data and explained the nature of the process) then what is the real motivation for this work? What goals will this work serve?

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 5 of 13 reviewers)

- If the project is to be granted it ought to clearly address how it ties into the experimental work of Lyle Pickett at SNL.
- A modeling approach that can be incorporated into a three-dimensional modeling code would be desirable.
- Get more experimental data, test the analysis techniques on the data, show the usefulness of the model in predictive mode.
- Need a better definition of the work scope, technical approaches. Right now, investigators are trying to mix and match different pieces of work being done at different places. Don't see a strong contribution evolving from the center of this work!

In-Cylinder Combustion Studies and Modeling

Automotive HCCI Combustion Research, Richard Steeper of Sandia National Laboratories



Brief Summary of Project

The focus of this project is to develop and apply quantitative optical diagnostics to understand in-cylinder fuel-air mixing in an automotive-scale HCCI engine. This project is being performed in the Automotive HCCI Optical Engine Facility on gasoline-like fuels.

Question 1: Relevance to overall DOE Objectives (Written responses from 12 of 16 reviewers)

One of the reviewers commented that the project is focused on developing useful diagnostics for gasoline HCCI. Correlating probability density function (PDF) profiles with combustion, emissions, and performance data (as is planned) will be very helpful in developing new combustion concepts. A reviewer noted that this is a hot topic in today's business. Another added that advanced combustion is critical to achieving overall objectives. One of the reviewers felt this program is relevant because it is aimed at developing diagnostics useful for quantifying stratification of equivalence ratio in HCCI engines. Stratification is thought to be a method to control ignition and combustion duration, so this technique will be useful. A reviewer commented that the project is providing the fundamentals for gasoline HCCI engines, and that investigating the fuel-air mixing is very important. Another person said that there has not been much gasoline research sponsored, and that gasoline HCCI is a worthy pursuit for emissions and energy independence. One reviewer was concerned that he did not see the linkage of fuel-air mixing to combustion in the work. Another felt development of techniques to study HCCI in an optical engine can provide substantial insights into how to manage and optimize HCCI. Another person felt it was not clear why it was necessary to develop a second HCCI optical lab at SNL, and questioned what the relationship is between this work and John Dec's. One reviewer commented that the experimental work employs a 11.9 CR engine, noting a higher CR engine would yield better fuel efficiency, if it is not limited by the optical measurement technique.

Question 2: Approach to performing the research and development (Written responses from 9 of 16 reviewers)

Several reviewers felt the research team has used a very solid approach, with good understanding of fundamentals that combines results from other programs and that the researchers have shown a clear analysis. Others stated the approach to configure an optical HCCI engine, and to develop PLIF diagnostics for equivalence ratio measurements was the right approach. They suggested identifying LIF tracers that would track well with fuel, and apply to effects of fuel injection timing. One of the reviewers felt it would be good to see a larger engine map of experimental investigation. Another felt the approach is well thought out, but that it would be useful if the focus of the work was shifted from diagnostic development to combustion analysis.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 10 of 16 reviewers)

Several reviewers felt that there has been good progress in applying a technique and getting the optical engine operational. Others commented that, since this is a newer project, it is too early to fully assess data generated to date. Others felt there was good progress toward DOE goals, although one person commented that the progress seems slow. One reviewer noted that the researchers configured a “low residual” version of the optical HCCI engine and test fired for reference fuels, showing that there are fuel types that cannot be used in the engine in neat form, although this work has just begun. Firing the test engine with a LIF tracer within the engine was done to study the fuel-air mixture preparation. One reviewer commented that much required initial effort was spent quantifying tracer behavior and follow-on engine evaluation has just begun. The tracer work has been intensive, identifying the Azeotrope tracer. Another reviewer commented that it may be too early to gauge technical progress. He went on to say that now that the tracer/method has been developed, it is time to apply the tools. The final reviewer acknowledged the development of a useful technique for measuring stratification in automotive HCCI engines, which has been thoroughly validated and proven. He added that he would like to see more work on combustion in the future.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 12 of 16 reviewers)

Many reviewers commented on the good team of partners and collaboration/technical exchange with industry (regarding the injection systems), SNL and LLNL activities. One person noted the groups are participating in Advanced Combustion Workshops, sharing information with university and industrial partners, and using industry-supplied hardware and some industrial liaison in FY2004. However, one reviewer commented that the project has not yet demonstrated a strong interest from industry. This reviewer felt that considering the investment, it would be desirable to see greater industry involvement. Another felt that there needs for more involvement and buy-in from OEMs and first-tier suppliers. The final reviewer added that the collaboration seems to have taken place at reviews. He felt it was not obvious that industry or institutional collaboration was significant, but maybe such interaction is not a necessity at this time.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 9 of 16 reviewers)

One of the reviewers felt that the future work plan contains key topics which are focused to push the technical barriers and that the relevance of the proposed future points is high. Another agreed, adding that the proposed experiments are well posed, especially the correlation with emissions and natural luminosity. Another person commented that the plan is to characterize the liquid injection process, the extent of wall wetting and the link to combustion and emissions tests, and to extend research to consider variable residual gas content. A reviewer commented that it is an absolute necessity now to start correlating the PDF-profiles with combustion data. Another stated that the researchers will look at various cams, but was not sure there is sufficient knowledge of the effect the cams have on in-cylinder conditions. One person questioned how this is going to advance the state-of-the-art. One of the reviewers thought the principal investigator had outlined a good game plan; his only suggestion was to include a broader range of engine operating conditions.

Specific Strengths and Weaknesses (Written responses from 11 of 16 reviewers)

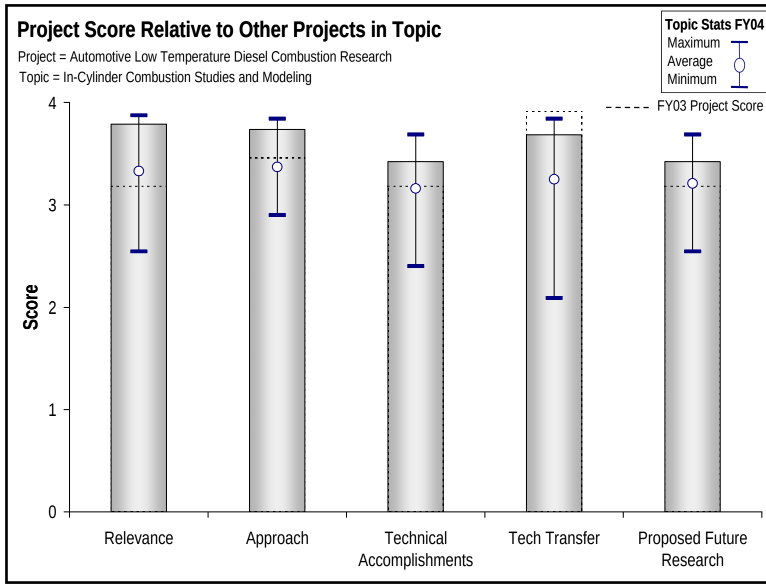
- Specific Strengths
  - Thorough characterization of tracer evaporation / contentious selection of tracer.
  - Good approach for determining mixedness.
  - Offers direct comparison with numerical models (development and validation).
  - Work is rigorous and convincing.
  - Capabilities and experience that led to development of such an impressive test facility. Clear and very informative research plan.
  - The project addresses the fundamentals of the fuel-air mixing for HCCI engine conditions.
  - Good capabilities and overall plan.
  - This technique is very useful for studying fuel/air mixing.
  - The technique was only applied to gasoline-like fuels.
  - Good tools.
  - Utilization of optical technique.
  - Outstanding experimental capability and associated PI to complete and perform analysis of generated HCCI mixing data. Also, the collaboration with metal engine experiments at the PI's lab should further aid in analyzing and understanding generated mixing data.
  - Developed a thorough understanding of the fuel tracer species to insure that the tracer co-evaporated with the fuel. They are applying their diagnostics to a basic understanding of combustion in a typical automotive engine. They have done a good job trying to meet their engine configuration close to the specifications of productions engines.
- Specific Weaknesses
  - No combustion data was discussed. Why is this taking so long?

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 9 of 16 reviewers)

- Start focus on combustion (correlate with emissions and performance).
- Determine effect of wall impingement.
- Focus on combustion. Use the air-fuel mixing to interpret the combustion process.
- Limitation to the PRF fuels, while it provides good foundation of information, is somewhat limiting. May be worthwhile to survey other fuels to examine the impact on mixture preparation, particularly with regard to boiling range.
- The installation of the recompression cams is highly recommended.
- It seems to me that there is more industry interest in the development of Diesel HCCI than in gasoline HCCI. If that is the case, this project may be somewhat redundant.
- Expand and keep going.
- Recommend correlating PDFs with burn rate (connected to John Dec's work).
- One recommendation is to include a broader engine operating regime.
- A lot of effort was spent developing the lab, the LIF tracer diagnostic and other diagnostics. This was essential work before testing could begin. I would like to see future emphasis on testing to understand the effect of stratification on combustion.

In-Cylinder Combustion Studies and Modeling

Automotive Low-Temperature Diesel Combustion Research, Paul Miles of Sandia National Laboratories



Brief Summary of Project

The overall objective of the project is to investigate in-cylinder, low-temperature combustion and emissions formation in a HSDI diesel engine. In this project for FY 2004, SNL has enhanced the capabilities of the facilities (including acquisition of multiple injection capability and enhancement of swirl capability), has developed an extensive matrix of experiments to characterize low-temperature, late-injection combustion, identified role of large-scale flow structures in assisting late-cycle oxidation, and developed new insight into dominant turbulence production mechanisms.

Question 1: Relevance to overall DOE Objectives (Written responses from 14 of 19 reviewers)

There was general consensus among reviewers that the 2004 project goals were relevant to DOE Program objectives. Individual comments suggested that the project is well organized, has a clear focus, and is well connected to core issues. The project is well directed toward combustion regimes being investigated by industry. The shift in focus to low-temperature combustion regimes has been good and should be maintained, since it is an essential component of advanced, efficient, low-emission engines. The research provides fundamental knowledge that will enable engine designers to develop cleaner diesel engines while maintaining high fuel economy. Improving in-cylinder understanding for achieving low emission and low-cost solutions will enable best possible fuel efficiency and lowest life-cycle costs. One reviewer felt that the objectives are somewhat narrowly defined and it would be better to include emissions and fuel efficiency in the project statement. One reviewer mentioned the idea of achieving engine out-emission level of Tier II through LTC.

Question 2: Approach to performing the research and development (Written responses from 13 of 19 reviewers)

In general, reviewer comments on the project approach were positive. Reviewers felt that the project is being conducted very systematically, and has a good balance with the "big picture" effect on combustion. The combination of optical and metal engine testing with numerical modeling is outstanding, complementary, and hard to improve. The approach combines the advanced testing and the latest simulation technology. The combination of turbulence measurements with modeling has the potential to extract the maximum from the work. The approach efficiently uses time and resources and provides a fundamental understanding of the combustion and science. The research is focused on highly premixed, late-injection combustion with the intent of understanding rate-limiting processes and preferred hardware configurations. Collaboration with industry and academia is excellent. The working group consists of a large number of industrial partners. One reviewer suggested additional input from the experimental metal engine would be desirable. Another stated that an expansion of the range of operating conditions could be considered to make sure the theories being developed still apply.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 13 of 19 reviewers)

Reviewers felt that the technical progress made in this project has been significant and 2004 goals have been met, although there is still a considerable amount of work to accomplish. The project has progressed from flow field experiments into quasi-homogeneous combustion regimes. One reviewer stated that the approach of tying the CFD-derived flow field with the experimental was good. Another said the relation of fuel economy and soot luminosity with swirl ratio provides engine designers some direction. The project has enhanced the facility and testing capabilities (injection and swirl), and has provided a good understanding of the turbulence field and mixing in the bowl, and its effects on soot oxidation, as well as low-temperature combustion processes and their linkage to flow structures. The project has also identified the role of large-scale flow structures in assisting late-cycle oxidation processes. The new multiple injection capability is important and should lead to key insights.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 17 of 19 reviewers)

In general, most reviewers viewed the technology transfer and collaborative efforts of this project positively. The researchers are collaborating with UW in exchanging experimental and numerical data. As part of the Advanced Combustion Engine MOU, the collaboration has been good between industry, universities and laboratories, and this has enhanced the quality of the work. All major players are engaged and active in the project, and every major diesel-related company is involved. The results have been excellent with significant insights for industry. The researchers have demonstrated a strong publication/presentation record as related to the project. One reviewer did express some concern about the involvement and contributions of Wayne State University. Another offered a suggestion for the DOE Program Managers: hold focused seminars or workshops for advances in diesel combustion targeting industry partners (senior industry R&D personnel) such as the crosscut members.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 13 of 19 reviewers)

Reviewers generally agreed with the approach to proposed future research plan while offering some additional recommendations. One reviewer stated that the future approach builds on past progress and focuses on key diesel engine technical barriers, and plans to move toward combustion-based work are good and could lead to a better understanding of soot formation. Further, the plan to focus on early HCCI combustion only increases the value of the project. The objective of the research should explicitly target Tier II emission levels through combustion improvement and without the use of NOx catalysts. A better understanding of LTC fundamentals and emphasis on the effect of EGR will also be beneficial. Validation of results will be important to the future work. Other reviewers offered that more focus should be placed on simulation with less investment (at least in the near term) on laboratory upgrades, and noted the work has made little mention of fuel effects. One reviewer stated that the project should include more combustion-related research and less turbulence model development work. Another reviewer stated that the FIE upgrade is critical, and it will be strategically important to investigate early injection strategies as well. Further, the benefits of optimizing in-cylinder swirl (and hence late-cycle combustion) for improving engine performance or reducing engine-out emission are limited. Finally, a reviewer questioned the effects of the "combustion" chamber, offering that they are probably very significant for combustion chamber robustness. A move toward 1,800 bar injection pressures would be more relevant to future engines.

Specific Strengths and Weaknesses (Written responses from 18 of 19 reviewers)

- Specific Strengths
  - Visual models and explanations are excellent.
  - Well-aligned with current diesel engine research. Lends significant insight into the influence of macroscopic and microscopic flow structures on combustion and emissions.
  - Combination of visualization, velocity measurement, modeling, and emissions highly desirable. Data used to draw conclusions on combustion process.
  - Team and depth of the examination due to the facilities and tools available.
  - The validation through metal engine, and the incorporation of modeling in the research.
  - This project is very valuable to the goals of DOE and is directly supporting the work in industry
  - The quality of the work and the results!
  - Complementary effort among three groups. There is good coordination of metal engine, optical engine, and CFD results.
  - Solid team with active involvement. Good presentation.
  - Collaboration (industry/academia/NL), broad tool application test - simulation. Very solid R&D!
  - Excellent facility and researchers. Directly applicable to DOE's objectives. Excellent understanding of the diesel combustion process.
  - Detailed, focused and capitalized on the strong team arrangement.
  - The effective use of the three-pronged approach.
  - A strong PI, good industrial communications and concurrent modeling.
  - Sound research.
  - Very thorough experimental approach; good connection between flowfield modeling and experimental visualization data and maintenance of realistic combustion chamber geometry and conditions.

- Helps to further our understanding on the combustion processes, in particular during late-cycle combustion
- Great CFD. Need more time for discussion.

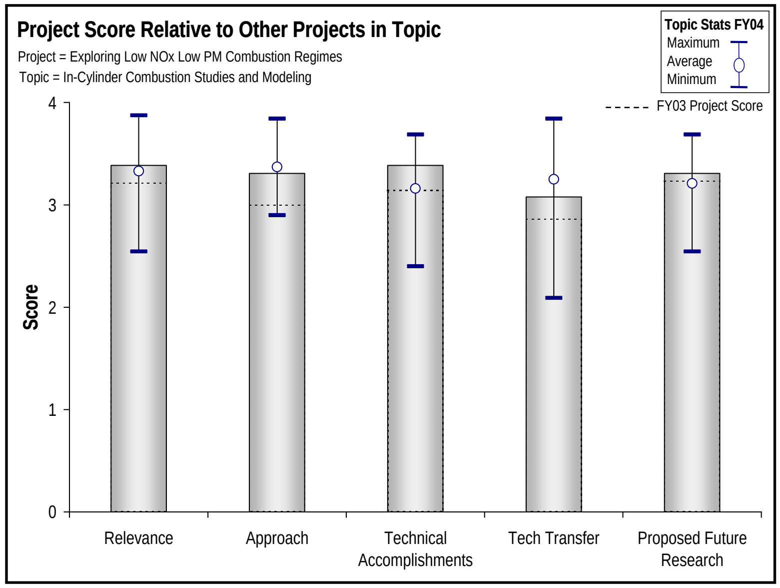
- Specific Weaknesses
  - Further work is required in order to better understand the effect of swirl.
  - Any thoughts on how to best overcome the rate-limiting processes?
  - Scope of work could be limited to give faster progress.
  - Not focused for real world engine applications!
  - I would like to see this project move away from turbulence models and toward more investigation of the low-temperature combustion regime.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 15 of 19 reviewers)

- Put more emphasis on fuel economy implications. Look at possible effect of "over-swirling" (study r-theta plane, for example). Prioritize investigations of early type of injections (PCI).
- Continue work in combustion. Look at other combustion strategies to achieve low-temperature combustion.
- No mention of any incorporation of fuel characteristics, perhaps a range of fuel types could be included to elucidate the most desirable fuel characteristics to maximize the benefits of these combustion modes.
- Work is very valuable and should be backed up with more resources!
- Need to follow up and look at multi-injection events and examine the effects of size and shape of orifices.
- These results should be compared with mixture preparation methods other than late DI (e.g., external atomization).
- It is important to understand combustion processes with early injection and with post injection.
- Continue direction of work into combustion. This appears to be a fruitful opportunity.
- I would add additional, higher-load conditions. Also consider including simulation modelers into the game.
- Pioneering work that has maximum impact to DOE's goals of fuel economy and emissions.
- Understand the fundamentals, then push the operating limits of LTC. Some lower-hanging fruit may be at hand.
- A greater emphasis on the effect of EGR would be helpful.
- Keep in the scope and focus on efficient emissions reduction. Target should be meeting Tier II (Bin 5) or heavy duty 2010 without the use of NOx catalyst of any form.
- The effects of post injection and/or late-cycle air injection would be more appropriate for understanding the physics during late-cycle combustion.

In-Cylinder Combustion Studies and Modeling

Exploring Low-NOx Low PM Combustion Regimes, Robert Wagner of Oak Ridge National Laboratory



Brief Summary of Project

In this project, the goals are to investigate the transition between normal combustion and an advanced combustion mode, and to maintain efficiency during the advanced, LTC mode. Additionally, the team will investigate effects of fuel properties on achieving LTC operation, and will perform thermodynamic analyses of the non-traditional combustion modes.

Question 1: Relevance to overall DOE Objectives (Written responses from 10 of 13 reviewers)

Several reviewers felt the program is directly applicable to the DOE primary objectives of low emissions and good fuel economy. One reviewer had very positive comments, stating that the project is focused on developing one of the most promising methods for clean, efficient combustion. Another commented that low-temperature combustion may provide a means of achieving high-efficiency and low-emission operation. Another commented that the fuel impact on LTC is important and useful and that some speciation is good to understand if there is anything to avoid regarding unregulated emissions. One reviewer agreed that research on low-temperature diesel combustion is relevant, however, he felt this research offers little added value to activities carried out elsewhere. Another reviewer felt this was an excellent project that explores the interaction among fueling, air delivery, combustion regime, and exhaust emissions and that can serve as experimental validation for many of the fundamental combustion/emission studies conducted in other laboratories. The final comment was that the work was pragmatically relevant and superior work.

Question 2: Approach to performing the research and development (Written responses from 7 of 13 reviewers)

One reviewer comment was that the approach identified is an enabler for low-temperature, low-emission, fuel-consumption neutral diesel combustion, displays strong similarities to what is commonly referred to as Premixed Charge Compression Ignition (PCCI or PCI); however, it does not seem the investigators have identified the real issues associated with this combustion mode. Another reviewer had a related comment that the range of possible experiments is so vast that it is very difficult to propose a systematic approach. He felt that it would be helpful to see some sort of matrix of objectives, correlated with different families of experiments. One person commented on the highly instrumented, RPECS controlled engine with advanced combustion monitoring capability and EGR and injection timing to achieve low-NOx, low-PM operation. Others felt that the team had taken a solid well-thought-out experimental approach that covered all bases. The final reviewer felt that the approach is adequate for the objectives of the project.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 6 of 13 reviewers)

Several reviewers had commented that the researchers had made decent progress for the time and effort, but the real issues have not been touched upon. A reviewer discussed the work that had been done and is being done to upgrade the engine control and the monitoring of the combustion process and noted that the group has performed a fuel screening in the low-NOx, low-PM regime. He noted that biodiesel did not behave in this regime in a stable manner, unlike other fuels considered. The team mapped out the limitations on transitioning from normal to LTC and back and looked for ways of reaching “efficient” LTC operation, and found it to be difficult with boost. One reviewer felt that the researchers accomplished much this year and will provide good guidance on the next year's experiments. Another commented that the detailed analysis of hydrocarbons in the stream is much- needed and extremely useful. Another person said they did not agree with the conclusion that the ability to recover efficiency is an exclusive function of EGR rate transition and suggested that the researchers probe it more for a better understanding.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 9 of 13 reviewers)

Several reviewers acknowledged the lab's connections established with Ford, LLNL, SNL, Catalytic Solutions Inc, and GM and the lab's participation in the Advanced Combustion Engine MOU. One felt that the interactions had significantly improved from last year. Another stated that the collaborations were satisfactory, but could use more industry guidance now that system capability has been demonstrated. Another noted that open collaboration between the DOE labs is emphasized by the exchange of equipment and expertise in this project. The collaborations with universities next year will only add to this. With such detailed analysis of species in the stream, these experimental data should be ideal for theoreticians interested in complex simulations of the evolving exhaust stream. One reviewer cautioned that the research group should keep an eye on intellectual property (IP) protection.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 8 of 13 reviewers)

One reviewer felt the fuels work and the premixed combustion element looks good. He went on to say that he would not recommend going into any vehicle work, but rather try and apply the fuels sensitivity at other conditions, especially at higher loads. He also felt that more comparisons of fuel chemistry impact across load conditions should be investigated rather than refining any specific point. Another commented that some issues that ought to be of high priority now are how LTC can be expanded to higher loads, and how acceptable transient behavior with a low pressure EGR system can be ensured. Neither of these is listed as future investigations. One reviewer commented that the group is on the verge of significant breakthrough discoveries. Others felt that the group may want to be more specific about the path forward; they feel currently it is a little vague. A reviewer questioned whether the researchers should continue with single point demonstrations or try for higher loads and speeds. One reviewer suggested that the addition of fundamental thermodynamic analysis is essential in determining future directions. The final comment was a suggestion to lower boost pressure to enhance stability, and to implement advanced combustion system.

Specific Strengths and Weaknesses (Written responses from 11 of 13 reviewers)

- Specific Strengths
  - Good approach. Using combination of suitable diagnostics.
  - Tremendous experimental capabilities and background of the team.
  - Outstanding experimental capabilities.
  - They have demonstrated very good operating conditions for a conventional diesel engine.
  - Good idea to include controls and engine analysis.
  - The detailed analysis of the exhaust streams is very impressive as is the push to optimize the engine with different fuels. The use of only production-like hardware is greatly appreciated and aids in the dissemination of the technology to other labs.
  - Good combination of advanced fuels impacts, a little speciation and good look at LTC.
  - Very relevant to today's diesel engine requirements.
  - The practical approach to develop a clean efficient combustion system.
- Specific Weaknesses
  - I believe some of the results presented are known to industry. Need to have better coordination and information sharing.
  - Field of experimentation is too large.
  - Focus on light load only - at least for the data shown.
  - Can this engine pull full power or is it only directly related to Light Duty Engines?
  - Lack of substantial 3-D simulation such as KIVA-4. Not a weakness but an opportunity.

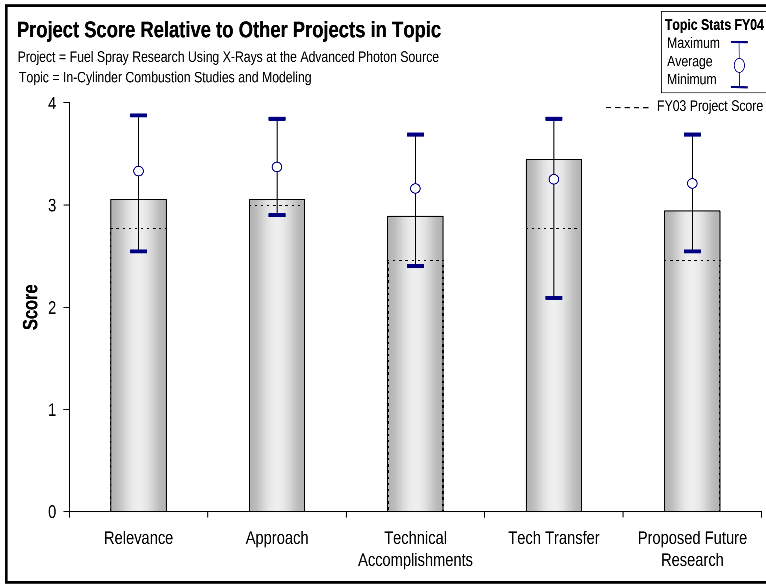
Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 8 of 13 reviewers)

- Why not study efficient low temperature combustion at a variety of speed-load points to understand how things change as function of speed and load?

- Consider other fuels and fuel blends beyond those in this year to include more exploration of fuel properties, such as volatility (different cuts), [and] cetane number (dope with EHN or run an F-T fuel).
- Further collaboration with partners is suggested to help narrow the focus on a set of truly important experiments.
- They need to study how to maintain the efficient, low-emission combustion over the engine speed and load range.
- The one-page project summary as the last page to emphasize the take aways to the reviewers was a very nice touch.
- Fuels work and the premixed combustion element looks good. I'm interested in why you have such variation with the biofuels. I wouldn't recommend going into any vehicle work. Rather try and apply the fuels sensitivity at other conditions - especially higher loads. I'd rather see more comparisons of fuel chemistry impact across load conditions than to refine any specific point.
- Introduce "assisted boost" to control the intake pressure. Investigate boost as a significant parameter influencing the results / outcome of low temperature combustion, especially for recovery of BSFC (taking into account the cost of boosting in terms of needed work.) Also, consider effect of swirl (air kinetic energy.)
- Transitions from conventional combustion to LTC are readily attainable in a realistic fashion. Seems to be on track to cover this base too.

In-Cylinder Combustion Studies and Modeling

Fuel Spray Research Using X-Rays at the Advanced Photon Source, Chris Powell of Argonne National Laboratory



Brief Summary of Project

The goal of the project is to understand the mechanisms of fuel spray atomization through the use of the quantitative X-ray techniques at Argonne's Advanced Photon Source. Current work is focusing on the near-nozzle region, which determines downstream behavior of the spray. Spray measurements have been conducted at a pressure of 10 bar, and the team is working on development of a rapid compression machine to increase pressures, bringing them closer to engine-like conditions.

Question 1: Relevance to overall DOE Objectives (Written responses from 12 of 18 reviewers)

Several reviewers felt the work showed good focus on realistic conditions. One person simply stated that this was solid basic work. Another said this work contributes to the improvement of injector technology. One reviewer commented that a thorough understanding of the spray structure resulting from a specific nozzle design will assist in developing low emission combustion systems. Another added that understanding fuel spray phenomena is critical to advancing combustion research, since spray formation and mixing are critical to conventional and advanced combustion regimes. A similar comment was that information in the near-nozzle spray region could be useful for development of spray models. One reviewer offered very detailed comments, stating that successful development of this technique should enable better understanding of spray formation in diesel engines and this type of understanding has greatly improved engine overall operating behavior over the last twenty years. Better understanding of early jet formation may reveal the link between early break-up/evaporation and the subsequent pre-ignition and post-ignition events, i.e. flame front development, NOx formation, PM formation, etc. Exploration of fundamental aspects of cavitation, air entrainment, stripping, etc. in this unique facility is an excellent opportunity to support more informed design and development of injection systems. In addition, supporting enhancement of numerical models of spray formation is very important for better predictive tools. Another person felt that the work fundamentally examines the optimization of dispensing fuel into the cylinder, a key means to improve fuel efficiency and emissions. The work probes holes in current knowledge. There was another comment that the program may have some impact on improved fuel economy, but it is difficult to predict whether this technique will result in the improvements. Significant effort is required to use this technique under realistic conditions. One person cautioned that the researcher talked about increased collaboration, but the impact of results on combustion or injector design seems lacking. Another reviewer cautioned that in the absence of correct density background, parametric studies involving the effects of nozzle geometry or injection conditions are mere academic exercises.

Question 2: Approach to performing the research and development (Written responses from 15 of 18 reviewers)

One reviewer commented that progress seems slow, wondering whether this is due to funding level or approach. Others commented that so far this has been very fundamental and interesting work. Another said this approach is an excellent utilization of a difficult technology for an automotive application. Another reviewer added that the project team seems to be in an early phase of understanding how to use the new tool and that the approach hasn't delivered real data yet. The comparisons shown did not provide a clear description of why the injector tips performed differently. Another reviewer commented that there is a long way to go to attain realistic pressures. There has been much investment in lab hardware with likely limited half-life, and they will have to generate (create) new programs / activities to use funding in the future, which is OK if affordability is not an issue. Several reviewers had questions/comments regarding the use of the rapid compression machine. One felt that the approach is reasonably well thought out, but could be improved in a few areas. The project team urgently needs to move toward testing in more realistic environments. The reviewer did not understand how the researchers will be able to do all the required experiments in the rapid compression machine, because thousands of cycles will have to be run to get a full map. Another reviewer added that the researchers had made attempts to model the observations, but taken together these provide marginal value to the overall program goals. He felt the researchers did not explain/address the need for the rapid compression machine or how it will be used to carry out x-ray fuel experiments. Another commented that there is a very good grasp of R&D and industry needs with ways to address the challenges (pressure, temperature, etc). One reviewer commented that this is an excellent setting of the context and the advantages of x-rays, but questioned whether fluorescent measurement instead of absorption of x-rays has been considered. The mass distribution of fuel is very useful to modeling and the researchers have an exhaustive search of imaging agents and their respective energy benefits. He concluded that there has been a good balance of experimental and theoretical work. Another reviewer commented that the technique is novel and can yield exciting results, but cautioned that the approach is severely limited by the type of seed molecules that must be used for the imaging to work and the need to average the spray events to complete an image. A key aspect of fuel injection and advanced combustion research is the consideration of fuel formulation. Without the ability to freely adjust fuel characteristics, these studies of fuel injection are severely limited. Also, the reviewer could not examine the interaction of turbulence with the spray at present. Nonetheless, the imaging of fuel mass in the near-nozzle region is very important and a unique capability of this work. Another commented that X-rays appear to be very well-suited for performing quantitative spray measurements in the near-nozzle region. The challenge now is to make the technique capable of handling higher pressures. Another person agreed, adding that it seems that PIs are spending too much time studying low pressure sprays with very little applicability to real diesel engines; past spray work has shown that bulk spray behavior under low pressure-temperature conditions does not scale well into relevant, high pressure-temperature conditions. One person commented that X-ray penetration in high-density gases is difficult and the effects of turbulence and swirl and interactions between sprays are limited. The resulting information may provide basic modeling of spray technologies for the modeling. The final reviewer commented that replacing cerium tracer with zinc has improved the ability to measure spray formation.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 13 of 18 reviewers)

Several reviewers felt there was excellent progress so far, that there appear to be good applications and also felt that progress toward DOE goals is good. Another was more cautious, commenting that reasonable progress had been made, but quantitative information is lacking and that the Detroit Diesel injector used is obsolete. Another reviewer felt there is good progress toward the goal of applying this technique to engine-like conditions, but it takes a lot of time and resources. Another, similar comment was that progress should be more rapid if this tool will be employed to address engine emission spray related issues in the near future. Another reviewer was concerned that the progress on the x-ray work is slow, partly due to the limited access to the x-ray facility, and partly due to the complex nature of the experiments they are trying to perform. Another reviewer said that high-energy x-rays are a very difficult technology to adapt to the measurement of droplet dispersion within, and just outside, an injector nozzle, but the ANL group has done a good job in solving the problems associated with using that technology. One person questioned how the x-ray measurement correlates with the work by Dennis Siebers at Sandia. The implementation of a RCM is very valuable and documents good progress. One person felt that the progress toward meeting the DOE goals is OK, since the direct contribution at this time is limited. One reviewer was pleased that the research team was finally showing high-pressure data and plans for higher temperature. This reviewer was concerned that the 2-D detector does not appear operational in spite of two years' work. Another reviewer thought there has been very interesting data generated thus far. The researchers quantified the loss mechanisms in the absorption of the x-ray beam for operation of elevated pressure. They have also been working past the challenge of needing windows that pass x-rays but have the strength to operate at elevated pressure. The impact of nozzle geometry effects has been considered by comparing nozzle types as shown in subtle differences in mass distributions. The team has built a rapid compression machine to work with the x-ray experiments for operation under high pressure and temperature. Another person stated that it is too early to gauge progress and accomplishments. Achieving higher ambient densities and post-processing the data into meaningful findings is important. Initial findings should concentrate on the near-orifice hole conditions, since there are no other means to look at these conditions. The final reviewers commented that understanding the effects of nozzle geometry on spray at 10 bar pressure is a good step toward a deeper knowledge of the final application, and reaching 10 bar was a major breakthrough in increasing the background density.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 15 of 18 reviewers)

Several reviewers commented on the excellent, diverse group of industrial and academic collaborators and applauded the use of the web site to enhance the rapid dissemination of information. Industry collaborations were established with Bosch, DaimlerChrysler, Visteon, GM, Detroit Diesel, and Caterpillar. Academic collaborations for model development with University of Wisconsin/ERC, Michigan Tech, University of Massachusetts\-Amherst, Wayne State University, Cornell, and Helsinki University were also noted. One reviewer commented that collaborations and technology transfer will be challenging, since the efforts required to make a measurement are large and the output has limitations. Another person commented that ANL is open to testing samples, although it is not yet clear what has been learned from these. It may be too early to judge progress. One person questioned how connected these results are to modeling. One reviewer commented he had not seen any injector manufacturer use this information in designing new injector nozzles. Another reviewer had similar comments, stating that it was difficult to see the result of the collaboration, i.e. not much data or information had been transferred, mostly plans for collaboration. Others were encouraged that there seems to have been advancement in the knowledge, indicated by the fact that several universities are using the x-ray data for model development. They were left wondering how the industry partners have benefited from this work, and how the x-ray measurement has enhanced understanding of diesel spray and atomization. The unique experimental facilities and the novelty of the x-ray absorption techniques have attracted many equipment makers and universities.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 13 of 18 reviewers)

One reviewer commented that the direction of the future work plan is correct, and must be toward time and space resolved measurements in a high-pressure, evaporating atmosphere. One of the reviewers felt that modifying a rapid compression machine to have x-ray access is a major accomplishment; the ANL group is headed in the right direction. Another said the future work plan builds on past progress and generally addresses removing the key barriers, but will take a lot of effort and time. One reviewer stated that the work is directionally connected to fundamentals of combustion. It was commented by several reviewers that the drive to higher charge temperatures and pressures (10 to 20 bar, i.e., more "diesel-relevant") with greater resolution is an excellent vision. Another agreed adding that the research group has a very good grasp of R&D and industry needs, with ways to address the challenges (pressure, temperature, etc). One reviewer recommended extending the technique and considering additional geometric issues in injectors, based on industrial interest, but since there is a need to use the metal additives under high pressure operation to maintain x-ray attenuation, the interference of the metal additive with spray formation and evaporation may bias the results significantly. One person commented that he would like to see more details on how ANL plans to characterize injectors and the data collection strategy. Another reviewer recommended focusing on near-hole conditions with higher ambient density. This approach puts less emphasis on high-temperature conditions. Combining this work with spray modelers is important and should be clarified or emphasized. One reviewer was concerned that he did not see a clear approach to where the researchers want to go and could not see the relevance of proposed work in fulfilling advanced combustion engine program objectives. The final reviewer was concerned about the project focus, stating that the work continues to give the impression that it is focused on finding new applications for x-rays rather than solving problems.

Specific Strengths and Weaknesses (Written responses from 17 of 18 reviewers)

- Specific Strengths
  - Unique.
  - Only approach to study interior of fuel spray.
  - Unique capability, excellent partnership arrangements.
  - Useful for developing and modeling spray. It's good to see the increased focus to application to modeling validation.
  - The measurement technique gives mass distribution in the spray. This fact can give fundamental new insight in hollow cone sprays. Technique can give input for spray modeling.
  - Readily aware of technical barriers and lays out plans to address the key issues. Multidisciplinary team from many areas assembled to resolve the numerous fields of expertise needed.
  - This work is innovative and provides data that is not obtainable by other methods.
  - Could be used to support model development.
  - Very impressive characterization capabilities.

- Only technique to look into near-nozzle hole spray liquid core!
  - Unique tool, project moving in the right direction in evaluation of high pressure and high temperature. Basic work will assist in development of improved models of fuel injectors.
  - Plowing new area.
  - The APS source.
  - The X-ray technique is promising and initially shows the capability to resolve early spray behavior in a manner previously difficult to acquire.
  - X-ray as a new measurement tool/methods.
  - They have access to a unique facility and they can provide unique measurements.
  - APS, team of physicists who know x-ray absorption technique and x-ray optics quite well.
- Specific Weaknesses
  - Based on presented material, impact of the project is low. I only see some qualitative pictures and discussion about how much data required to make images. There is limited conclusion.
  - Need for the metal additive. Leaves this panelist concerned over bias from the additive.
  - Pressure limitations – will be difficult to achieve typical in-cylinder pressure.
  - The technique is limited due to a low signal-to-noise ratio and a low output-to-effort ratio.
  - The pace at which the drive to real engine conditions is projected should be accelerated if possible.
  - Research has been slow.
  - No attention to fuel properties.
  - Low ambient density is not really applicable. Perhaps too ambitious in terms of vision. [This reviewer would] prefer a focus on near term deliverables such as identifying liquid core characteristics and trying to compare this with existing models. Let's try to get good results and then get this understanding covered in our spray.
  - Chemical reactions at high temperature and pressure may overwhelm the effects of the fuel spray. Difficult to transmit through high pressure due to loss of transmission at 25 bar. Modifications of fuel, additives, etc may result in differences in the fuel spray. Not apparent how this will translate into transient conditions observed in a diesel engine.
  - Long way to go before it is relevant or applicable.
  - This measurement technique seems to be pressure limited and thus its practical applicability to realistic diesel pressures and temperatures is dubious.
  - They need to become more familiar with the needs of the diesel industry with regards to understanding sprays. Need to understand state of the art and current needs in modeling. They need to have a clear understanding of how much the spray model really affects the overall CFD model and what improvements in modeling capability they can contribute.
  - Severely lacks technical focus. Efforts are more focused to please different OEMs than advancing the measurement technique/capabilities!

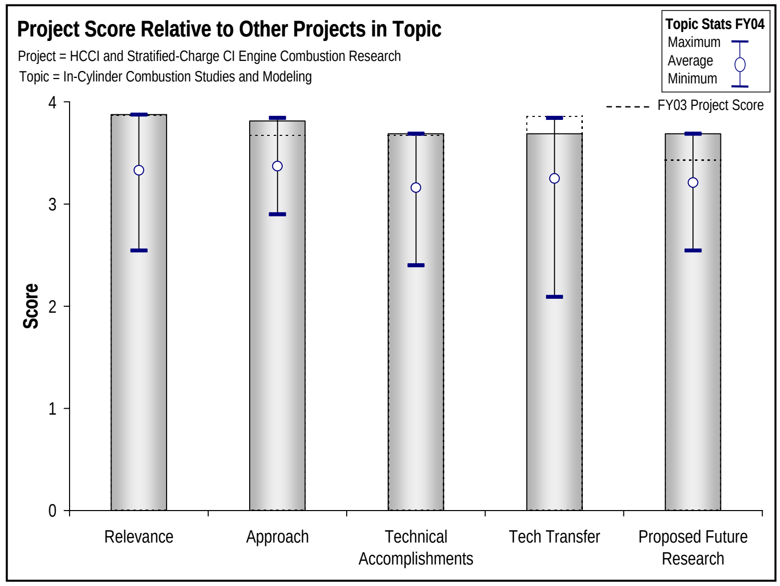
Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 13 of 18 reviewers)

- Work towards on-line data processing, and towards expanding the operating range.
- This project has high visibility and seems to involve a lot of resources in DOE and at ANL. A longer review of this project to assess benefits and future directions is required.
- Work to extend the technique (as mentioned in Session #1) to eliminate the need for the additive. Continue to extend the techniques to more relevant injectors AND injection conditions. While the low ambient pressure and temperature measurements can help to validate models, the results are limited in their application to real engine environments.
- Elaborate measurements with this technique on a hollow cone gasoline spray (for gasoline HCCI) to use the strength of this technique.
- There needs to be close attention to how the metal imaging agents perturb the properties of the diesel. Is there a chance for utilization of this technology in another field, specifically in the field of sprayed material precursors at reduced pressures that evolve on the way to a desired target? Particularly with the focus beam you could probe the evolution of metal and ceramic precursors to fundamentally understand their genesis and drive the thin film technology with a greater understanding and control of the species before they are formed into a device. Is it also possible to carry out fast XANES to look at how the geometries of the imaging agent/metal is changing in the spray at temperature and pressure?
- This research has the opportunity to map out important spray vaporization effects, including effects of

volatility and multi-component vaporization. The great power of this tool makes it incumbent that key questions to scientific community are addressed.

- Specifically add a spray modeling contingent. Perhaps link this spray modeling ot the ANL fixture as well as the SNL spray work - together there is much experimental data that could be "harvested."
- How difficult is it to obtain fuel without metal fuel additives? Lubricity may be an issue but it is probably worth it to test as such.
- Will the use of any gas, other than N_2 reduce gas absorption of the X-ray?
- Can the new X-Ray Fuel Spray web site be made available to others such as reviewers and participants in this annual review?
- Not sure how this approach can provide quantitative data to the modelers. This has been implied during the presentation but this reviewer couldn't relate or correlate it as such. Long ways to go to attain realistic pressures.
- Strong emphasis on interactions with injector suppliers, higher pressure measurements and measurements in the rapid compression machine.
- It is paramount that the apparatus is improved toward much higher ambient pressures that are representative of actual engine operating conditions.
- NSF joint funding would be great.
- The rapid compression machine was just mentioned briefly. What are the plans for using it?
- If x-ray optics and windows are limiting the future experiments, why rapid compression machine? I think efforts should be made to improve the technique rather than bench mark dozen different nozzles at ambient background pressure. Need to prioritize research goals and tasks!!

HCCI and Stratified-Charge CI Engine Combustion Research, John Dec of Sandia National Laboratories



Brief Summary of Project

This project team will provide the fundamental understanding required to overcome technical barriers to development of practical HCCI engines. The team has developed a laboratory for HCCI research (including optical and all-metal engines) and has also been working with multi-dimensional modeling groups at LLNL and the University of Michigan.

Question 1: Relevance to overall DOE Objectives (Written responses from 10 of 16 reviewers)

Reviewers mostly focused on the fundamental research nature of this project. A reviewer noted that this project represents fundamental research in the HCCI arena that fully supports DOE's goals of improving fuel efficiency of the gasoline engine and the emissions of the diesel engine. Another reviewer echoed this, noting that the project focuses on understanding and developing a high-efficiency, clean combustion system. Further, a reviewer pointed out that HCCI engines would reduce aftertreatment costs and reduce NOx. This program is developing information which will be useful in understanding low-temperature combustion and how it can be applied to diesel-fueled engines, said another. Reviewers said that HCCI is an important alternative compression-ignition engine design and operating mode, potentially a critical component of advanced engine design, and that HCCI technologies have the potential to bring engine-out emissions down into a range where present or planned aftertreatment technologies may be sufficient to meet Tier II emission standards. Reviewers also complimented the quality of the work, noting that the objectives are clear and concise, and that it is well-connected to industry and university needs (and as a result is aimed at issues on which the industry is focusing). Other reviewers added to this, noting that the work is an outstanding basis for the industrial community and is providing the fundamentals to overcome key technical barriers to development of clean, efficient diesel engines. Finally, a reviewer said that this program has a strong relevance to the advanced combustion engine program; it attempts to provide in-depth data and analyses on the understanding of HCCI combustion.

Question 2: Approach to performing the research and development (Written responses from 11 of 16 reviewers)

Reviewers were impressed overall with the approach, noting it was solid, with good progress and follow-through, and that the approach was clear and well-thought-out. Others felt the approach and analysis used were highly effective, and that the work was "world class." A reviewer said this is a well defined program: he wished every program could have laid down the objectives and technical approaches this way for better understanding of the programs. Another reviewer said the approach is well-designed to identify the dominant factors that control HCCI combustion. Incorporating modeling into the approach is very effective, and no obvious areas are being missed in the approach used by this group. They take a very thorough, detailed approach to their work, said another reviewer, who felt that the conclusions drawn from this work are well-documented, well-described, and relevant. This reviewer noted that the research goals are planned for a year or more into the future and then the plans are carried out systematically, leading to detailed results. Another reviewer also approved of the approach, mentioning that using a "metal" engine and optical engine provides the means of performing practical and fundamental experiments that, when combined with detailed kinetic and multi-dimensional modeling, enables authoritative and highly informative research. One reviewer commented that, as always, the principal investigator presents a very systematic approach to the problem, aiming at isolating individual factors thought to be important to the overall process. Finally, one reviewer referred to the project as being fuel study basics (basic R&D) so far.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 10 of 16 reviewers)

Reviewers approved of the technical accomplishments of this project, noting that the work was well-done, that there had been excellent progress on several fronts (with several SAE papers documenting the results of the work), and that the presentation showed a "firework of results." Another felt that there had been several accomplishments with progress toward understanding fundamental combustion issues. One simply said that the stated objectives for FY04 were all completed successfully: "great job". One reviewer said the accomplishments of the project are valuable and are leading the technical community toward a better understanding of the combustion regime. Another reviewer said the researchers have made excellent progress from last time and that the objectives have been exceeded. He felt it is great that the optical engine is running and is looking forward to see fundamental in-cylinder data next time). Among the accomplishments singled out by reviewers were identifications of the factors affecting changes in HCCI combustion phasing; the potential of employing boosting to extend HCCI operation towards higher loads explored for several fuels; the initial studies on the influence of thermal stratification; the investigation of factors affecting combustion phasing that showed that fuels have a lower required input temperature with increasing equivalence ratio, and the completion of development of the HCCI optical engine.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 12 of 16 reviewers)

Reviewers provided generally positive comments on the technology transfer/collaborative efforts as well, referring to the project having effective collaboration with other national labs, universities and industrial partners, and strong sustained connections with industry and university partners. Reviewers noted the continuous, close cooperation with industry that is strengthening the project, and mentioned the multiple industrial, university and national laboratory partners (including Cummins as a supplier of engines and high-pressure fuel systems, International as a supplier of variable valve actuation, GM as a provider of guidance on GDI-like injectors, Delphi as a supplier of the high-pressure GDI injectors, and Deere as a possible supplier of variable valve timing equipment). Another reviewer singled out the modeling interactions with Lawrence Livermore National Laboratory and the University of Michigan. Reviewers talked about the progress reporting on a regular basis at the University HCCI Consortium meetings, and the fact that the principal investigator has been taking every opportunity to work closely with industry partners of the AEC Working Group. Finally, one reviewer expressed the opinion that this was the kind of collaboration this he liked to see, where thoroughly researched and analyzed results are presented in a timely manner. This reviewer was not concerned with day-to-day test operations, just plans and results).

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 8 of 16 reviewers)

Reviewers were generally approving of the future research plans, but offered some comments for improving them. Reviewers felt that the work plan looked good and was very appropriate, and were glad to see that diesel fuel work will return to the workplan next year. One reviewer noted that the future work plan was based on past progress and has been clearly pushing the barriers. Among the aspects of the future work that were highlighted were the fact that future research on well-mixed HCCI will remain fuel-inspecific to leave open the issue of what type of fuel is best suited for HCCI-operation, and that the metal and optical engine experiments will offer significant insight into effects of thermal and mixture stratification. One reviewer said that the various ideas for potentially extending high-load range and improving low-load combustion efficiency (through thermal- and mixture stratification, respectively) seem well worth exploring. One reviewer noted that additional testing details would be worthwhile. Finally, one suggested that developing methods to extend high-load operation is the most logical follow-up step; studies related to thermal/mixture stratification are relevant.

Specific Strengths and Weaknesses (Written responses from 13 of 16 reviewers)

- Specific Strengths
  - Focuses on the fundamentals of HCCI.
  - They are developing good fundamental understanding of HCCI combustion.
  - High-class, fundamental research into the aspects of HCCI. Outstanding work. I think the proposed work (and continued) work into olefins and aromatics is vital.
  - The detailed fundamental investigation and analysis of HCCI combustion using optically accessible engine

- Meticulously conducted research.
- Excellent experimental planning and technique, excellent data analysis, very thorough and well thought out work.
- Excellent methods, systematic approach, deep knowledge of how to perform meaningful experiments.
- Not fuel-specific.
- Lends useful insight into answering questions such as what fuel is optimal for HCCI.
- Well-established connections to industry.
- Good team and very good interaction with industry.
- Industry connection, relevant work, continue this work, solid team.
- Excellent team with strong participation of industry, laboratories and universities. Definitely dives into the details and understanding of combustion processes.
- Tremendous experimental capabilities.
- Very carefully constructed experiments that yield substantial insights.
- John "hits the nail on the head" regarding the understanding of HCCI combustion in the optical engine in cooperation with combustion modeling.
- This project is very valuable to the goals of DOE and is directly supporting the work in industry.
- The quality of the work and the results.
- Center of excellence in "in-cylinder" combustion research.

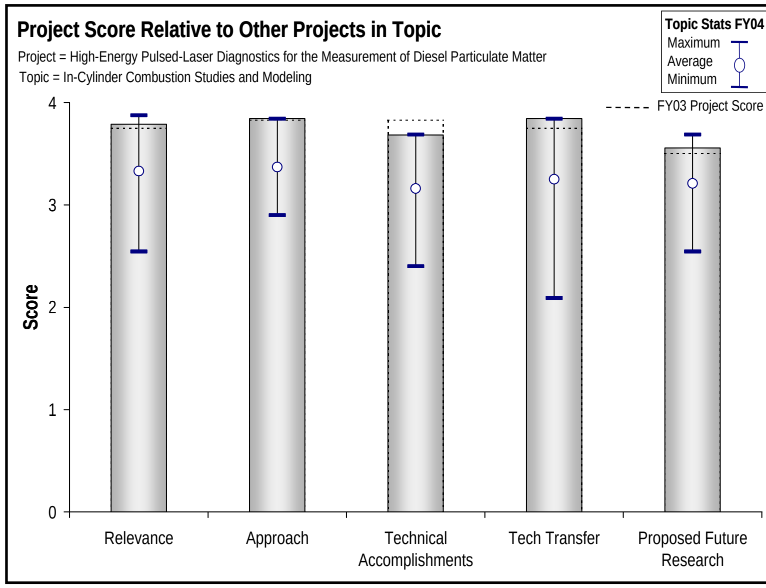
• Specific Weaknesses
  - Very incremental in nature, maybe not always focused on pragmatic deliverables
  - Too much work is concentrated at lighter loads.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 9 of 16 reviewers)

- By ensuring that research is conducted on the fundamental processes of HCCI combustion, it will remain relevant to a large community.
- Work is very valuable and should be backed up with more resources.
- They need to work more at higher loads and with diesel fuel instead of gasoline-like fuels.
- May need to increase size of project to fit scope of work.
- No changes.
- Keep funded. Suggestion for DOE managers: organize an advanced combustion workshop for cross cut team members targeting senior RD engineers who are working in the area of combustion development. This can enhance the efficiency of technology transfer to industry that SAE meetings can not achieve.
- Suggest considering density in lieu of temperature at BDC as a variable for future studies.

In-Cylinder Combustion Studies and Modeling

High-Energy Pulsed Laser Diagnostics for the Measurement of Diesel Particulate Matter, Peter Witze of Sandia National Laboratories



Brief Summary of Project

The project team is developing a technique for real-time PM measurement using a high-energy, pulsed-laser combined with a PC-based control system. Real-time PM measurement is key in investigating transients and in achieving sufficient sensitivity for PM measurement in cleaner vehicles. In-situ

Question 1: Relevance to overall DOE Objectives (Written responses from 12 of 19 reviewers)

This project was considered relevant to DOE Program objectives by the majority of reviewers. Specifically, the techniques developed in the project can be readily used as a development tool by engine designers enabling better PM controls and control strategies and providing a better understanding of engine combustion and emissions. The project results have been readily integrated into academic and industrial markets, providing for unforeseen real-time, in-situ PM measurements. The measurement technique developed in this project is useful for obtaining the transient data necessary to model DPF soot loadings. Further benefits will include the capability to be an opacimeter for aiding engine calibrators. Other DOE Programs could benefit by collaboration with the researchers.

Question 2: Approach to performing the research and development (Written responses from 13 of 19 reviewers)

In general, positive comments were provided by reviewers concerning the project's approach. The use of LII and its ability for continuous PM sampling is a good approach. The tool is very practical, robust, capable of operating in test cells or on the road, and should be easily transferred to and used by industry. This unique approach along with the researcher's detailed understanding of laser analysis has led to several novel PM characterization methods. The PM signal during the rich spike was especially impressive. The use of "off-the-shelf" components will enhance the dissemination of the approach. Extending the LIDELS technique to real-time measurement was viewed favorably. Working with other laboratories should help shakedown and calibration efforts on the tool.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 11 of 19 reviewers)

Most reviewers viewed this project as making significant progress toward project and DOE objectives. One reviewer characterized the project as a "true success story." The project has made continuous progress toward benchmarking the tool and is now testing it in the field where it can collect data for weeks unsupervised. The project has created a unique suite of laser diagnostic tools for PM analysis. The tests performed at Cummins and ORNL should provide a means of assessing the non-linearity of the LII response under steady-state conditions, thereby allowing correction/calibration under transients. One reviewer did state that the project's drive to the market could have benefited from more acceleration, but the demonstration in the field is excellent.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 14 of 19 reviewers)

On technology transfer and collaboration, reviewer's comments were generally positive. The project has shown favorable transfer to both industry (Cummins) and laboratories (Chuck Mueller's in-house SCORE lab) and has been commercialized through Artium Technologies. Clear benefits have been shown from these partnerships in the large amounts of useful data generated by having the tool available to other laboratories. These technology transfer approaches are excellent (a few systems have already been sold) and will be hard to improve upon, but the researcher should keep pushing the technology transfer.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 11 of 19 reviewers)

Comments on the project's future research plans varied. In general, comments supported proposed work on the project, indicating that it appears focused on the key technical barriers and offers several opportunities for further progress. One reviewer commented, "I can't wait to see the next entry in the toolbox!" The future benefits of the approach will include basic combustion development and DPF modeling. The LIDELS validation at ORNL will benefit both programs. The demonstration of ELS for PM sizing, development of LIBS for metallic ash, quantification of ELS and correlation with SMPS and TEM will be very important and will help further evolve the real-time technique. This technique may also be interesting to more partners. One reviewer suggested that cost of the political and press publicity should be considered in the future work. Another reviewer considered the future plan to be less important since the project is likely to be concluding in the near future.

Specific Strengths and Weaknesses (Written responses from 17 of 19 reviewers)

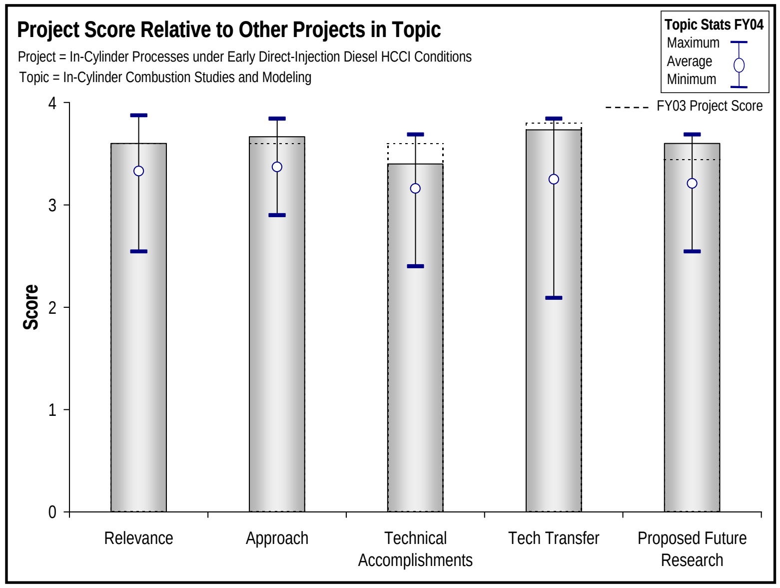
- Specific Strengths
  - Enables in-situ investigation of real driving conditions on engine-out soot (dry PM as well as VOF). Connections to industry are well-established. Well-tested.
  - Work has demonstrated interesting transient PM measurements that are valuable during calibration and development. Good job.
  - Experience with LII, development of previous approaches (LIDELS and LIBS) and the lessons learned, collaborative studies with partners which generated lots of data for evaluation of the LII response.
  - Valuable tool, which will be more valuable in the future. Tool can be easily transferred.
  - Very good sensitivity.
  - Demonstrated in the field and probed robust nature of technology. Drove technology to actual product.
  - There are no specific comments in the earlier sections because this project has been very successful.
  - This is one of the best projects that DOE has funded. It has led to a useful instrument that will assist engine development considerably.
  - Well founded in principles of the subject.
  - Very solid, fundamental work. Good attention to industry interface.
  - Excellent technical capability. Tool that can reduce the time to conduct and understand particulate emissions data. Gives excellent information on transients. Very sensitive technique.
  - Seems to be a unique approach to solving a relevant problem.
  - Moved to utilization of the equipment in transient tests.
  - Good PI and good partners.
  - Outstanding project that has led toward development of a commercially available engine system diagnostic and calibration tool.
  - It's being commercialized in time for US industry needs.
  - Center of excellence in optical measurements.
- Specific Weaknesses
  - Unclear whether research is focused on using measurement results to recommend improved operation.
  - LII system in production. Are there plans to offer enhancements in this system?
  - Would like to measure SOF and elemental carbon. Addition of second laser to get real time.
  - What is the prospect of rendering this approach to a viable tool for engine R&D dev. in industry? Affordability?
  - Work is spread around; perhaps more focus in key areas.
  - I want one.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 10 of 19 reviewers)

- Expand the on-vehicle tests to well-defined on-road test cycles at a test track under more controlled conditions.
- Work out the scatter in the data when correlating LII to gravimetric (more data averaging?)
- Will need to address differences between gravimetric analyses and LII quickly. May want to expand upon the temperature calibration of elemental carbon and its subsequent compensation with the LII.
- DOE should continue this work and fund engine investigations using this technology.
- Keep going. More can be learned.

- Take the next step to reduce the setup to a lab and/or onboard configuration: 1) Combine / refine the LIDELS; and 2) Accelerate the development pace!
- Resolve why there appears to be a non-linear response at high soot volume fraction.
- Has this project reached completion?   It is not clear that additional work needs to be done past FY05.
- This should now be stopped and let the private company take it forward. When there are already sales of the product, it should no longer be funded as a research program by DOE.

In-Cylinder Processes under Early Direct-Injection Diesel HCCI Conditions, Charles Mueller of Sandia National Laboratories



Brief Summary of Project

The Sandia team is using an optical engine in a heavy-duty size configuration to understand in-cylinder combustion processes, and the effect of differing injection profiles on combustion and resulting emissions.

Question 1: Relevance to overall DOE Objectives (Written responses from 11 of 15 reviewers)

Relevance of this work to DOE objectives was generally felt to be good. Reviewers noted that the project is sharply focused on key technical barriers to developing clean, efficient diesel engines, is very well aligned, poses strong potential for progress, and is focused on developing and understanding a practical, clean, efficient combustion system. Pre-mixed injection technology is well suited to achieve DOE objectives, noted one reviewer. A reviewer said that the relevance is outstanding, and the data supports directly observations made in the industry, so this is very valuable work toward the DOE objectives. Another offered the view that research focused on exploring new combustion concepts in the area of alternative fuels in general and diesel and gasoline in particular is relevant to DOE overall objectives. In opinion of one reviewer, the project is focused on answering key, fundamental questions about in-cylinder processes and their relation to pollutant formation, and extending those observations to understanding limitations and controlling factors for advanced combustion mode. It provides great insights to surpass technical barriers. This opinion was restated by another reviewer who noted the work is very relevant to the DOE objectives because it is addressing the problem of developing a fundamental understanding of low-temperature combustion modes. Multiple injection strategies are in common use but the implications of those strategies are not always clear, and this optical engine work provides great insight into the combustion effects that these strategies cause. One reviewer offered the suggestion that expansion to other operating conditions could improve progress in understanding multiple injection implications, since to date this work is focused on a very small portion of the engine map, so results are not universal at this time.

Question 2: Approach to performing the research and development (Written responses from 10 of 15 reviewers)

Reviewers offered generally positive comments about the approach of this project, noting that the quality of the work (both experimental and simulation) and the subsequent analysis is outstanding (and that the approach is difficult to improve). The research is well-planned and -executed, in the opinion of one reviewer, and the program goals are developed over a longer term to investigate fundamental phenomena. The approach to combining the experiment and the analysis is outstanding (in one reviewer’s view) and is very time- and resources-efficient for giving the detailed and fundamental understanding of this combustion. Reviewers noted the advantages conferred by the equipment and facilities available for this project, specifically the SCORE engine which lends itself well to the study of in-cylinder processes governing combustion and emissions formation; the in-cylinder LBD; visualization and combustion analysis; instrumentation; and the tremendous experimental facility. One reviewer said that this was a good application for optical engine to see in-cylinder processes, combining optics and simulation while incorporating previous Sandia results to a new topic. This reviewer liked the study organization by key questions, which gave a good comparison to optical and verification in metal engines. One reviewer singled out the effective use of available experimental tools for improving the fundamental understanding of the processes. Another said it appears all the correct variables (EGR, flame structure, equivalence ratio, injection timing and overlap of injection events, etc) are being considered in this study. Finally, a reviewer felt it would be good to expand the study to more operating conditions.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 10 of 15 reviewers)

Progress was generally felt to be very good or excellent, the contributions seemed to be well-founded, and the approach was generally regarded as robust. One reviewer noted that the results support and closely reflect the work currently being done in industrial circles. Another said that the principal investigator's work has been key to a better understanding of in-cylinder processes and has helped the research of many others. One reviewer noted several accomplishments, including the dual injection studies to explore relationship between pilot and main; the exploration of the combustion efficiency penalty in diesel HCCI; the study of mechanisms of NOx emissions for dual-injection operation; and the study of the relationship between stoichiometry at the lift-off length and soot emissions using LII. Another reviewer was impressed with the effort to estimate the stoichiometry at the lift-off length and to tie this in with the soot measurements. This is using the results from one program to advance another program. One reviewer found the results puzzling, but wanted to see this investigated further to understand what is going on. One reviewer spoke of the principal investigator's good publication record and good interpretation of the combustion regimes produced by the injection strategies. Now that the origins of the poor combustion efficiency under early direct-injection diesel HCCI conditions have been explored, noted a reviewer, solutions can be proposed and tested. A reviewer felt that much progress had been made, but it is limited to an engine operating condition at this time.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 10 of 15 reviewers)

Technology transfer and collaborations were generally thought to be good, and several noted the collaboration with Caterpillar as being useful. Several reviewers commented on good collaboration with industry partners, universities (especially the University of Illinois), and national laboratories (and one felt the group was well-connected to the right organizations). This collaboration was felt to enhance the quality of the work. Participation in AEC working group meetings was also felt to be useful, as were the numerous publications of the team and the links with modelers and supporting experimentalists at the labs and universities. The combustion CRADA with Caterpillar was characterized by one reviewer as being well integrated into the broad industry team. One reviewer, however, said that the evidence for good industry collaboration in the presentation was weak, as it seemed to be primarily the working group and Caterpillar (which was decent, but not extraordinary).

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 10 of 15 reviewers)

The future work plan builds on the past progress and is sharply focused on one or more key advanced combustion engine program technical barriers, in the opinion of one reviewer who also said that the plan to move to an early HCCI approach increases the value of the project. Others noted that the work is pointed at fundamentally challenging aspects of combustion, that the plans for future work are good, and that the fuel-enabled combustion aspect is important. One reviewer singled out the study of fuel-enabled LTC; the extension of biodiesel research; the examination of fuel effects on achieving low emissions and high efficiency; and the continuation of NO diagnostic development. A reviewer said that continued NO diagnostic development is highly relevant to all modes of combustion; another said that the focus on EGR and in-cylinder NOx diagnostics is very relevant. A reviewer said that this project sets the stage for future work in use of optical measurements to assess the capability of multiple injections to control combustion in an HCCI-like engine, but that much follow-on work is required to expand understanding in a more general sense. Another suggested that a stronger focus on soot oxidation/formation conditions would be helpful. This reviewer agreed that fuel effects need to take a very prominent role in the studies. The 46 cetane fuel originally used in this project may not be relevant to what will be found in the marketplace: lower cetane is far more likely. Many of the pre-production engines show a high sensitivity to cetane number. This reviewer questioned the value of the biodiesel studies, noting that there are far more pressing problems that this technology can address. Fuel-enabled LTC is of limited, short- and mid-term value in the opinion of one reviewer, but if DOE believes that diesel and gasoline will likely be replaced by alternative fuels, there is definitely a long-term relevance to the project. A reviewer said that the team could be looking at a range of topics that is too broad, and suggested more focus on early injection. Another reviewer wondered why it took so long to study EGR, which this reviewer believed should be done this year.

Specific Strengths and Weaknesses (Written responses from 14 of 15 reviewers)

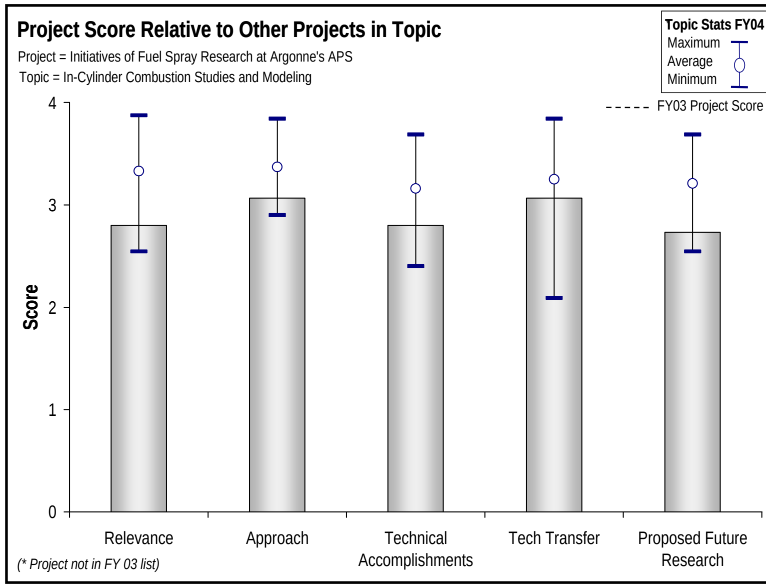
- Specific Strengths
  - This project is very valuable to the goals of DOE and is directly supporting the work in industry.
  - The quality of the work and the results!
  - Excellent project.
  - Excellent diagnostic techniques.
  - Responsive PI.
  - Good PI and good utilization of the SNL facilities and synergy.
  - He has made significant progress on a number of interesting topics.
  - Well rounded team and resource base.
  - World-class capabilities. Good focus.
  - Potential long-term value.
  - Realistic engine geometry - study over range of loads.
  - Facility, capabilities and partnerships provide excellent capability that is generating fundamental and important insights into {diesel engine] combustion and underlying processes.
  - Outstanding experimental facility and very qualified PI for this project.
  - Excellent experimental facility. Good industry support. Good past record of accomplishment. Useful publications from past work.
  - Excellent combination of technical tools - looking at the right questions.
  - The potential implementation of the studied injection strategy in an effective manner that would lead to a clean, efficient combustion system.
- Specific Weaknesses
  - Early injection diesel HCCI should be explored in more detail, i.e. various fuel distribution between pilot and main, different dwells, EGR-rates, intake temperatures etc. Without having run through such a test matrix, the conclusions drawn from the research may be premature.
  - The current work seems more like interesting science and not focused on problem solving.
  - Why did he study only one way to do HCCI?
  - Biodiesel???? I am not sure it is worth the effort at this point.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 10 of 15 reviewers)

- Add funding to accelerate the work.
- More extensive test matrix.
- It would greatly help the engine community if this work was expanded to include a broader engine operating map.
- Lower cetane "realistic" fuel studies and more direct work with industry.
- The investigation of biodiesel should be of lower importance because of its high cost and low availability.
- Prior to investing more resources in the area of alternative fuels, a discussion is due between the DOE, the automotive OEMs, and the energy companies on the likelihood of diesel and gasoline being replaced.
- May be interesting to expand studies into labeled aromatic compounds to probe the basics of the soot formation process in this engine - relevant to coal-liquids derived fuels and tar sands fuels.
- Add the EGR to the HCCI work.
- Looking at fuel injection techniques to get low NOx/robust early injection is advantageous - early injection deserves more attention and focus.
- I would like to see an explanation of the smoke vs. phi at lift off length question. Why were these contradictory? Would like to see this work more connected to the Livermore fuel mechanism development effort.

In-Cylinder Combustion Studies and Modeling

Initiatives of Fuel Spray Research at Argonne's APS, Jin Wang of Argonne National Laboratory



Brief Summary of Project

The objective of this project is to use the Advanced Photon Source at Argonne National Laboratory to provide X-ray imaging of high-pressure fuel sprays, and to validate CFD simulations of sprays with this imaging. Currently, researchers are obtaining systematic and quantitative spray data, and are testing sprays in a pressurized environment (10 bar).

Question 1: Relevance to overall DOE Objectives (Written responses from 13 of 15 reviewers)

Reviewer opinions on this aspect of the project were varied. One group was positive about the work. A reviewer commented that the technique developed by Argonne allows in-depth characterization of the spray structure in the near-nozzle region, which will serve as an excellent basis for development and validation of numerical models. Several comments focused on spray characterization. One person commented that research is important to better characterize spray with models, especially for HCCI. One of the reviewers felt that understanding fuel spray phenomena is critical to advancing combustion research, since spray formation and mixing are critical to conventional and advanced combustion regimes. Another added that quantitative spray data, in particular the near-nozzle regime, would help both spray-combustion modeling and tip design. One person felt that answers are needed as to whether a spray is good or bad, according to DOE objectives, which is difficult to get. One person said that this work addresses the fundamental need of genesis of the fuel as it is injected into the cylinder. Another reviewer agreed that the project entails solid fundamental research, and that the technique is potentially useful, but was not sure it will lead to combustion improvement. Another person echoed elements of this, stating that it was not clear how one gets from the basic fuel spray work to combustion in this talk. Another person went further to suggest that this proposal is of a scientific research nature, and is well suited for National Science Foundation or DOE funding. Its relevance to diesel is of a fundamental research nature. Another agreed, stating that this is very fundamental work, and is a contribution to science, but since there is a long way to characterize a spray under real diesel engine conditions, the contribution to the development of clean, efficient diesel engines is small. Others were more critical of the work; one person stated the researcher's objectives included efficiency and emissions, but the presented data shows no connection to this goal. Another reviewer, while not sharing the researcher's aggressive vision, felt the process needs to show its value and should focus on getting the quantitative data at the near orifice liquid core rather than suggest all nozzles will be characterized on such a device. Another person said the work is focusing more on developing a technique than on contributing to the development goals. The final reviewer stated that it is difficult to see a significant relevance in some of this work; the experiment is complex and expensive to run which will result in little data.

Question 2: Approach to performing the research and development (Written responses from 12 of 15 reviewers)

Again the comments were varied. One person simply stated that the researcher has used good reasoning, proactive proposal, and good use of LDRD. Others stated that this was very fundamental work so far. Another felt the approach is well-thought-through and has strong academic merit. One person said a lot of effort/capacity is currently spent on developing this technique. One reviewer thought the researcher has used a systematic approach, continuously improving the technique and expanding it towards higher ambient pressures. One commented that the information presented are the very early results of a new approach, adding that the mass info in jet and the liquid core is great, but not much in the way of real information or results can be seen so far. He suggested getting good results focused on the liquid core and comparing those to current spray models (rather than just taking pictures) should accelerate the work and get the best results. Another reviewer felt the high-level content is a good approach, but *details* are needed: specifics of the testing approach would be worthwhile for further R&D. This could result in a very complex test plan, with potentially several key projects to be funded. Others felt that there was much room for improvement. One reviewer felt the researcher needs improved connection to goals of efficiency and emissions. Another thought the x-ray absorption technique is sound and proven, but the phase contrast approach for cavitation imaging is not clear. Another person said that the researcher shows information about the capability of the technique, but not enough information about how the data collected in the experiment will be used to advance the state of understanding and modeling. A reviewer commented that the technique is novel and can yield exciting results, but the approach is severely limited by the type of seed molecules that must be used for the imaging to work and the need to average the spray events to complete an image. A key aspect of fuel injection and advanced combustion research is the consideration of fuel formulation and without the ability to freely adjust fuel characteristics, these studies of fuel injection are severely limited. The inability to examine the interaction of turbulence with the spray is a limitation. The final comment was that a direct comparison to optical methods to clearly demonstrate the technique's additional capabilities would be useful. It was not clear why there needs to be specific orientations/angles of measurement. To aid in the description of the fuel plume and increase speed, an array of detectors would simultaneously capture the information for all the angles in parallel. Are the very best/fastest detectors being employed? Has an exhaustive study of this field been carried out? The data are collected in transmission mode, but has a fluorescent mode been considered? Has an exhaustive screen of different metal additives been considered as soluble imaging agents?

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 13 of 15 reviewers)

Here too, reactions were varied. One comment was that researchers have already shown good progress, and demonstrated a unique technique (an industry first). Another thought that there has been good progress towards the goal applying this technique to engine-like conditions, but it takes a lot of time and resources. Another noted the very interesting data generated thus far, that the work has clear signs of evolving capability, and the team is looking to have dedicated staff and experimental setup to permit a more effective program, particularly by enhancing researcher access to the facility. He went on to note the conflict over beamtime access, and the resultant need to establish a partnership/collaboration to gain guaranteed access to APS. Others were more critical. One person simply stated that the presentation presented old results. Another commented that although the early results and analyses including tomography were quite promising, the technical accomplishments over the last year were rather limited. Another felt it was not clear anything has actually been done yet. Another offered a similar comment, namely that comparisons of injectors at 1 and 10 bar have already been done, so no knowledge has been gained so far (or at least this insight was not presented). One reviewer felt the progress toward meeting the DOE goals was weak, since the direct contribution at this time is not large. One reviewer suggested the researchers consider higher temperatures and pressures. One person commented that the results are useful for understanding multi-phase flow. It's not clear how the results will improve industry products. The final reviewer suggested the researchers discuss 1) the test method/process status versus 2) empirical fuel spray results.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 12 of 15 reviewers)

The reactions in general were positive. Several people acknowledged, or commented on, researchers' significant effort to look for collaborators and opportunities to work with partners, including many university and fuel injection equipment manufacturer industrial partners. One person wondered whether the motivation is commercially based. Several people suggested extending the work to a larger share of the injector and fuel system industry. One reviewer commented that ANL seems very open to testing hardware. He was pleased that spray modelers seem interested in getting involved, and encouraged this to continue. One reviewer commented that there was no mention of LLNL's combustion work. This reviewer felt the industry interactions were limited, but that the researchers collaborated well with universitries, and that the relationships with fuel injection system suppliers could be strengthened. Another reviewer commented that collaborations and technology transfer will be challenging, since the efforts to make a measurement is large and the output has limitations. The final reviewer felt that it was not clear that the information is disseminated at conferences, publications and websites. This could be demonstrated.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 13 of 15 reviewers)

The reviews were varied on this question. One reviewer felt that the implementation of more focused optics is excellent. Another commented that enlarging the partnership further is a good plan to enhance the strength of the effort and the continued access to beamtime, but problems remain with the approach that were not addressed in the presentation. This reviewer felt it was a good idea to expand into tie-in with simulation studies, and that this is a good way to apply the results for system. Another reviewer commented that the direction of the future work plan is correct, toward time- and space-resolved measurements in a high-pressure, evaporating atmosphere. The future work plan builds on past progress and generally addresses removing the key barriers, but it takes a lot of effort and time. One person acknowledged the future research plan includes both testing and CFD simulation. One reviewer commented that many firms have expressed interest in using APS facilities and the ANL expertise; such efforts would lead to develop a quantitative spray database on different injectors/fuel systems. A comment from a previous question was repeated, stating that the high-level content is a good approach, but details are needed: specifics of the testing approach would be worthwhile for further R&D. Another person thought that a strong focus should be placed on how to use the experimental data to improve and validate models describing primary and secondary atomization, effects of internal nozzle flow specifics, cavitation etc. One reviewer questioned the use of the rapid compression machine, noting that high pressure is needed, but there is also a need to focus on the liquid core. One reviewer suggested encouraging the PI to engage fuel injection system suppliers. Another felt he needed a better understanding of how this work will actually benefit combustion. Another person cautioned that it will likely take many years for this to pay-off in a combustion research setting and then in a product application. Another reviewer said, he is still waiting for high-pressure fuel sprays, and that nothing on this was presented in the talk. The final reviewer commented that there was very little information contained on the future plan; the researchers simply saying they were planning to do more work. This reviewer added that he would like to see much more detail about what they plan to do and how it will be used in their collaborative efforts to improve understandings of spray physics.

Specific Strengths and Weaknesses (Written responses from 14 of 15 reviewers)

- Specific Strengths
  - Unique technique in offering time-resolved, quantitative information on spray structure in the near nozzle region. This allows air entrainment to be determined. Effects of nozzle-design such as k-factor, and degree of hydro-erosion on spray structure and mass distribution can be studied in detail.
  - Unique approach and capability, partnership developed to enhance access to beam time.
  - Research addresses both test and simulation. Potential to image internal motion is important.
  - The measurement technique gives mass distribution in the spray. This fact can give fundamental new insight in hollow cone sprays.
  - The optimal delivery of fuel into the cylinder is a key means to improve fuel efficiency. Real time imaging is advancing the fundamental knowledge.
  - This research provides information that has not been available in the past.
  - Innovative technique.
  - New approach not available elsewhere.
  - Exceptional capability of the radiographic source. Initial modeling is excellent.
  - Its new application for spray research towards fundamental understanding.
  - They have a unique facility.
  - The technique and the facilities are quite unique.
- Specific Weaknesses
  - The presentation was too qualitative. I presume the data is presented elsewhere or shared with the partners and the partners directed him not to divulge it. A 2D detector is still lacking.
  - The approach, requiring particular cerium additive level at 4 weight percent, has limitations in applicability. How does the cerium additive affect the spray geometry, spreading and mixing, and how does this spray compare with the spray without the cerium additive?
  - Limitation of environmental conditions. Relies on point averaging rather than full field.
  - The technique is limited due to a low signal to noise ratio and a low output to effort ratio.
  - Need to look at conditions that are closer to those used in the application
  - The need for repeated injections and averaging to obtain data is a weakness. Also, it is unclear how this work will lead to better engines.
  - Connection to combustion improvement is not demonstrated.
  - Limitations on pressure. No conclusions on the sprays were made that was presented. I recommend focusing the project on specific technical objectives about the liquid core that this set up is uniquely

qualified to test.
- Did not supply information how this program would lead to improvements in combustion research or how it will apply to improved fuel economy.
- It's not clear with respect to industrial application.
- The images that are shown are composites of point source measurements which are ensemble averaged. This presents two problems. First, it takes them a long time to produce results. Second, the images cannot capture shot-to-shot variations in the spray. This makes it impossible to see many of the interesting features of the spray such as droplet phenomena and local mixing phenomena.
- Extremely difficult to replicate in-cylinder density or evaporative spray imaging conditions

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 12 of 15 reviewers)

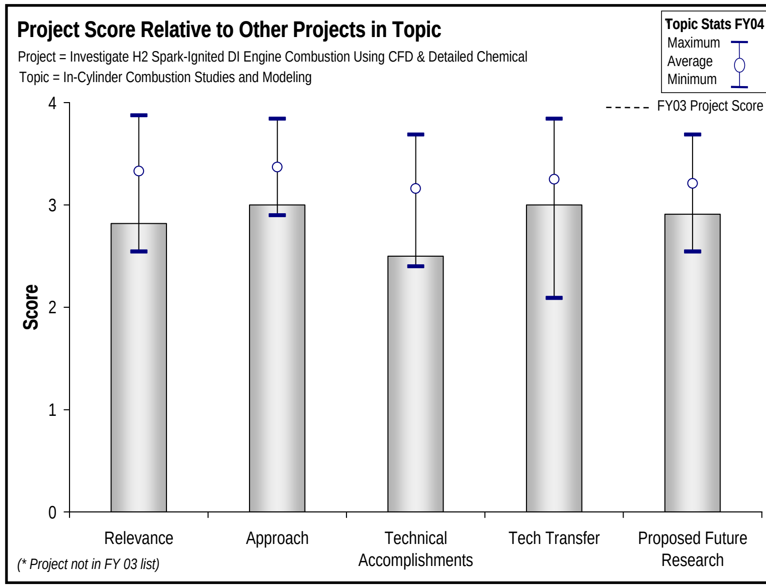
- Work towards on-line data processing, and towards expanding the operating range.
- He is asking for support for future plans. Based on this material (only), there is no reason to support this. Results were too qualitative and only showed interesting capability and not detailed understanding and conclusions. This is troubling after several years of funding and effort.
- Continue growing the partnership, expanding link with CFD modeling and improve techniques so as to eliminate need for cerium additive.
- Elaborate measurements with this technique on a hollow cone gasoline spray to use the strength of this technique.
- Need to build a detailed cost/benefit chart to justify designation of a dedicated beamline for this work at a user facility. Even should it be decided to not dedicate a beamline to this work with the number of collaborators a large number of proposals could be submitted and beam time obtained. The modular design of the equipment will aid in set up and moving the experiments. Could this work be extended into the realm of materials? There are several coating techniques were plumes of inorganic/metal precursors are sprayed/vaporized and the species evolve before hitting a target. This work has the potential to probe those plumes at reduced pressure and higher temperatures to help optimize coatings. This talk would have benefited greatly if it had been after the more technically detailed talk by Christopher Powell.
- They need to investigate higher chamber pressures and higher injection pressures. Also, they should investigate fuel spray interaction with surfaces since these are quite important in engines.
- Focus on specific systems and correlate to combustion improvements. Find a way to increase funding.
- Walk before we run.
- Very interesting approach, but does not seem to be connected with other work in this area. Recommend detailed discussion with LLNL and the industry to get feedback to determine what the near term pay-off of this approach. It is not clear how this will assist in either fuel economy improvements or emissions. The potential to impact these areas is not clear, but certainly the technique is impressive.
- Fund this work by National Science Foundation because it's too fundamental unless fuel injection system suppliers can fund part of the work. Potential fuel system suppliers are Siemens, Bosch, Delphi, and Denso.
- I would like to see a more detailed description of why this technique is better than optical techniques and what it offers that can't be done using an optical technique. The x-rays are capable of resolving much smaller features than light, but it seems that these features are lost in an ensemble average. Also, it is imperative to see a more detailed description of what they are planning to do and how the work will be used to improve spray modeling.
- Given the test setup/conditions limitations, the team needs to develop more specific program targets for each year. In my opinion, repeating x-ray absorption measurements on different injectors does not add any more value because test conditions depart quite significantly from the target conditions. For example, the team needs to develop target background density. Similarly, the potential workscope and benefits of phase contrast experiments need to be stated clearly.

In-Cylinder Combustion Studies and Modeling

Investigate Hydrogen Spark Ignited Direct Injected Engine Combustion Using CFD & Detailed Chemical Kinetics, Salvador Aceves of Lawrence Livermore National Laboratory

Brief Summary of Project

To meet the need to develop a fundamental understanding of hydrogen spark-ignition engines and hydrogen combustion, LLNL is working on several simulations of hydrogen combustion, and has identified a method that can promise accurate results with reduced computational effort using KIVA. This project is a collaboration between DOE and Ford, with the participation of LLNL, SNL, and ANL.



Question 1: Relevance to overall DOE Objectives (Written responses from 7 of 11 reviewers)

Reviewers generally found the relevance of this research to DOE's goals to be good, but questioned its relevance to the advanced combustion engine program. One reviewer characterized this as overall good, fundamental R&D work. Another said that the hydrogen ICE is underexplored and needs more work: this is good. A reviewer offered that this program may help develop hydrogen ICEs, but does not share the rest of the advanced combustion engine program's relevance to near-term improvements of emissions and efficiency due to the impracticality of hydrogen fueling in practice.

Several suggestions on the relevance were made. One reviewer noted that the project objective isn't clear and a better statement of it should be provided to better determine the relevance to DOE objectives. Another said that the argument concerning the potential of the hydrogen ICE should be made more effectively; this project does not fit within the stated goal of clean, efficient diesel engines. One reviewer pointed out that it will be many years before hydrogen will be available for personal transport. Efficiency improvements offered by the hydrogen ICE are not much better (relative to current vehicles) than diesel, if there are improvements at all. A diesel-electric hybrid would have impact on DOE's goals much more rapidly than a hydrogen SI DI engine. The hydrogen ICE has been studied and characterized by industry in the past. BMW is referenced in the study. TNO (Netherlands) and possibly IFP have done work in this area, too.

Question 2: Approach to performing the research and development (Written responses from 8 of 11 reviewers)

Reviews of the approach were generally good. A reviewer said that this is a reasonable approach, but suggested more sharing of combustion chamber designs for lean-burn SI hydrogen. Another said that the approach to better understand combustion through modeling is important. "Good approach," said another, with a unique approach to computational methods. Reviewers noted the use of decoupled fluid mechanics/chemical kinetics modeling approach in combination with KIVA (as successfully developed for HCCI combustion) along with a similarity approach to permit a variable geometry mesh. One reviewer said that looking at hydrogen introduction into cylinders at modest pressure is risky and intriguing. One reviewer said that the project was in the very early stages, and it is difficult to assess whether the approach will be effective. Finally, a reviewer commented that the project had a low budget and a limited scope, both of which may compromise the outcome. The KIVA approach with nozzle similarity approach may require more fundamental checks and further enhancement. Also, it seems that the analysis is 2-dimensional. Finally, geometry and location of spark plug, tumble, etc. are substantial influential factors. This renders this study of "very lean combustion" near the spark plug of a fairly limited value.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 6 of 11 reviewers)

Most of the comments concerned the fact that this is a new-start project that was just getting underway. One reviewer felt that there had been very rapid progress given the short time since inception, and that this was good key work in support of the hydrogen ICE FreedomCAR concepts.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 7 of 11 reviewers)

Ford's collaboration in the project (referred to as an industry leader) was noted by several reviewers. Other comments included the approval of a reviewer in the involvement of both experiments and modeling (a good idea). One reviewer said that solid collaborations existed between industry and the DOE labs, but the project could use further university involvement and dissemination of results at conferences and in publications. "Good team," commented a reviewer. One reviewer felt, though, that it was too early to grade this project and did not fully understand the extent of the collaboration.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 6 of 11 reviewers)

Several suggestions were made relative to the approach and relevance of research. One said that the team might want to define better the barriers in the hydrogen direct injection project. Another said that this was a reasonable approach and good fundamental R&D work overall, but suggested more sharing of combustion chamber designs for lean-burn SI hydrogen. "Very promising opportunities," said another, but said this project needs to be focused on real engines. One reviewer specifically mentioned the plan to use charge stratification to reach lower NOx by preventing excessive temperature in the region of the spark plug. Modeling of hydrogen seems to duplicate large eddy simulation at Sandia, said a reviewer. One reviewer felt that more information was needed to properly assess the planned work.

Specific Strengths and Weaknesses (Written responses from 6 of 11 reviewers)

- Specific Strengths
  - Low-cost computational work can be very useful when appropriately validated by experimental data from other programs at Nat'l Labs or from industry partner.
  - Understanding soot formation in low-temperature combustion is important.
  - Unique computational approach. Key work in support of hydrogen full utilization.
  - Building on existing programs and models.
  - Computational tools and approach and teaming arrangement.
  - Modeling will help to interpret/guide experiments.
- Specific Weaknesses
  - Hydrogen engine research should be low priority.
  - Small scope. Much more could and should be done.
  - Reliance on hydrogen as the primary fuel limits potential near-term impact.

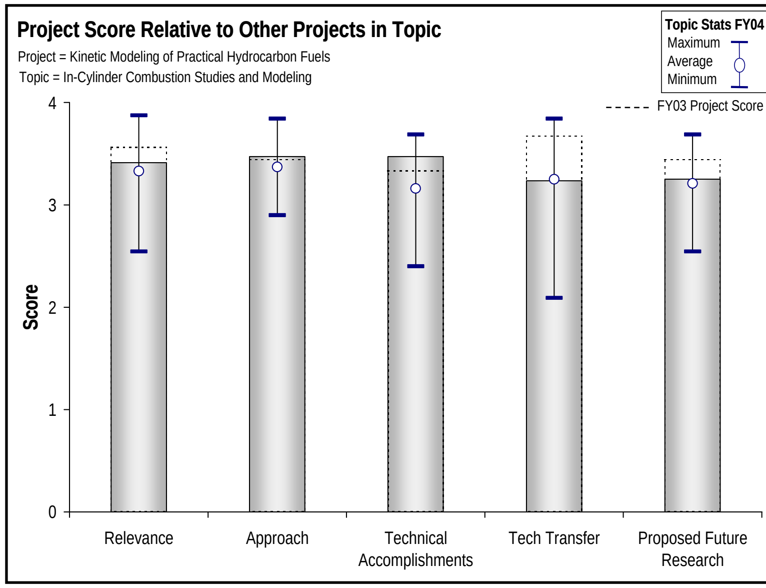
Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 6 of 11 reviewers)

- Because this is a new project, a clear scope is work is needed. I struggled to really understand what the scope is, but perhaps that is coming as the project matures.
- The work should lay out the fundamentals for hydrogen combustion to provide the fundamentals for industry
- The project on modeling low-temperature diesel combustion is much more important than the hydrogen engine project.
- Expand project to move more quickly; move into metal engine work.
- Not sure of the funding level, may not have the minimum critical mass to sustain a worthy effort? Assumptions and premises for the applied approaches may be valid, but this is outside the immediate area of my expertise.

Kinetic Modeling of Practical Hydrocarbon Fuels, Charles Westbrook of Lawrence Livermore National Laboratory

Brief Summary of Project

This project develops and applies chemical kinetic modeling techniques to the analysis of key combustion processes in diesel, HCCI, and spark-ignition engines. In this way, this technique can address important practical concerns for limiting pollution emissions (including NOx, soot, and hydrocarbons).



Question 1: Relevance to overall DOE Objectives (Written responses from 13 of 17 reviewers)

Reviewers were mostly positive about the relevance of this project to DOE goals. One referred to the project as a unique core competency in a relevant area, while another said that this project is much needed by the engine modeling community and will be very beneficial to the community upon its completion. This work is directed toward developing useable kinetic models of real fuels, noted one commenter. The fundamental nature of the work was highlighted by several reviewers, who said that the project represented solid work in fundamental areas that was valued by vehicle OEMs. The project provides some fundamentals of the kinetics of HCCI combustion. This program represents on going work in developing appropriate chemical kinetics models for better diesel and HCCI combustion – an important part of the advanced combustion engine program, noted a reviewer. One reviewer suggested, however, that research should be aligned more closely with current directions of OEMs and energy companies. Another was unclear as to the relevance of the work to DOE objectives.

The essential nature of the kinetics work was a subject of several comments. Gaining a deeper understanding of the kinetics of fuels is an absolute necessity in the development and optimization of future combustion systems applying analytical techniques. A reviewer said that an extremely practical implementation of the modeling and calculations is to be recognized and recommended. The need for the fundamental science to support the drive to better fuel efficiency while reducing emissions cannot be stressed enough and this research is directly aiding in this thrust. Developing extended models for the combustion of realistic fuels is critical to advancing the ability to simulate diesel engines and therefore can help overcome barriers through numerical support of advanced combustion regimes. This is an enabling technology, in the opinion of one reviewer, to allow HCCI combustion simulation and is a useful database at a very fundamental level. The LLNL projects have always supported DOE's experimental projects well, noted another. The interpretation of kinetic work is an effective supplement to the experimental work. The multi-zone modeling for HCCI (not included in this presentation) has been clearly beneficial.

One reviewer characterized the project as having a very fundamental and interesting approach. The movies illustrating what happens on a catalytic surface are interesting and can help to demonstrate to management how heterogeneous catalysis works. But for experts, this is nothing new and this reviewer wondered if it is worth it to spend large amounts of money on these simulations. This reviewer felt the question of whether to work on simulation movies should be discussed in an extra workshop together with experts in catalysis and simulation.

Question 2: Approach to performing the research and development (Written responses from 12 of 17 reviewers)

Several reviewers offered positive comments about the researcher and the approach. One noted that the group under Westbrook represents the leading-edge in the community of chemical kinetics. Another said that the group represents a unique core competency in a relevant area. A reviewer said the approach presented is thorough and begins with a fundamental understanding of fuel behavior and chemical kinetics of fuels. Another reviewer referred to the approach as an excellent one for modeling practical fuels. A reviewer commented that the researchers are developing kinetic models for individual compounds in practical fuels and combining them to simulate the combustion of practical fuels. This approach builds fundamental rigor into the models and thereby gives them robustness. "A good, solid approach by a good person" was the opinion of another commenter. Finally, a reviewer pointed out that the studies with surrogate fuel mixtures offer much-needed rate information for HCCI development work.

Suggestions for improving the approach were offered by reviewers, including one who noted that the "by hand" development of kinetic mechanisms is difficult and time-consuming. This reviewer believed this group should begin to use the computer-generated mechanisms. The value of the computer-generated mechanisms is that they provide an extra level of confidence that no reaction/reaction type has been neglected. Another said that the research is attacking several areas: the evolution of oxygenates in fuel, NOx adsorption on surfaces to name but two. The researchers must remain watchful not to allow their scientific zeal to dilute their impacts too much. One reviewer characterized the project as an effort of the principal investigator to "look for projects". Experts in heterogeneous catalysis should be integrated, said another.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 12 of 17 reviewers)

Several reviewers had positive comments about the project accomplishments. One noted that this was one of the few talks with simulations and models that went from the total system all the way down to the molecular level (crossing from the complex engineering issues all the way down to the fundamental chemistry). This depth of study and diversity of expertise is "terrific." Others said that the capabilities with outstanding computers are impressive, and that the team is making progress building surrogate diesel and gasoline fuels. One reviewer commented that the team has a good understanding of the impact of oxygenate fuel structure on formation of soot precursors and has developed interesting first results on NOx-trap modeling. Other comments included a note that great progress had been made on a very difficult problem: the key results will be generated next year and "it's well worth the wait." "Good use of experimental data from other sources," said another reviewer, who highlighted the interesting fundamental work on surface chemistry. A reviewer singled out several aspects of the research, including development of a kinetic model for methyl cyclohexane to serve as a surrogate for cycloalkanes, and for toluene, an aromatic surrogate, along with separate MD of adsorption of NO_2 onto LNT catalyst surfaces and continued work on understanding combustion of oxygenates. Another noted that the researchers modeled a realistic NOx trap surface. Finally, a reviewer said that the team reported significant progress on methyl cyclohexane and toluene kinetics, and it seems that efforts were split among different tasks that include surface chemistry (LNT), diesel oxygenates and soot chemistry in diesels.

Other comments on the accomplishments were that the temperature domain is higher than "low-temperature combustion", and that very few details about specific progress were provided. This reviewer noted that more specifics would have been useful, and that he knew from this presentation what the principal investigator is working on but not what he has done. Finally, one said that the continuing work on the oxygenated fuel additives is interesting. The interest in the oxygenated species is beginning to drop. The new work on the barium oxide surfaces is very interesting. Often the work presented at these meetings is a collage of applications. It would be helpful if the reviewers got a comprehensive presentation on the direction of the modeling work at Lawrence Livermore.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 12 of 17 reviewers)

Responses to this question were mixed. Several researchers were enthusiastic about the collaborative aspects ("always well done"), noting that the knowledge transfer/sharing was effective and that the team has good, solid relationships with working groups (including good collaborative efforts through the AEC MOU and the university HCCI collaboration), and that the team is interacting with various communities and serving them quite well. Others highlighted the solid interaction with other DOE labs and universities, as well as the good dissemination of research via papers and presentations and the work with Sandia. Many industry and university personnel are awaiting the outcome of this project. A reviewer said that although there is no direct industry participation on this program, the results are quickly being disseminated to different HCCI programs that are taking place elsewhere (OEMs, labs, and universities).

Other comments included one that the combustion CRADA is a good mechanism to disseminate the intermediate results/findings, but expanding the collaboration to include the HCCI CRADAs would be beneficial. It was unclear to one commenter how the researchers are leveraging the industrial sector to help in this work, and another said the collaborative aspects were not really clear, but the presenter also asked for input from industry.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 13 of 17 reviewers)

Several suggestions were provided to improve the future workplan, although one reviewer noted that the future work proposed can be a significant addition to the understanding of several systems. Proposed future work aims at addressing real-life issues, said one reviewer. "Continue to build model for surrogate gasoline and diesel fuel," suggested another reviewer (the surrogate fuels are eagerly awaited by researchers). Another reviewer would like to see the surrogate fuels projects reach a point where engine tests are being compared to predictions and would like to see a plan for who is going to do the surrogate testing and how the testing will be compared to the modeling. A model description of diesel fuel is needed for HCCI/advanced combustion predictions and should continue, said another reviewer. Good ideas, said a commenter, but the team may need better equipment. Finally, a reviewer said that the project was more focused toward surface chemistry, which is helping many LNT studies.

Several other comments were offered. The molecular dynamics modeling is highly relevant in determining trapping efficiency of NOx traps. Research on oxygenated fuels appears somewhat academic, considering current industry direction. One reviewer offered that the future work could be more structured and more detailed: at present it seems to be rather vague to say "we hope to get more involved with ...." A comprehensive direction for the research is rarely given, noted a commenter. The work on fuel surrogates is especially interesting, but a more rigorous approach to mechanism development would provide additional confidence that no reactions/reaction types have been neglected. Finally, one reviewer felt the future workplan was not clear, and was very fundamental. In case of limited budgets, there might be other projects could have higher priority. This project is in the nature of long-term research.

Specific Strengths and Weaknesses (Written responses from 14 of 17 reviewers)

- Specific Strengths
  - Offers a way of gaining a fundamental understanding of mechanisms responsible for trapping of NO_2.
  - From a scientific point of view, the research on oxygenates is highly interesting.
  - Building upon the database already assembled to create the surrogate fuel kinetic model. Array of capabilities and supporting facilities that are brought to the creation of the kinetic models.
  - This work provides good understanding of the kinetics of fuel combustion.
  - The drilling down in the levels of complexity through the system is rather impressive. The ability to expand the research horizons and translate the work to explosives demonstrates cross-fertilization and open collaboration at government labs. This example provides a case study for why research and funding at DOE labs should be increased.
  - Focus on representative fuel surrogates. Proven track record.
  - Strong expertise on chemical kinetics modeling and computational facilities.
  - Good integration with industry/NL's and academia.
  - Interesting approach in modeling of surface chemistry for NOx adsorbers. Basic chemical models may be instrumental in understanding combustion.
  - Computer capabilities.
  - Excellent fundamental/practical approach that is essential for developing successfully a clean and efficient combustion system
  - Strong research group and good collaboration with the experimental measurements.
  - Outstanding research activity throughout the last few years that few in the U.S. are capable of performing from an engine-relevant perspective.
  - The Livermore group is renowned for their development of chemical kinetic mechanisms. Everyone uses some form of a Livermore mechanism. I hope to see them continue this kind of work in the future.
- Specific Weaknesses
  - Surrogate fuels still not identified. This is a formidable task, but if any group is going to make it, it's the LLNLs. Research ought to focus strongly on this task and less on oxygenated fuels, considering their rather modest significance in today's (and most likely mid-term future) commercial fuel industry.
  - The detailed kinetics of fuel combustion are only of relatively minor importance to improving engine

combustion and emissions.
- May need to do a better job using the results.
- The next steps should be modeling the systems at temperatures that are closer to practical scenarios to avoid classic comments from experimentalists that activation energy at low temperatures in a gaseous state does not reflect actual experimental conditions.
- It's not clear how this work will get implemented into a new KIVA sub-model, for example.
- Difficult to determine the outcome of this research program. Appears to be pioneering work but the connection to DOE goals was not obvious. Probably needs additional industry direction to focus the research.
- Lack of a systematic approach to mechanism development.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 10 of 17 reviewers)

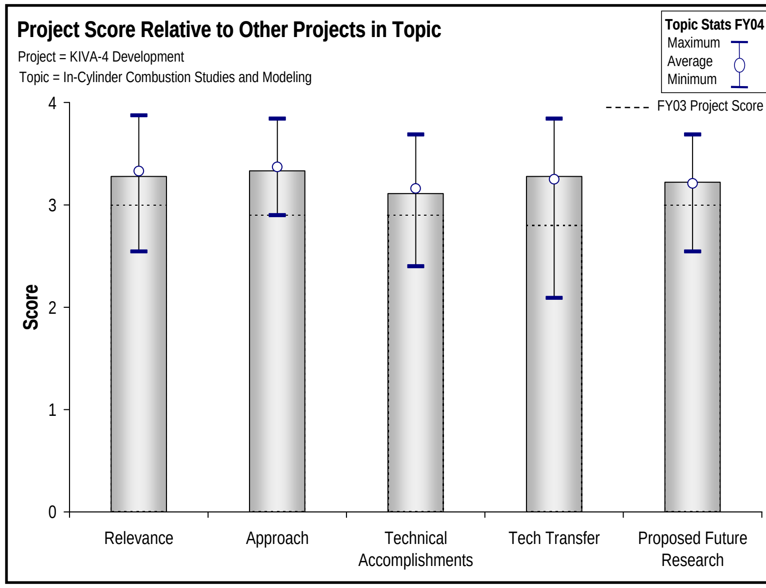
- Focus effort on identifying suitable surrogate fuel for gasoline, diesel, and any other relevant fuel.
- In response to the question of whether to continue the MD simulation of adsorption on LNT catalysts, this work should continue and the interaction with SO_2 and the impact of high temperature (if possible) should be considered.
- With regard to using a carbonate as a surrogate for biodiesel specifically and esters in general, the researchers may like to examine the different chemistries and electron densities in the two functional groups and demonstrate this is the best molecule to work with. Have the researchers considered ethyl acetate? The branching ratios might be different when cleavage is non-symmetrical. It would be interesting to look at trajectories of NO_2 on the surfaces and examine the average population at a certain temperatures.
- Forget further oxygenate studies - new insight opportunities seem scarce.
- Don't see the priority for work on oxygenates. As PI identified, interactions with universities (U of M, ERC) and other labs working on LNT shall benefit all the programs.
- It would be nice to develop a technical roadmap for better kinetics, thus leading to sub-models for use by industry/others. I think CLEERS is a good opportunity to build the kinetic databases for aftertreatment. Perhaps the combustion CRADA should formulate some approach to get a database for in-cylinder kinetics.
- Workshop mentioned above with experts coming from industry and academia.
- Introduce a systematic mechanism development approach into the projects. At the next review provide a clear framework for the future directions of the whole modeling effort.
- Would like to see a plan for who is going to do the surrogate testing and how the testing will be compared to the modeling.

In-Cylinder Combustion Studies and Modeling

KIVA-4 Development, David Torres of Los Alamos National Laboratory

Brief Summary of Project

KIVA is used extensively at universities and some industry for engine modeling, and is an open-source code for modeling. The current work revolves around development of unstructured meshes for the grid generation, which can provide increased accuracy and can be generated more easily. This work was designed to accomplish the unstructured meshing with minimal impact on computational speed.



Question 1: Relevance to overall DOE Objectives (Written responses from 13 of 18 reviewers)

KIVA is generally accepted as quite relevant to DOE objectives by these reviewers. KIVA is still widely used in universities, laboratories and industry worldwide to develop clean, efficient diesel engines, and has a long track record as a reliable, useful engine computational tool, thus clearly fitting the overall DOE objectives to assist in advanced engine development. The tool is felt to be very useful and the KIVA-4 represents a good improvement in the computational field. KIVA has become the standard for simulating DI engine processes, said one reviewer, who went on to say that expanding its capabilities will have extremely important benefits for design and development of more efficient, low-emission engines and moving to an unstructured version of KIVA-3V will enhance efficiency and accuracy of mesh generation for complex engine geometries. A predictive combustion simulation tool for 2010+ conditions is crucial for optimizing future engines in the opinion of one reviewer. The open source nature of the code was noted by several reviewers, who commented that the development of open code is a noble and needed function for DOE (and if linked with the model's ultimate use, the code is relevant to the DOE's objectives). The big advantage of this project to one reviewer is that it provides an open source analytical tool for the engine research community to conduct combustion modeling, which enables new models to be tested on a broad basis. This project seems to have quite a bit of return on investment, noted several reviewers. The principal investigator has done an outstanding job in modifying a very difficult and lengthy combustion computer code to include improved mesh structures and computational performance, but it is too early to determine if these improvements will aid engine designers (this will be more evident as the updated code is distributed to various organizations). One reviewer said that the objectives were excellent and focused, and that this modeling is a national core competency that is worthwhile to maintain. The project is focused on developing reliable tools that would eventually lead to development of clean, high efficiency combustion systems, and many lessons learned have been applied to this well-thought out new code. The improvements in KIVA to create the version 4 code should be useful to modelers at universities, labs and in industry.

Question 2: Approach to performing the research and development (Written responses from 11 of 18 reviewers)

Most reviewers felt that the approach was appropriate and solid, using previous work and making refinements on the known issues. One reviewer noted that this principal investigator is probably one of the few researchers in the country qualified to carry out this type of work. Another reviewer noted that the team has presented a very organized approach to addressing the needs of their users. They have focused their limited resources on achieving the stated goals of KIVA-4. The goals were well defined to address specific problems with KIVA-3 and to make practical and useable improvements. Modifying the well used KIVA is a good choice, in the opinion of a commenter. This reviewer also said that it appears CHAD was just too complicated to get wide usage, and that going to unstructured meshes is important. Furthermore, good documentation is crucial and modifying the code to work in a parallel environment is a high priority. A reviewer highlighted the project team's activities in developing an unstructured mesh capability by permitting multiple cell geometries, while maintaining efficiency and accuracy. A commenter said that the various approaches undertaken in the development of unstructured KIVA-4 address some of the shortfalls of KIVA-3. This was echoed in the comments of another reviewer who said that key deficiencies of predecessor (KIVA-3V) have been identified and are being addressed in the development of the new code. However, possibly due to insufficient resources, certain areas are not being addressed to the extent that would be desirable, such as grid generation and post processing. A reviewer was not clear on how this new KIVA release will incorporate existing sub-models and also include current work on HCCI and detailed chemistry. Finally, a reviewer added that some good modifications have been made to the code, but to make this really useful, the team needs to parallelize.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 14 of 18 reviewers)

Most reviewers felt that progress on this project was good or excellent (especially given the short time and small investment), in that the team has completed the majority of code development and a beta version is ready for release. One noted that given the fact that the results presented so far have essentially been achieved by a single full-time staff member at LLNL, the progress is outstanding (but it would probably make sense to allocate more resources to this effort). Another reflected this view in saying that significant improvement in the model was achieved with little loss in processor time, all with what sounds like a modest-sized team. This is a significant effort. A third reviewer said that the team members were very practical and organized in their work this year.

Several reviewers mentioned unstructured grids as a key point. One noted that an unstructured KIVA tool would be welcome, but asked if it will include advanced sub-models. This reviewer also asked if there are benchmarks on real engine simulation case studies, and if LANL has a plan for building a KIVA tool for 2010 and beyond. Another reviewer felt that development of a code using unstructured grids is the right direction.

The work was characterized as being a very useful addition to the capabilities of the previously developed tools. A reviewer highlighted aspects of the work, discussing the identification of two strategies (two KIVA versions that had too low efficiency) that did not provide performance in unstructured calculations. Based on this the team developed a scheme for KIVA-4 that meets the performance requirements while achieving unstructured computation, understanding the need for code that is no more than 10%, but more likely only 5% slower than KIVA-3. This reviewer mentioned the plans to distribute a beta version in two months.

Much effort has been spent by the principal investigator (noted one reviewer) in including more flexible meshing in an important engine combustion code used by many parties. There still seem to be potential issues in using commercial meshing codes with KIVA-4V, but the PI is aware and believes they will be overcome with time. Another reviewer said it is good to see that KIVA 4 will be coming out soon, and that KIVA-4 will be compared in performance against KIVA 3 in its ability to predict combustion process and emissions. It was not clear to this reviewer how KIVA should have coordinated validation with industry and academic partners.

Finally, one reviewer noted that the team still needs to test several features (what percentage of degenerate cells are too many, for example). Another felt that progress on modeling development has been slow, and that the redirection back to KIVA has been wise.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 13 of 18 reviewers)

This project includes very good coordination with industry and research institutions involved in multi-dimensional spray combustion simulation, in the opinion of several researchers, and collaboration with other government labs was judged to be good as well. One reviewer said that the key academic institutions were involved, but this commenter was not clear about how other partners are contributing to the development of KIVA-4. One reviewer said that the mix of collaborators was right, but the team should consider the addition of John Abraham from Purdue. Several reviewers noted the efforts by the team to contact and work with parties interested in testing the beta version of the KIVA-4 code. It was particularly impressive (in the opinion of one reviewer) to see how the researchers were engaging the scientific community at large and allowing the whole community to test and avail themselves of the code. The suggestions from users were readily incorporated in a new version of the code. It was obvious to one reviewer that there is much interest from industry and academia but this researcher was not sure there is strong collaboration. Perhaps it is a question of resources available to do this work. One reviewer said that code transfer with good documentation is important, and appears to be on track.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 13 of 18 reviewers)

Reviewers had several suggestions to improve the future work plans. In addition to comparing to KIVA-3V, one reviewer suggested the team compare KIVA-4 results to experimental results. Another reviewer felt that there is a clear direction to distribute a well documented code that works well in the full engine modeling environment, and this would be the best choice for future research directions. Another reviewer said that the team needs to ensure feedback from partners in both academia and industry. The next steps appear logical but additional resources would be helpful, said a reviewer. One noted that it was a good idea to add examples in the suite of information to be distributed, and another said that documentation and test examples can be essential to the continuous progress of the tools. One reviewer highlighted the plans to test out the code in beta version with outside partners and debug features to enhance operability, and the efforts to parallelize and release a parallel version as an update.

Some reviewers noted the project is coming to a close, and offered suggestions for close-out tasks. One reviewer said that benchmarking will be concluding soon, documentation is under development, and benchmark cases with industry and universities will begin. These items should properly conclude this project; relevancy will be addressed later as industry and various institutions evaluate the new unstructured code. Another felt that the research team is doing a good job finishing up all the details. One reviewer said that further refinements such as bowl snapping, moving valves, interface with other meshing tools (strategies), and more validation are essential for the success of KIVA-4.

Other comments on the future plans included a reviewer's opinion that helping the users interface with the new software is critical and the principal investigator has laid out plans that clearly move to expand in this direction. Another noted that an unstructured KIVA tool would be welcome, but will it include advanced sub-models? Are there benchmarks on real engine simulation case studies? Does LANL have a plan for building a KIVA tool for 2010 and beyond?

Specific Strengths and Weaknesses (Written responses from 14 of 18 reviewers)

- Specific Strengths
  - Open source code (cost, licensing etc., implementation of in-house models).
  - Wide user base.
  - Good long-term track record of KIVA.
  - Building from KIVA-3V, a program widely used in lab, university and industry for engine modeling.
  - Improves on a good tool.
  - Captures technology developed in previous projects (i.e. CHAD).
  - Improving KIVA code is valuable for universities, laboratories, and industry.
  - Flexible.
  - Have improved code without sacrifice to execution speed.
  - Quite open to suggestions from users and incorporation of desired additional features in the code.
  - KIVA-4 seems like worthwhile update for engine CFD calculations.
  - Unique capability and much needed for future engine developments.
  - The development of a reliable effective tool for modeling in-cylinder processes.
  - This project provides a needed unstructured mesh capability for KIVA that should allow more accurate assessment of complex combustion chamber geometries.
  - Excellent resources available to develop codes and models. LANL is good at this.
  - LANL has the lead group, which has the expertise and tools toward development of KIVA-4.
- Specific Weaknesses
  - Lack of personnel.
  - Increase the effort and funding.
  - Low level of support. Also the need to keep focused on the main tasks. I think they have done better at this in the past year, though.
  - Support?
  - Documentation.
  - Grid generation (ICEM planned to be tied in, but…)
  - Post-processing.
  - Code validated by comparing to previous version. Is there other data (may be experimental) to compare to

calculations?
- Still has some limitations.
- Lacks parallel computing capability, which is essential during optimization studies.
- Not a clear road map - there is a tremendous amount of in-cylinder work ongoing - there should be a plan and funding to capture these results into our simulation models.
- This work needs to keep on focus and not try to jump to far ahead.
- Integration of commercial meshing codes may be an issue.

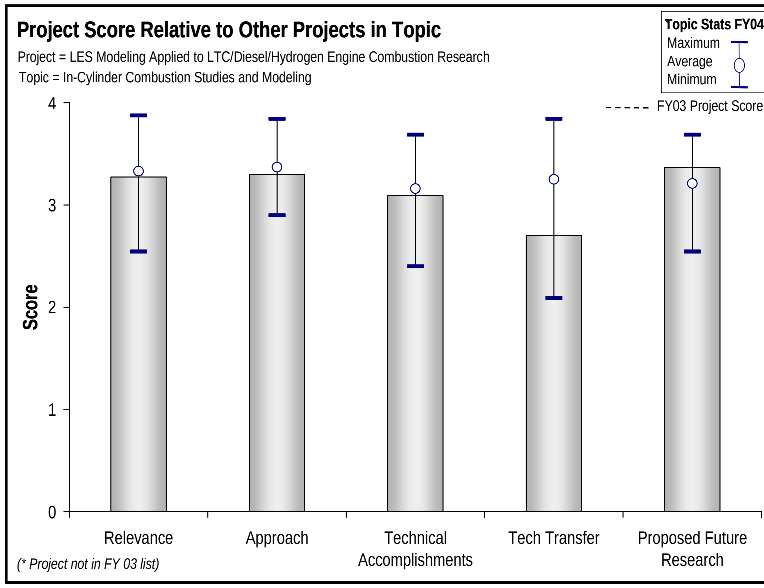
Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 12 of 18 reviewers)

- Allocate additional staff, put stronger focus on grid generation and post processing.
- Parallelize code. Gridding programs. Both are part of future plans.
- Create a converter to permit earlier-version files to be used with the new code.
- Has the DOE ever considered a modeling/simulation center of excellence to consolidate and complement all the modeling/computing efforts?
- Continue work with goal of reducing issues.
- I recommend adding more sub-model development, perhaps including some of the HCCI CRADA activities, perhaps a new spray model based on SNL and ANL data.
- Obviously, this reviewer is an advocate of engine simulation and its value to R&D and DOE's OFCVT mission. Very good presentation of a challenging subject to a wide audience. Open for further industrial collaboration? Some type of intellectual property protection for DOE / Federal Government in contrast to transferring it
- Continue the interaction with industry and promptly distribute versions of the code.
- Keep.
- If the program really is winding down, then continue completing the details. If the program is going to continue, they need to define some new goals and objectives.
- Needs more code validation and quality assurance tests, close ties with beta evaluators and set up a closed loop correction procedure.

LES Modeling Applied to LTC/Diesel/Hydrogen Engine Combustion Research, Joseph Oefelein of Sandia National Laboratories

Brief Summary of Project

The key objective of this project is to use high-fidelity, large-eddy simulation modeling to complement combustion experiments to extract detailed quantitative data not otherwise available. The project team will be performing a joint analysis of the unsteady and transient in-cylinder processes in actual cylinder geometries over full engine cycles.



Question 1: Relevance to overall DOE Objectives (Written responses from 9 of 11 reviewers)

Reviewers were comfortable with the relevance of this project, stating that it is fundamental work that can help general understanding, and that the program has some relevance in that it could be used to improve CFD modeling capability. One reviewer felt that the project is complementary to the engine measurements at SNL, but does not stand on its own without supporting the engine studies. One reviewer stressed the importance of credible modeling being performed in conjunction with ongoing experimental efforts in LTC combustion. Another felt the work was a good and necessary addition to ongoing experimental work. Still another thought the project is “a perfect fit” but felt the scope and budget cast some doubt on the expected results. The last reviewer had very detailed comments stating that this new project is focused on modeling a hydrogen SI engine with LES. This CFD technique is very time-intensive but is advertised to more accurately handle turbulence in comparison to standard KIVA approaches. It was not apparent to the reviewer whether this type of project will contribute to future engine design, but he felt that time will tell whether the trade-off in supposed turbulence accuracy is worth the associated computational time scales.

Question 2: Approach to performing the research and development (Written responses from 8 of 11 reviewers)

Reviewers felt the approach was satisfactory and that the researchers have taken a systematic approach to the problem followed by a good work plan. One person stated that this is an appropriate improvement that is the best next step in engine modeling. One reviewer cautioned that in order to properly initialize the flow field modeling the intake stroke must be modeled as well. One reviewer felt that the approach is good, but was not sure how well the audience understands the approach and what the program is trying to achieve. He felt that it would be good to provide a little background info for the uninformed.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 8 of 11 reviewers)

Reviewers seem generally satisfied with progress and milestones achieved (on time) for the funding level. One reviewer commented that this work has made a lot of progress in its initial months, has built on a large amount of background work, and has multiple resources in place. The program has a consistent flow even though the principal investigator has moved from one place to another. One reviewer felt that the LES code appears to represent a very refined approach compared to most other methods currently being used to simulate flows and combustion in internal combustion engines. However, they have concerns that there seems to be quite limited validation with experimental data of engine-relevant conditions.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 7 of 11 reviewers)

One reviewer felt there were solid H_2ICE partners and relevant work in place, while another acknowledged that one engine manufacturer is involved, with the potential for more. One person commented that several collaborative efforts were described, centered mostly around getting data to model, but they felt that it would be useful to get the code developers at LANL and the universities more involved. The final reviewer simply stated that the effort here appears to be very rudimentary at this point.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 6 of 11 reviewers)

Reviewers were comfortable on the relevance of the future research. One reviewer acknowledged that further validation is planned, but added that more information on what the H_2ICE development involves would be desirable. He wondered about using hydrocarbon mixtures and which chemical kinetic mechanisms will be utilized. One of the reviewers felt that the proposed work is well tied in with experimental work at Sandia. The final reviewer stated that there appear to be opportunities to move this forward and broaden the range of work.

Specific Strengths and Weaknesses (Written responses from 8 of 11 reviewers)

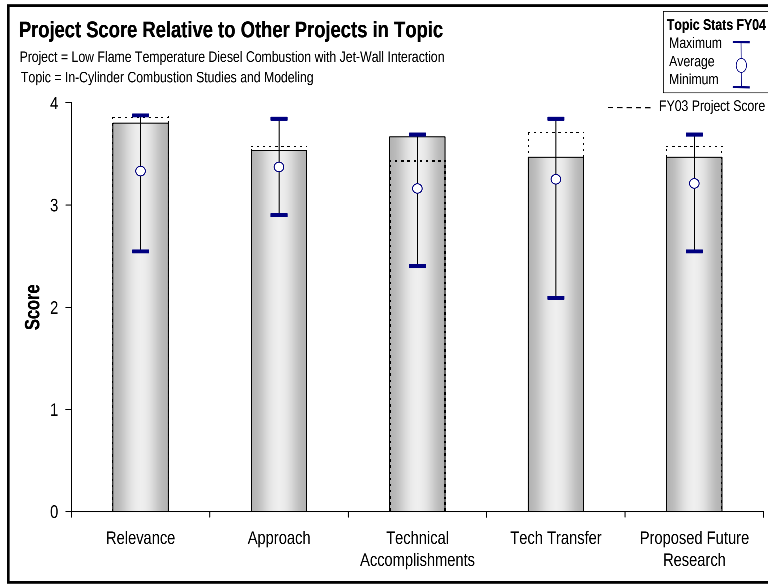
- Specific Strengths
  - Rigorous modeling approach.
  - This modeling technique seems powerful and useful.
  - Concerted effort of experimental testing and numerical modeling.
  - The support of the experiments.
  - Fresh work into challenging area where limited work is being done.
  - The primary strength of this project is the intimate working arrangement with all the engine measurements and a very experienced numerical working on the project.
  - The relationship with one OEM will be of great value benchmarking the CFD model.
  - This is a unique piece of work which requires the resources of a National Lab. The results could be very useful in developing submodels for CFD codes.
- Specific Weaknesses
  - Too little focus on hydrocarbon fuels.
  - Too little focus on quickly generating complex geometries.
  - Too little interaction with other partners.
  - Does this simulation stand alone or can this tool also be used by the industry?
  - It is not clear that there will be good applicability to hydrocarbon fuels, since hydrogen is an impractical fuel.
  - Speed and scope may be limited due to low funding.
  - Very weak approach to rolling out the software to industry.
  - Time will tell if this approach will become a practical engine design tool.
  - The modeling approach is very complex. The work described here uses hydrogen as the fuel which greatly simplifies the chemical kinetics part of the simulation. Going to a hydrocarbon fuel would extend the already long run times.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 6 of 11 reviewers)

- Having such a solid modeling tool and expertise in-house, it would make a lot of sense for Sandia to tie this activity to experimental turbulence measurements, such as those conducted by Paul Miles, to some extent.
- Does everybody agree this project should focus on hydrogen rather than on hydrocarbon fuels?
- The real problems associated with hydrogen combustion are infrastructure and storage. Until these issues have been properly addressed, the resources in this project are best spent looking at hydrocarbons.
- Continue to work the process and make it relevant to this underserved area.
- Is this competing with KIVA-4?
- Will it give further insight that is not available elsewhere?
- Not sure of the value of this work in the context of the big picture.
- More suitable for an NSF grant?
- Please develop a plan for rolling out and testing this software in industry.

In-Cylinder Combustion Studies and Modeling

Low Flame Temperature Diesel Combustion with Jet-Wall Interaction, Lyle Pickett of Sandia National Laboratories



Brief Summary of Project

The SNL team is examining the effects of fuel type on soot production and the effects of low flame temperature diesel conditions (including jet-wall interaction effects). These studies are being conducted in an optically accessible combustion vessel.

Question 1: Relevance to overall DOE Objectives (Written responses from 11 of 15 reviewers)

Most comments about the project were positive. One person simply stated this was small project, and was interesting work. Others added that this project is investigating new combustion strategies to reduce or eliminate soot and to reduce NOx; the in-cylinder advanced combustion work is highly relevant to the DOE objectives. Another positive comment was that this research is instrumental in understanding the fundamental processes underlying diesel combustion and the results will provide engine developers with a mental picture to guide their thinking. Others added that developing a better understanding of the low-temperature combustion modes will enhance the ability to develop advanced combustion engines, and that this is outstanding fundamental work to support and understand phenomena of "classical" diesel diffusion combustion. One reviewer suggested that it may be beneficial to look at high-load, multi-mode strategies. Several reviewers felt that the program pulls together many unanswered questions and begins to answer them in a systematic fashion and that the work capitalizes on SNL core competency. The final reviewer felt that overall this project explores combustion regimes that may help with simultaneous soot and NOx reduction and also on the effect of jet-wall interaction on soot. The latter study is not fully comprehensive since it is focuses on a very limited engine map regime; nevertheless is does open up the discussion of wall interaction-soot formation mechanisms again. The former is an important effort that may help with regeneration strategies and should be explored in much detail.

Question 2: Approach to performing the research and development (Written responses from 10 of 15 reviewers)

Most reviewers felt that the researchers had used a good, well-thought-out approach to use the injection fixture to understand the fundamental question of the onset of soot formation; however, some areas may need additional focus. One reviewer noted that new techniques for mixing and combustion are evaluated and analyzed; the goal of understanding and explaining the fundamentals behind the combustion modes was felt to be extremely useful. This reviewer supported the multi-year, long-term approach as shown in this project. Another reviewer thought the approach with the transparent box was very interesting and that the strength of the high-pressure vessel is being consequently used in this work. Another reviewer commented that the jet-wall interaction study could include more variation in the impingement-to-nozzle-diameter ratio. Experiments were focused on roughly a 280 ratio and pushing this limit down to 200 would be worthwhile since it will affect the mean jet fuel-air ratio at impingement. The final reviewer noted that the research team had identified the methods to produce low-flame-temperature, mixing-controlled combustion and generate little or no soot using an optically accessible combustion vessel. They have extended to high EGR combustion at temperatures below the soot inception limit and have investigated jet-wall interactions and jet-jet interactions by inserting a plate and a ceramic box into the combustion vessel, respectively. The reviewer was concerned that the studies of jet-wall interaction involved a cool plate (500K) which seems too cool to be relevant to a burning spray interaction with the combustion chamber of a diesel engine (DI or IDI) and wondered on what basis this temperature was chosen.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 8 of 15 reviewers)

One reviewer said the results were impressive so far, and another said it was "great work." A reviewer indicated the team has made excellent progress against the objectives: the SAE papers produced by this program are very useful. A reviewer commented that the studies on low-temperature diesel combustion have already contributed significantly to the understanding of soot formation mechanisms. This kind of information will be critical in designing future clean diesel powerplants. A reviewer pointed out that the team has identified regimes where low-temperature, rich combustion can yield non-sooting combustion under mixing-controlled conditions. Several researchers commented on the fuel jet work: one noted that the principal investigator provided information on how jets interact with walls and each other, while another said that the examination of jet-jet interaction and jet-wall effects is providing needed insight. A reviewer felt that the extension of the work to include EGR modes is significant. Finally, a reviewer said it is good that the PI is plotting his strategies on temperature-equivalence ratio plots, thus improving communication of what he thinks is happening in-cylinder.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 10 of 15 reviewers)

Several reviewers commented that collaboration was lacking. They went on to say that it is not immediately obvious that industrial partners are actively participating. One comment on this subject was that this project seems autonomous in nature; there appears to be very little industry interaction, but this might be necessary given the nature of this work. Others commented on the good collaboration with many players including international and domestic universities. One reviewer thought the new collaboration with IFP is a positive step. Another felt that the interaction is mostly through papers published in the literature as well as personal communications at the meetings. Another added that the PI has done a good job collaborating with industrial and university partners; he has collaborated effectively through the AEC MOU and also one-on-one. Another person added that this work is part of the SNL combustion CRADA, which has very good collaboration. The final reviewer acknowledged the researcher was part of the Advanced Engine Combustion working group and collaborates with industry and universities.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 9 of 15 reviewers)

One comment was that the proposed research involves applying advanced laser diagnostics to investigate the low-temperature limit of LTC. The residence time, fuel composition and injection rate are important factors that need to be considered. There would appear to be significant synergies with John Dec's work on HCCI (e.g. threshold temperature for CO burnout). One reviewer stated the plans are to identify the low temperature limit for sooting, impact of fuel composition and how mixing-controlled combustion limits at low temperature are similar to HCCI limits. Another reviewer felt the planned future work does a good job of using the fundamental understanding of soot and NOx formation in the equivalence ratio versus temperature space to guide the work. He continued that by answering questions as they pertain to the fundamental space, the researchers are providing information that is more universal and useful. One reviewer recommended mixing modes to expand the range, and adding a pre-mixed mode would help. Another suggested a closer planned linkage to modeling. Others were positive, one simply stating: "keep going." The final reviewer felt the researchers had good plans to determine effects of the low-temperature combustion on emissions.

Specific Strengths and Weaknesses (Written responses from 12 of 15 reviewers)

- Specific Strengths
  - Helps in obtaining a deeper understanding of various routes towards clean diesel combustion
  - Offers systematic study in well-defined environments.
  - Well aligned with industry research.
  - Interesting from a scientific point of view as well.
  - The detailed and very careful investigation of individual effects to address these important questions.
  - Work provided definitely a new understanding of jet-wall vs. -jet-jet interactions at diesel conditions. Work used an effective combination of different diagnostics which focuses on answering the key questions.
  - Good methods and systematic approach.
  - They have identified important combustion concepts for future low emission engines.
  - Good leverage to design of engine system.

- Good work on establishing soot-wall interactions and developing techniques that can have broad applicability to DOE's goals. Provides basic framework that can be helpful to the combustion community.
- Effective utilization of the experimental facility and excellent analysis.
- Experimental facility is fantastic and includes an outstanding PI who has shown a history of providing relevant engineering analysis of acquired optical data.
- A unique and well designed facility for investigating direct injection combustion phenomena. Excellent record for producing very useful results over many years.

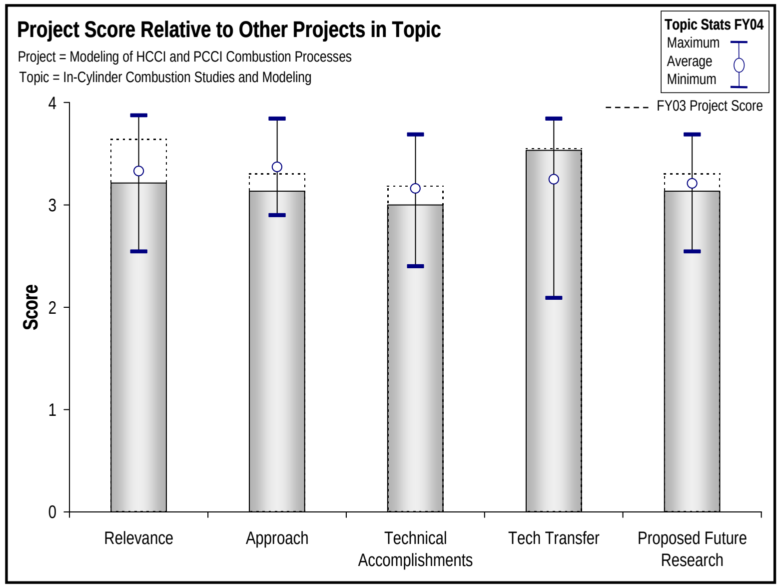
- <u>Specific Weaknesses</u>
  - Soot measurements involving wall impingement are inconclusive. In order to evaluate the influence of wall heat transfer on soot formation, some degree of modeling would be helpful in supporting the experiments. Effect of various methods on combustion and thermal efficiency not well-established
  - The wall-jet interaction work seemed to provide a rather trivial result that the flame would quench and that would shut down soot formation processes.
  - The spray-wall interaction studies ignore the very confined space in real engines.
  - The alternatives suggested all seem to be load limited, as are most advanced combustion approaches. Suggesting a means to increase load while maintaining low NOx/soot would be useful. Not including a total diesel engine cycle simulation is a weakness: for example, 5% oxygen suggests 75% EGR rates. This can be done at low loads but high loads make this difficult to realize. Consider mixing modes to expand range.
  - Expansion of the piston in real world applications may change the results through quenching of the reactions. Question of how much efficiency is lost through this low-temperature process. Need to verify which avenues can be taken from the "bomb" test to a diesel engine, additional guidance may be required.
  - Jet-wall interaction should include various impingement-length-to-diameter ratios to cover a more broad perspective. The original parameters were chosen to represent a heavy duty engine, but the ratio seems a bit high for current engines. This difference will affect the jet head fuel-air ratio at impingement and thus could impact PM formation behavior.

<u>Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 10 of 15 reviewers)</u>

- Take a step back and look at the various approaches in order to select a good candidate for testing in an engine.
- Perform modeling to quantify effect of heat transfer on soot formation and oxidation.
- Consider a range of wall temperatures in the wall-jet interaction to probe that interaction more thoroughly.
- Check out the effect of very high EGR (60% and above).
- Compare results to comparable engine experiments, tie in with other Diesel engine research programs at SNL, other labs, and involve industry partners more closely.
- Sandia needs to apply these low-soot, low-temperature combustion concepts to engines, especially one with optical access.
- I know that this would be hard, but it would be nice to look at opposed flame jets and soot formations at the interface. Also, fuel composition effects beyond oxygenates would be useful.
- Most combustion modes will be combined, so we can expect LTC to follow a pre-mixed heat release for example. I suggest altering initial conditions to reflect a pre-mixed heat release at the onset of the LTC
- Provide / develop the measure of combustion efficiency. Work on a bridge between the combustion bomb and more realistic conditions. SNL did so in the early 90's (Siebers - Dec collaboration.) It can be done!
- Expand jet-wall interaction study.
- I would like to see a little more effort to recognize the differences inherent in this experiment as compared to a real diesel engine combustion chamber. This is a minor thing, though.

In-Cylinder Combustion Studies and Modeling

Modeling of HCCI and PCCI Combustion Processes, Dan Flowers of Lawrence Livermore National Laboratory



Brief Summary of Project

The approach to this research is to apply multi-zone chemical kinetics models to understanding of low-load HCCI operation, and to extend multi-zone modeling tools to handle nonhomogeneous combustion regimes that are similar to HCCI. The team is performing both modeling and experimentation to understand the practical and fundamental issues related to HCCI combustion.

Question 1: Relevance to overall DOE Objectives (Written responses from 10 of 15 reviewers)

Reviewers were generally in agreement on the overall relevance of this project, noting that the project is providing an important basis for developing HCCI-like engines, and good work has been done in moving modeling tools forward. In addition, the title of the research fits “almost perfectly,” in the view of one reviewer. Other comments included the view that this work is addressing the need for practical ways to model HCCI / PCCI / SCCI-type engines, and that the work is directly applicable to DOE’s goals of low emissions and high performance. Another reviewer said that, in general, this project supports future HCCI R&D through simpler modeling approaches (relative to full computational fluid dynamics approaches), but that it appears much work is still required to address realistic fuels and to quantify the exact start of combustion. The view was expressed that to date, no credible modeling of HCCI has been presented, and that the work presented shows good progress toward achieving the modeling that will enable HCCI combustion systems to be designed and optimized. This was echoed by another reviewer who said that combustion simulation for HCCI would be great and the state of the art is currently inadequate, but these are perhaps the first few easy steps. A reviewer said that advanced combustion modes have the potential to enhance efficiency and reduce emissions, and understanding them is critical for development of future diesel engines. Another reviewer pointed out the studies related to the low-temperature and/or stoichiometric diesel combustion are quite relevant, in particular for light-duty diesels at part loads. One reviewer was not sure that the statement of work quite fits the title of the research.

Question 2: Approach to performing the research and development (Written responses from 10 of 15 reviewers)

Reviewers generally expressed the opinion that the approach plan and use of resources were reasonable, referring to the plan as following a reasonable path and being directionally well-thought-out. One reviewer said that by incorporating detailed kinetic modeling, high-resolution CFD, and engine experiments, the project offers excellent prospects of success. Among the high points noted by reviewers were the combination of modeling and experimental studies to use complex chemistry calculations with validation against engine tests; the good use of KIVA to predict preignition temperature distribution; and the subsequent use of the temperature distribution in a multi-zone, detailed kinetics model. One reviewer said that correlating models to the experimental approach was excellent, and was particularly impressed that the modeling and experiments seem to be well balanced. On the other hand, reviewers also offered suggestions for improvement, including the need to have more experimental data to validate simulations and the need for a list of expected and actual “deliverables” in the program. This reviewer said that the principal investigators are doing a lot of interesting things, but he had some trouble visualizing how the program has progressed and where it is going. A reviewer suggested that the approach could include a more realistic incorporation of heavier fuels and more focus on eliminating start-of-combustion perturbations due to assumed equivalence ratio. Another said the approach described for the homogeneous charge engine is understandable, but the approach for the non-homogeneous charge engines should be developed more. One reviewer felt the current work was good but the next steps (such as in-cylinder fuel injection for PCCI/SCCI) will be very difficult with this approach. A reviewer did not see a well defined technical approach to this problem.

According to him, this project needs a better focus in identifying the technical challenges and a comprehensive method of overcoming them, offered a final reviewer.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 8 of 15 reviewers)

Several reviewers felt that progress has been good and steady, and that there have been several worthwhile accomplishments. Incorporation of new data from Sandia National Laboratories was noted as a good accomplishment, along with results showing the impact of stoichiometry on pollutant formation within the chamber using the KIVA+multi-zone model approach, and demonstration of some effects of fuel type/chemistry on HCCI behavior. One reviewer offered the opinion that this was the first real modeling of hydrocarbon and carbon monoxide emissions in a diesel engine. On the other hand, a reviewer felt the work was still lacking from a fuel chemistry viewpoint, since the benchmarking to date has been limited to light and pure fuels that are probably not realistic. Since it is a new program, mostly in the literature review stage, progress is limited, said a reviewer. Finally, one reviewer emphasized that publishing papers is not a metric for performance, per se, a comment he felt should apply across the board to all projects. This reviewer added that the computational fluid dynamic results and conclusions seem difficult to substantiate, at least within the scope of the presented information. Also, the multi-zone model "full integration" seems to be an over statement and the transition point curve fit is not a viable approach.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 9 of 15 reviewers)

Reviewers liked the collaborative aspects of this project. One reviewer noted the excellent contacts and collaboration within industry, universities and national laboratories, while another talked about the extensive interaction with various industrial, laboratory and university partners and the significant and productive collaborations. Others noted the good collaboration with Sandia, some industry partners, and some university partners and the longstanding partnership with industry and academia, as well as the good progress in technical documentation. Coordination has been good with fundamental researchers at various universities and engine manufacturers that include a natural gas engine product portfolio, one reviewer wrote. A reviewer felt that the principal investigators seem to be working with academia, but this reviewer would like to see their advanced combustion and kinetics presented to Los Alamos for consideration in development of KIVA-4. Finally, a reviewer expressed the view that the non-disclosure agreement with Ford has no meaningful implication for tech transfer, nor does it show any interest from the industry. He went on to say that it was good to see collaborations with other labs, but the team needs to develop stronger association with at least one of the engine manufacturers to provide regular feedback on the progress of the program.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 9 of 15 reviewers)

Opinions on the relevance of the future workplan were mixed. Some reviewers felt the plan appropriate and the team to be moving forward with reasonable next steps. Aspects of the plan that were singled out for praise included: the move toward validation of non-homogeneous PCCI strategies;, the plan to look at high load HCCI; the validation of models for non-homogeneous configurations and investigation of these modes; the work to incorporate the KIVA and multi-zone models, and the study of practical strategies for combustion phasing in multi-cylinder engines. A reviewer offered that the team plans to use their expertise on chemical kinetics modeling - much of the input will come from other labs or OEMs that will define the technical tasks and guide the goals of the program. On the other hand, reviewers suggested improvements to the future plans, including closer ties with the diesel work being done at other labs (mainly the work at Sandia). Another reviewer felt that the relevance of this work to ground transportation is doubtful at this time, and this project should focus more on realistic fuels and resolving temperature and fuel concentration maldistribution issues with pressure rise. He also said that more attention could be paid to heat transfer effects. Another reviewer said that adding very early in-cylinder direct injection will make the kinetics expensive to retain (this reviewer was interested in following this). One reviewer said he either missed the goals and objectives of this work, or viewed it as a nice graduate work type of exercise. Finally, a reviewer was not confident that the best approach to simplify the modeling has been selected, as the results seem dependent on assumptions.

Specific Strengths and Weaknesses (Written responses from 12 of 15 reviewers)

- Specific Strengths
  - Excellent kinetic modeling.
  - Detailed CFD.
  - Sound approach to combine modeling effort with engine experiments.
  - Collaboration, combining simulation and experiment for validation.
  - Work is providing the fundamentals in the area of chemical kinetics for HCCI-type combustion.
  - Further development and application of detailed chemical kinetics modeling shall benefit our understanding on rich combustion and low temperature combustion regimes.
  - Uses tools that are accepted in the area of study and moves the work forward.
  - Carbon-14 experiments with dual fuels very nice. Should continue.
  - Practical approach to achieving HCCI combustion simulation capability.
  - Excellent modeling and result correlations. Development of the basic building blocks for this technology.
  - Very good approach incorporating CFD and multi-zone modeling toward answering HCCI combustion questions. Project leverages other DOE programs focused on fundamental fuel chemistry issues.
  - Strong background in chemical kinetics. They have access to this expertise and use it well.
- Specific Weaknesses
  - Transition point from CFD-code to multi-zone model still TBD.
  - Zones should exchange mass and energy.
  - Computationally costly.
  - It seems that relatively simple cases have been modeled.
  - Limited depth of work so far.
  - Transition between KIVA and HCT tricky - would be nice to confirm robustness.
  - Not being considered as part of KIVA4 development - could use some more links for eventual comparison to experimental set ups and actual engine tests (in-cylinder information).
  - Not sure how one progresses from steady-state conditions through transients. Mixing uniformity and interactions between cylinders may be an issue that should be looked at earlier rather than later. What level of control will be required?
  - Seems to over-simplify a very difficult phenomenon. Not sure what the end objective is.
  - Main weakness is lack of relevance to a practical HCCI combustion system - more effort should focus on practical fuels.
  - They should expand their approach to modeling. Don't just look at modifications to the KIVA / HCT multizone technique. It would be good to see some new techniques under investigation.
  - If the investigators have already developed a detailed multi-zone chemical kinetics (which the presenters claim predicted soot emissions identical to Toyota's measured data and explained the nature of the process) then what is the real motivation for this work? What goals this work will serve?

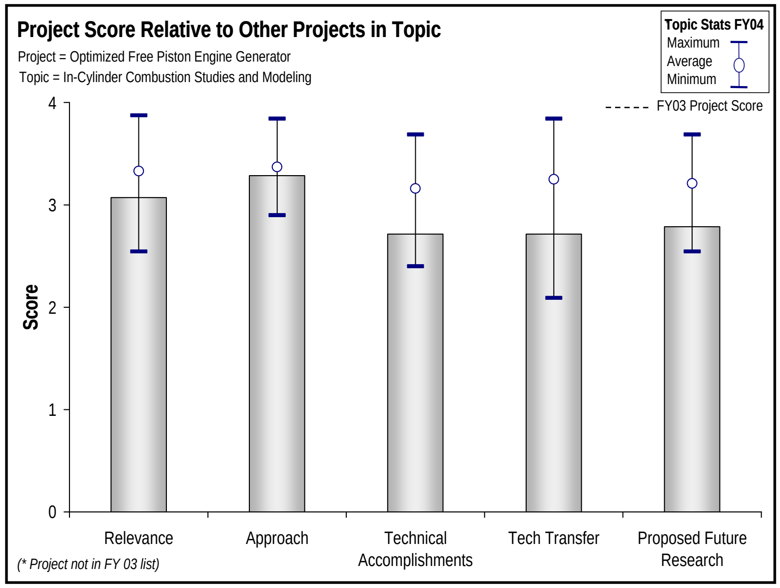
Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 8 of 15 reviewers)

- More work where simulation used to suggest experimental studies.
- Unclear how engine configuration guidance will be evaluated experimentally. This should be explained more fully in future presentations. How will the practical strategies being recommended by the modeling efforts be tested in experiments, if they involve changes in combustion chamber configuration?
- Expanding the work to other fuels would be valuable.
- Need a better definition of the work scope, technical approaches. Right now, investigators are trying to mix and match different pieces of work being done at different places. Don't see a strong contribution evolving from the center of this work!
- Expand commercial links.
- Would be very nice to look at dual fuel/multicomponent HCCI.
- I respect the research team to a high degree. I think they should refocus their work.
- Maybe DOE is better off funding UM to come up with the so-called "transition point" determination, if the premise of this work is valid.
- Do not get into ion sensing and/or C-14. This is a diversion of the effort and validates the need for refocus.
- Use the team's CORE COMPETENCY in Chemical Kinetics, etc. into a refocus effort, instead of conducting this type of graduate work.

- Focus on practical fuels and answering thermal and species maldistribution effects on combustion (pressure rise).

In-Cylinder Combustion Studies and Modeling

Optimized Free Piston Engine Generator, Peter van Blarigan of Sandia National Laboratories



Brief Summary of Project

The SNL team is developing a free-piston engine that can operate in HCCI mode to demonstrate increased efficiency and reduced emissions. The engine employs a linear alternator to transfer power from the pistons to a load.

Question 1: Relevance to overall DOE Objectives (Written responses from 11 of 14 reviewers)

Reviewers were essentially positive about the relevance of this new, advanced-concept engine development project to approach ideal Otto Cycle performance, which may provide important information for advancing to practical HCCI engines. Several people commented that it was an interesting project with a very unconventional approach; the project has high chances for success and also high risk. One person added that there is much work required to see any benefits. A reviewer said that the project does not focus on advanced combustion regime engines, but has many interesting characteristics. Others felt that this program is relevant in that it proposes a clean, efficient combustion system resulting in a high-efficiency method for generating electric power. Some reviewers were not sure what it can be used for if it is successful. They added that it is nice to have a diverse portfolio of projects including these high-risk investments. They felt that it is very positive that high-risk technologies are about 10% of the total. One person added that we need to understand fully how this approach compares to others. The final comment was that opposed-piston, linear alternator technology has potential to offer higher fuel efficiency than standard SI technology at low NOx, but faces stiff competition from both standard genset DI diesels and natural gas engines. It was also deemed questionable that this technology is easily scalable for ground transportation.

Question 2: Approach to performing the research and development (Written responses from 10 of 14 reviewers)

Reviewers found the approach to be strong overall, one stating that the researcher had taken an effective approach to overcome practical and technical barriers. Reviewers described the approach as very solid and systematic, well planned and executed, with a good combination of advanced simulation tools. One person commented that this approach addresses some of the basic difficulties with the reciprocating engine technology. It raises unique difficulties for its own technology; however, reasonable approaches to solving those difficulties are presented. One reviewer noted that each component of the free piston system was considered carefully, adding that using modeling to guide decisions was a good idea. However, another felt that the theoretical analysis and simulation should be used more intensively and more broadly. Another wrote that the project realized the potential benefits of avoiding the slider-crank limitations on compression and handling high-pressure loads with a goal to reach efficiency greater than 60% using a high compression ratio (about 30:1) and an equivalence ratio of about 0.4. A negative comment was the slow schedule for the project – nine years. Another reviewer added that the approach is good and really in the early development stages, considering little scavenging and fuel injection system work has been addressed at this time; these developments will be key in determining the final overall engine efficiency and combustion system behavior, and should be addressed as soon as possible. The final person commented that the program appears to be well-planned and the plans have been carried out over the course of several years.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 8 of 14 reviewers)

Reviewers noted the project has made slow progress, but has also had relatively low funding. One person added to this, stating that clearly the project has not had sufficient funding to progress at a more useful rate. Several people had positive comments, saying the project has clearly made progress since last year and has a definable direction.

It does not appear refereed papers have been presented on this approach; that would provide a wider critique of the approach. One person noted that early benchtop experiments without proper scavenging, cooling, and fuel injection systems have been completed with various fuels. Another person commented that there was a lot of work on the linear alternator and magnetic materials, which is not as interesting as the combustion related work but necessary. The KIVA program has been used for design of cylinder ports and for modeling the piston approach (compression and purge cycles). The final reviewer commented that this project seems more like an academic project and was not sure of commercial interest. The indicated efficiency of the free piston concept was found to be similar to a heavy-duty diesel, at about 0.7 g/hp-hr ISNOx in a 38 hp/liter power density. However, the concept offers to provide a projected 50% efficient electrical energy in a small package at low emissions which is interesting and may be worth looking into if the project plan is really technically reasonable/feasible. He added that attaining this will require a very efficient total system package, but based on the results so far he questioned the potential to achieve this target. The last question raised was whether the target efficiency of the generator was over 90%.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 8 of 14 reviewers)

Most reviewers found some collaboration with component suppliers but were not sure of the level. One person stated that he did not see the industry connection. However, others commented on the good collaboration with industrial partners. Another reviewer commented that this project has a long history of limited collaboration with industry, which may be acceptable given the scope of this project. One person added that the presentation did not show much industrial input in this project. The reviewers clearly want to see more collaboration in the future, especially with industry. One reviewer commented that, based on future collaborations aimed at prototype development, this could become outstanding. None of the reviewers mentioned university tech transfer or other relationships, past or planned. One reviewer commented that the researchers found good use of outside experts in the area of magnetic materials and generators, and the use of consulting houses to create prototypes.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 8 of 14 reviewers)

Reviewers look forward to construction of the opposed piston prototype, which seems to be the proper next step, to answer many fundamental questions, although they acknowledge that more questions will arise. Establishing a commercial linkage was suggested. The right technical areas have been targeted and depending on modeling results, the researcher may move from a single to an opposed piston. One reviewer felt that more time should be spent addressing key issues with this technology, including air handling, fuel system configuration, and cooling. Collectively these items could lead to an expensive engine with little fuel consumption and emission improvement over standard genset engine technology. One reviewer suggested he would like to see more info about the scavenging efficiency and closed cycle-efficiency. He went on to wonder what limits the efficiency in this engine, and to question how high the closed-cycle and scavenging efficiencies can go.

Specific Strengths and Weaknesses (Written responses from 13 of 14 reviewers)

- Specific Strengths
  - High-risk project that might have a payoff.
  - A new approach is opening our minds.
  - A creative idea and a company that should be able to provide a linear alternator.
  - Nice academic effort.
  - The long-term effort is a sign of commitment to the project objective and patience to do the job properly. Something this innovative clearly requires ample time to investigate the components and processes required to realize the engine.
  - Technical approach. This is a well planned and executed program. The work has spanned many years but the goals and objectives have remained clear.
  - Very careful analysis and systematic approach to the design.
  - The concept is innovative.
  - Novel approach - strong/robust development approach - not a “cut and try” approach.
  - Careful, well-thought out approach.
  - The experimental technique, and the potential for effective implementation of HCCI combustion.
  - One strength is the development of benchtop prototype. It does not include all relevant engine systems but is a good first step.

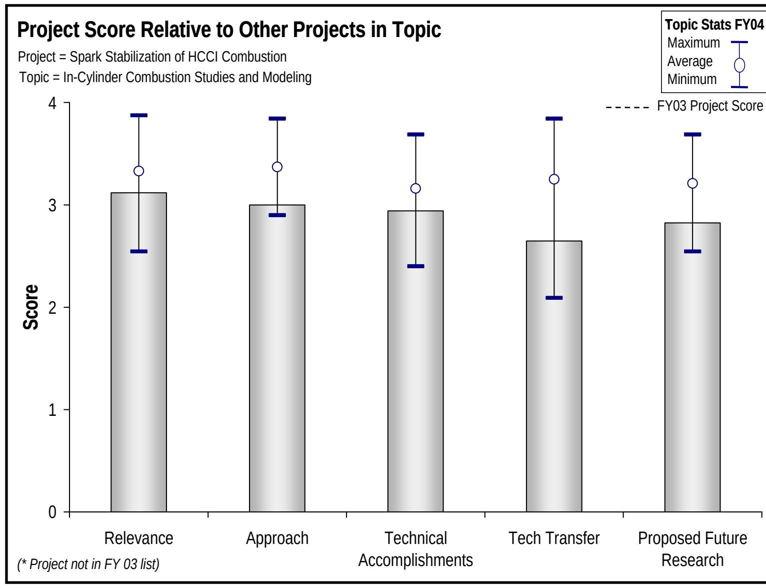
- Specific Weaknesses
  - Low interaction with engine manufacturers.
  - Project is risky.
  - None really, but much development is still needed.
  - The research is slow and will continue to be so. Also, there are many unsolved problems.
  - No commercial connection.
  - Twenty minutes isn't enough time to review results - gas sealing, lubrication, heat transfer and ultimate rejection.
  - More time should be spent realizing a final engine configuration in order to assess the real world performance of this technology. Again, air handling, fuel handling, and cooling are very important issues that will impact the performance of a realistic engine configuration.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 8 of 14 reviewers)

- Continue with work using his plan. Develop plans for continuous operation. I suspect efficiency will drop as parasitic losses of device and supporting devices will become more significant.
- None. Very interesting project and hope it results in a successful demonstration.
- Report figures on achievable mass and volume density.
- Explore the issue of fuel delivery to the combustion chambers very carefully. A low-cost method of providing a truly homogeneous mixture may be very desirable.
- Accelerate or stop.
- I would suggest a heat rejection test be shown that confirms all energy flows are being accounted for. I would look at combustion phasing impact - if heat release is complete much before TDC then there should be an opportunity to increase efficiency by retarding SOC - at 35:1 compression ratio I'm not sure how to do that - perhaps changing the fuel - or going to direct injection would be potential options. Direct injection would be the most straightforward approach, but then the same issues with a stratified mixture and diffusion combustion with NOx emission formation will appear.
- Spend more design time on the key issues.
- More investigation into what limits the efficiency and how much can be achieved realistically. Also, how do efficiency and NOx trade off?

In-Cylinder Combustion Studies and Modeling

Spark Stabilization of HCCI Combustion, Bruce Bunting of Oak Ridge National Laboratory



Brief Summary of Project

Through use of the AVL single-cylinder engine with variable valve actuation, the team will map the benefits of addition of spark to HCCI engines (especially as it relates to use during transitions). Additionally, the team will examine a new rotating-arc spark plug (RASP) and determine effects of the use of this technology on the HCCI engine operation.

Question 1: Relevance to overall DOE Objectives (Written responses from 11 of 17 reviewers)

Overall, reviewer comments were positive about the relevance of this project. A reviewer said this program is relevant in that it addresses stability and combustion control in HCCI engines. This is a good alternative to the challenges of lean aftertreatment, said another reviewer. A reviewer observed that this was a useful investigation into a key element of HCCI, and that the spark system is key. Controlling the phasing of HCCI is critical to incorporating it into advanced engine designs, said a reviewer, so this project contributes to the HCCI research. A reviewer noted that the team was trying to study HCCI combustion over a speed and load range. Another said the team was looking toward spark-ignited HCCI, and it would be nice to look into the control transition phase. This project is worthwhile (in one reviewer's opinion) since it looks at a complementary approach to control ignition through a high-power spark plug and very high trapped residual fraction. Results to date are limited and show comparable fuel consumption to a non-spark ignition HCCI engine, but increased NOx. More experimental work is required to answer the overall effect of the spark plug over a wider operating range since it seems only a few points have been explored in any detail. The work addresses some aspects of overcoming some barriers, but it has to be determined whether the rotating spark plug has an advantage. A reviewer summarized by saying that this is an interesting study that is limited in the results it can produce by the AVL HCCI concept: there are other means of inducing HCCI combustion. It is unclear that any of the engine manufacturers are interested in the RASP technology. No proof of value estimations (lower energy, better ignition, etc) was presented. This program aims to improve HCCI operation, said a reviewer, in particular transition from conventional diesel to HCCI operation, one of the technical barriers associated with HCCI, but he did not see the potential of RASP to meet these objectives.

Question 2: Approach to performing the research and development (Written responses from 13 of 17 reviewers)

Reviewers offered several comments in response to this question. One said that this was an innovative approach to improving HCCI capability. Another said this was a good approach that takes advantage of a potential new spark ignition system and VVT to push the operating limits of HCCI. He went on to say that the central focus of the entire program is to apply RASP on a single-cylinder HCCI engine. Another reviewer said the team was using good combustion diagnostics. One reviewer highlighted several areas of research, including the spark assist using rotating arc spark plug and considering fuel effects; use of the AVL Powertrain facilities, where there was an existing HCCI engine; evaluating the benefits of conventional spark plugs; modifying a head to accept the RASP; and using significant internal EGR for the engine. A reviewer asked how this work provides synergy with other HCCI work that has been funded by DOE. Further, he said that there was either no "designed experiment" or it was not obvious from the presentation. According to him, gasoline direct injection HCCI is a competing technology, world-wide, for fuel economy, CO_2 reduction and emissions reduction, and the team should consider working in this area vs. PFI. Another reviewer added that the combustion regimes (injection timing, spark assist and EGR) that are believed to be different from AVL and much of the rest of the industry. The approach seems to be predicated on using an untested spark assist technology and seems to have very weak justification, in the opinion of this reviewer. A reviewer suggested that the team look at the overall engine system more and consider the effects of operating conditions on the engine performance: the information that was shown was at a light load even for an automobile engine. Finally, a reviewer offered that some consideration should be also given to aftertreatment, there may be challenges in controlling A/F perturbations needed to get high 3-way efficiencies.

Reviewers' opinions were mixed on the issue of using AVL's facilities for this work. One said the work approach had merit, especially in leveraging this AVL resource. Another said he was not convinced the researchers made the case to do this work at AVL. There are pros and cons that the research used an AVL engine and facility, said another. A reviewer mentioned specifics: the test engine might be somewhat of a deficiency: how representative is the AVL SCE for this work? No HC emission information was given that relates to instability.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 11 of 17 reviewers)

Responses to the project's accomplishments were mixed. Comments included that this was excellent work and good results given the "small" funding level; this was a good first step; and that progress is good. The accomplishments so far are very beneficial in developing an applicable HCCI combustion engine. Another said that this research would be useful to advance HCCI combustion capability. One reviewer offered that the team has made good progress on the project, and the collaboration with AVL (who is subcontracted to generate single-cylinder results with RASP) really helped to move the project along quickly. Another reviewer pointed out several accomplishments: the team evaluated benefits of spark assist; demonstrated the benefits of the spark and showed clear understanding of impact of the transition to HCCI by varying exhaust valve closing timing. The information on transition would seem to provide important guidance on the practical implementation of HCCI. HCCI allows stable, high-EGR operation and the spark aids during transients. The team also showed correlation of peak heat release with MON rating of test fuels. The cylinder head is ready for RASP studies.

On the other hand, a reviewer felt that progress has been good but results have not purely shown spark assist with VVT to improve HCCI operating range. More experimental work is required to answer this question. Another reviewer characterized progress as being "not much," but the fuel matrix is "sort of interesting." Finally, a reviewer said that only one operating point was considered (or at least shown), and this reviewer was not sure if the conclusions are similar across the conditions.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 14 of 17 reviewers)

Assessments of the technology transfer for this project included that the collaboration with industry was "okay, but could be intensified;" that there was a good collaboration with an industrial partner; and that collaborative efforts could improve next year as more interested parties get involved. One commented that this work was unique in that it is primarily a one-partner project but also unique in its use of partners' resources. One suggested the team continue to share results, while another was curious about what the auto companies think of this work. A reviewer said that there was not much evidence of input from either engine manufacturers or system developers. The PI is working closely with a subcontractor, noted a reviewer, but interaction with engine manufacturers is lacking at this time.

Participation of an energy company was singled out by some reviewers. One said that collaboration or industry interactions are rather limited: a "major oil company" who assisted with fuel test planning/fuel blending is the extent of current cooperation, and the absence of HCCI players is obvious. Another was unsure that the gasoline manufacturers are directing the work or ensuring that the test engines are representative of what industry would target using current technology. Finally, a reviewer said that no information was given on who the collaborators are, but inferred that the participation of an energy company has been important.

Several reviewers mentioned the AVL connection, one saying that the work at AVL demonstrates the close coordination, and AVL appears to be fully supportive. Another said that the project team chose to have the experimental work done at AVL. This was probably more expedient and efficient in this case than doing the work in house since AVL had an existing engine debugged and ready to run. A reviewer noted that AVL is partner and subcontractor, an oil company is assisting with the fuel evaluations, and that there have been reviews by EPA and the Diesel Cross Cut team.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 10 of 17 reviewers)

One reviewer said the work was very relevant to future possibilities, and that there was good leverage to promote the understanding. Another said the future research is directionally very good but it would be helpful to explore a wider operating range. A reviewer suggested that the team quantify advantages of spark on load/speed, and it would also be nice to compare benefits of RASP with a regular spark plug. Another suggestion was that the team considers updating the test engine to something more representative if there are volunteers within industry. One commented that the team really needs a much better justification for investing all this effort in a particular spark technology. The team should ensure synergy among HCCI programs at DOE labs and university consortium. A reviewer offered that the future work plan should have more detail. This reviewer would like to see something that will demonstrate how this technique would be applied in an automotive engine and how the system would perform in a transient test. Finally, a reviewer said he saw no justification for going through a series of fuel matrices with the RASP system.

Specific Strengths and Weaknesses (Written responses from 12 of 17 reviewers)

- Specific Strengths
  - Using AVL resources in advanced engine to study the combustion process.
  - The partnership with AVL was clearly a wise choice due to the excellent capabilities of the single cylinder engine. This is moving to a practical implementation of "HCCI" type combustion and that is a significant strength.
  - Excellent leverage of AVL resource.
  - Access to AVL's single-cylinder engine with HCCI
  - A very interesting study, well designed and well executed.
  - Looking at transition conditions - which are often neglected.
  - Excellent initiative.
  - The integration of useful resources available at various facilities
  - There is an excellent test mule available to complete this work that is critical for this type of effort.
  - Good collaboration and use of existing testing facility.
  - Potential simplicity of aftertreatment system.
- Specific Weaknesses
  - This study is limited by the AVL HCCI concept in the results it can produce. There are other means of inducing HCCI combustion.
  - It is unclear how this engine concept will be significantly better than a conventional stoichiometric engine, although it will be more complicated.
  - May or may not be true HCCI.
  - Test engine set up and prototype hardware/technologies.
  - Gasoline direct injection HCCI is a competing technology, world-wide, for fuel economy, CO2 reduction and emissions reduction
  - The operating range of the engine was somewhat limited, the peak IMEP was 4.5 bar. This is not a high enough MEP to cover the FTP75 region.
  - There is nothing unique about RASP, one could find many multiple sparking devices that were developed in conjunction with lean burn SI engines, should the need for spark assist in HCCI arise.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 12 of 17 reviewers)

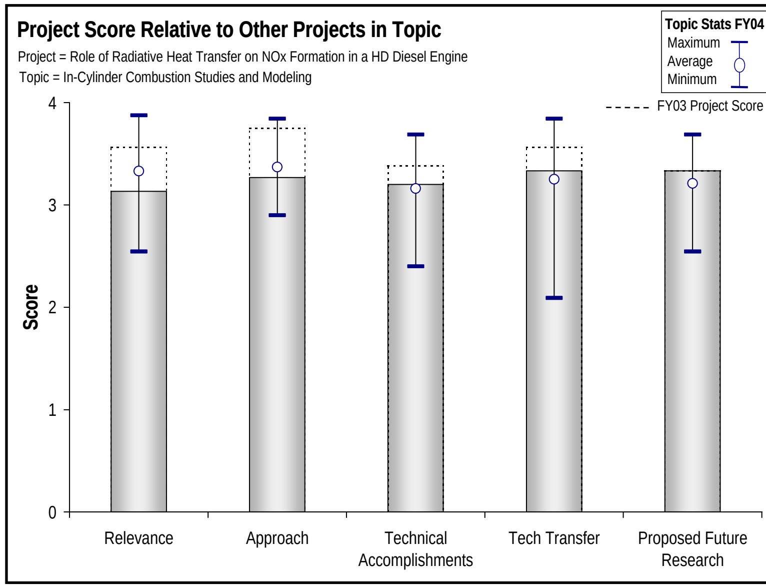
- Need to develop strategies for valving and assess if that can be implemented in a non-fully flexible system. This is probably beyond lab charter so you need to expand the participants. COVs and pressure rise rates seem a bit high to be practical.
- No mention of HC and CO emissions. If these are not also reported, they should be. It would be interesting to know whether the same behavior would be observed during the transition is external EGR was used instead of internal EGR.
- If funding permits, it would be useful explore other means of inducing HCCI combustion.
- Continue to develop the concept.
- More consideration to details of spark physics would be helpful.
- Include boost levels. Include simulation to guide experimental results, as well as to analyze the reduced

experimental data. Run tests at equal output / BMEP

- Good focus on Lambda = 1, to avoid need for NOx aftertreatment
- One comprehensive set of justifications for using RASP need to be presented. This does not mean experimental work. It refers to estimations of energy deposition, ignition probability, energy savings, etc.
- Future research should explore a wider engine operating map.
- Keep only if the program has synergy with other work at ORNL because the DOE total $ on HCCI need to be focused.
- Increase the range of operation to higher loads. Address how you would handle transient operation with this concept. Do you switch back to SI operation during a transient or do it in HCCI mode?
- Don't find technical justification to continue working on RASP.
- Would like to see aftertreatment and controls coupled with this project to show a complete system solution.

In-Cylinder Combustion Studies and Modeling

The Role of Radiative Heat Transfer on NOx Formation in a HD Diesel Engine, Mark Musculus of Sandia National Laboratories



Brief Summary of Project

In this project, the research team is updating the laboratory hardware and capabilities of the Sandia Heavy-Duty Diesel Laboratory and will explore factors that affect in-cylinder NOx formation under conditions with significant premixed burning. Premixed burning conditions will likely become important as companies move toward EGR and lean combustion to meet 2010 emission standards.

Question 1: Relevance to overall DOE Objectives (Written responses from 11 of 15 reviewers)

Reviewer responses to this question were generally mixed. They said the work is solid basic research in the area of "classical" diesel combustion (premixed), low-temperature combustion modes, and soot radiative heat transfer and the effects of compression heating of combustion products on NOx formation in heavy-duty engines, which is important to the DOE program. Reviewers indicated that a clearer understanding of in-cylinder combustion mechanisms is important, especially at low NOx levels, to better optimize thermal efficiency and integrate engine subsystems. This work provides some direction for reducing both soot and NOx during in-cylinder combustion, which should be very helpful in designing low-emission diesel engines. Alternatively, some reviewers felt the work was "an interesting scientific study" but poorly related to DOE objectives and showing only modest potential for reducing heavy-duty diesel engine emissions. The study seems to be more academic in nature since it focuses on a phenomenon that indirectly impacts engine control strategy. For example, if flame radiation does affect NOx formation, it has been neglected in the past and engine combustion system developers have addressed perturbations in NOx through changes in control strategy. It is not clear how understanding flame radiation effects will directly affect future control strategies in a manner different than today. Others said that while the project can support the development of advanced combustion regimes, it is not clear if this is the most critical issue or whether other barriers should be addressed first.

Question 2: Approach to performing the research and development (Written responses from 12 of 15 reviewers)

On the project's research approach, reviewer responses were also mixed. Reviewers praising the project felt that it has a good work plan that addresses the needs of the industry. They went on to say the approach employed a good mixture of optical and conventional diagnostics, and the new optical diagnostics are answering fundamental questions. One reviewer stated that the approach of correlating in-cylinder measurements with exhaust NO and applying 3-color thermometry were very effective for understanding premixed combustion. Another viewed the research as updating the SCE with the thought of bridging to LTC. Another reviewer stated that the project has introduced soot radiation aspects. Further, it was felt the approach simulated a "real-life" set-up. However, negative comments focused on the so-called "NOx bump." One reviewer said the research may have been sidetracked from program objectives by efforts to understand the NOx bump phenomenon. Another questioned whether investigating the NOx bump will contribute to developing low-temperature combustion concepts. One reviewer felt that two key elements were missing from the current approach: in-cylinder NO measurements and extensive CFD modeling. Further, a reviewer offered that detailed NO/NOx measurements should be coupled with in-cylinder optical diagnostics to understand NO formation. Finally, one reviewer felt that the approach is sound in general, but could benefit from the testing of a lower-sooting fuel (versus DF-2), possibly a hybrid diesel fuel.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 10 of 15 reviewers)

Some reviewers felt that the project has made good progress toward meeting the stated goals and in upgrading the common rail fuel system capability. Positive statements were made concerning the project's experimental analysis as well as additions to the scope including NOx analysis capability; a new high pressure common rail injection system; development of a three-color soot thermometry technique, and examined NOx formation using 2-color pyrometric data under large premixed burn conditions. Others would like to have seen more modeling prediction at this point in the project because of the importance of simulation to engine development. One reviewer stated that several project conclusions seem speculative (e.g., optically thin soot is cooler, and NOx is solely correlated with the temperature estimated from 3-color soot technique not accounting for any residence time effects). Another reviewer suggested that future work expand on the current evidence database supporting flame radiation effects on NO formation. Finally, it was stated that the NOx bump effect is probably not the best project objective for this facility. Additional publications were also deemed necessary.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 11 of 15 reviewers)

Reviewers generally agreed the project has had good collaboration with industry and academia. Several technology transfer interactions have been conducted and the project results can be used directly by industry in relation to current diesel combustion processes. The Advanced Engine Combustion Working Group collaboration ensures dissemination of results and consultation with industry, other laboratories, and universities. In addition, the researcher will be involving a UW student in modeling work on site. One reviewer stated a contrary opinion saying project has had "limited collaboration." Another reviewer expressed some uncertainty in regarding which industry partners have been involved in the project beyond the biannual reviews.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 11 of 15 reviewers)

Most reviewers agreed that the future plans of the project are generally in the correct direction and will further understanding of radiative heat transfer effects on NOx and soot emissions. The approach should include work with multiple injections and exploring injection timing concepts with emphasis on early-premixed injection and combustion. Other diagnostics should be applied to understand low temperature (EGR) early injections. The implementation of an HP-CR FIS is correct. One reviewer expressed uncertainty as to why the approach emphasizes radiation effects. Somehow radiation should be eliminated with a set of experiments to sort out its specific effect. Without these experiments, the proposed mechanisms will be unsubstantiated theories. It is also believed that there is no correlation between pre-mixed burning in conventional diesel combustion and HCCI/early premixed combustion. Another reviewer suggested that the project include a modeling phase to better explore/understand the phenomenon.

Specific Strengths and Weaknesses (Written responses from 14 of 15 reviewers)

- Specific Strengths
  - Given the right focus, the research could provide useful insight into processes relevant to low-temperature diesel combustion.
  - Good work, but I am not certain this is the main problem.
  - Project builds upon significant existing experimental capability.
  - Since the work is dealing with classical diesel combustion, it appears at first not to be spectacular, but it still deals with the primary path of improving current and future engines!
  - The optical engine is a useful tool.
  - Solid work, but perhaps not as glamorous as HCCI.
  - It has a significant legacy - and history of good solid work. This gives good confidence in the newer data and findings.
  - Excellent tools. The optical access to the engine is world class.
  - Probably one of the better projects at SNL at the present time.
  - Experimental technique used and effective analysis.
  - SNL has a good engine experimental group.
  - Great experimental and analytical capability that is not easily available at other domestic engine R&D facilities.

- The laboratory is in place, debugged, and has been producing good results for many years. One of the biggest strengths of this work is that it is not in a diagnostic development mode but in a combustion study mode.
- Unique experimental facilities and technical expertise; close cooperation with ACE.

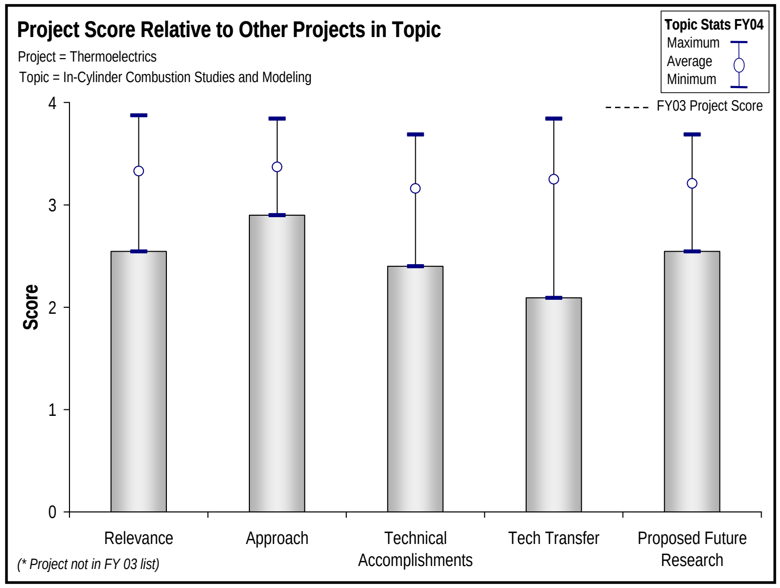
- Specific Weaknesses
  - How significant is the NOx bump? The operating conditions investigated are of limited relevance (e.g., high EGR rates would be desirable, in which case the NOx bump according to the investigator becomes less significant). Rather than using the three-color soot diagnostic technique combined with "back of the envelope" calculations, it would seem beneficial to apply the NO PLIF-technique utilized in Chuck Mueller's SCORE lab to measure in-cylinder NOx. Modeling has not been given any priority so far.
  - The focus in this year seems to have been on an issue that is not particularly important to overcoming key technology barriers.
  - NONE, the engine deserves a modern HP-CR FIS now!
  - The project has involved investigating an unimportant phenomenon when there are much more important issues to be investigated.
  - Only one point considered, i.e., fairly low load (4 bar). The project does not have a clear objective, or perhaps not an objective that I see tremendous value in (i.e., NOx bump).
  - May want to step back from the research to understand where the project needs to go. Concern is that some of the work may be too focused on a small issue whereas there are major items to be solved that need attention.
  - Lack of numerical simulation, so far. UWM work in the future will help!
  - No concurrent modeling.
  - The impact of flame radiation on NOx from a big picture point of view is dubious. It is not fully clear that understanding of this mechanism will truly provide the engine R&D community with information for developing future engines.
  - Need to better connect the previous work to the future work. Specifically, how does the NOx bump work relate to the future work that is being proposed?

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 8 of 15 reviewers)

- Re-focus research on conditions more relevant to industry direction. Apply proper measurement techniques. Accompany experiments with detailed modeling.
- Move to more commercially relevant injection strategies (as planned). The investigation of the NOx bump seems a topic that is more suitable to a numerical simulation, since computation would allow the specific issues related to the reasons for the NOx bump to be exhaustively studied.
- Study the fundamentals of LTC with EGR rates of over 60% (no soot formation!). Industry should give more input to this project.
- The project should investigate combustion and emission formation during low-temperature combustion (high EGR) conditions, since these are low-NOx conditions.
- I would suggest looking at early injection leading to pre-mixed conditions/combustion/emissions. It is good that some modeling activity is being integrated.
- Add concurrent modeling and develop a direct industrial collaboration.
- Strong consideration should be given to experimental work on either a lower sooting fuel or a very low sooting operating condition.
- Combine with HCCI work where radiative heat transfer implications are more relevant than late injection. NOx bump is non- trivial! Efforts shall also focus on higher fractions of pilot injection at different injection pressures, different charge densities at SOI.

In-Cylinder Combustion Studies and Modeling

Thermoelectrics, Larry Olsen of Pacific Northwest National Laboratory



Brief Summary of Project

Thermoelectric materials are being developed to harvest waste heat from vehicle exhaust. In this project, the PNNL team is working on an approach to scale up production processes for these advanced thermoelectric materials using sputter deposition techniques.

Question 1: Relevance to overall DOE Objectives (Written responses from 9 of 11 reviewers)

Reviewers had mixed comments on the relevance of this project. One felt it addresses DOE's primary thrust of reduced dependence on foreign oil while reducing emissions. Another reviewer agreed, stating the project was relevant to thermal energy recovery from waste heat. However one reviewer disagreed, questioning how the project fits into the program. Another reviewer commented that while the risk is clearly high, the payoff for the country would be huge and the potential energy savings enormous. Other comments were more restrained, including one that the project must be combined with other technologies to get to the goal. Another reviewer commented that this is very fundamental research and has little chance to be transferred to the automobile industry. Another noted that the true energy efficiency will be ~10-15% since a 500°C temperature differential is improbable, leading him to conclude that the potential payoff was small for the level of effort required.

Question 2: Approach to performing the research and development (Written responses from 8 of 11 reviewers)

Reviewers' comments on the project approach were guarded. One reviewer commented that the researchers have an excellent vision of the pathway to market in identifying scale-up or micro-scale successes as a major barrier and focusing research on this aspect. One person commented that this work focuses on manufacturing process technology. He had to assume there are other programs elsewhere that focus on developing the materials and application designs, but asked for some references as to who is working on materials and designs. One reviewer questioned why the work to scale up production was much different from that done in the integrated-circuit industry, such as Intel producing millions of integrated-circuit chips a year. He went on to question whether there are deposition techniques other than RF that are cheaper and better suited to produce these materials at faster rates. Another reviewer questioned how this work relates to overall combustion goals. A reviewer noted that the work seems a straightforward application of sputtering techniques. The final reviewer commented that the research team seems to have a robust approach to verify claims that values of 2-5 for figure of merit are possible.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 8 of 11 reviewers)

Reviewers recognized some progress toward project goals but felt less sure about the progress toward DOE goals and how project accomplishments could be used. A reviewer appreciated automation of the large-scale sputtering of targets as an advance, especially the ability to use alternate substrates for increased performance and cost effectiveness. Another was encouraged by claims that 2-5 figure of merit are possible. Another reviewer questioned the expected efficiency at a temperature difference of 200°C.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 4 of 11 reviewers)

Reviewers did not feel they had a clear understanding of the technology transfer paths or the level of collaboration with industry, other DOE labs and universities. Two reviewers mentioned the solid interaction with the industrial sector, including Hi-Z.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 6 of 11 reviewers)

Reviewers did not feel they understood where this research, if successful, was headed. One reviewer questioned how this technology compares with others, and wondered how much power was possible. Another reviewer felt emphasis on the next crucial step of how to implement the thermoelectric devices within a system to maximize the efficiency was good; in fact this may drive the optimization of the thermoelectric device itself when the confines of the final application are applied to the potential device. Another felt that a demonstrator generator would be interesting.

Specific Strengths and Weaknesses (Written responses from 8 of 11 reviewers)

- Specific Strengths
  - This is a key process required for economic production of thin-film thermoelectrics.
  - Strong deposition team.
  - Smart people. Long term idea. May pay off, but a long way to go.
  - Driving the research away from the single-crystal studies to a more practically implementable system is commendable.
  - Fundamental approach to confirm capabilities of thermoelectric technology.
- Specific Weaknesses
  - Need to show how this could be implemented into a device.
  - No cost targets.
  - There appear to be many problems remaining in this research area.
  - Lack of clear target applications. How much energy may be available?
  - It may be due to industrially proprietary information, but there was little analysis of devices/films and actual results from experiments to support statements. Scrubbed data would have been extremely beneficial. For instance, showing that results are virtually unchanged upon testing at different scales.
  - Lots of specifics missing related to key fundamental questions.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 6 of 11 reviewers)

- Need to show data that demonstrate that their thermoelectric films actually work. Data seems to suggest results were estimated.
- [A reviewer suggested] urgently that the economic sense of this work should be checked immediately before the work be continued with the goal of the application for engines.
- What is the cost and the gain under the most optimistic conditions?
- There needs to be some cost/benefit analysis presented to put the technology in perspective to other technologies.
- Keep the perspective that this is very long term.
- The presenting of simple background material was essential to educate this essentially “tough” crowd who may not yet appreciate how thermoelectrics, once they are efficient enough, will be able to dramatically aid the engine community increase efficiency while reducing emissions.
- A discussion of the cost analysis to implement this device in the field would greatly stimulate the audience and pique their interest earlier on.
- Some mention of controls and precision needed to lay down a large area thin coating would be advantageous and set some of the context. Repeatability and reproducibility studies of film and device control would be extremely interesting and help in the drive to market.

This category includes projects involving research into advanced post-combustion emission control technologies. Devices being investigated to control NOx emissions include NOx adsorbers, selective catalytic reduction, and non-thermal plasma catalysts. Research is also being conducted on diesel particulate filters to control PM emissions. These technologies are being investigated both for light-duty diesel vehicles and for heavy-duty diesel vehicles. Research is also being conducted on how these NOx and PM devices will interact with each other in an integrated emission control system.

Below is a summary of average scores for 2004 for the ten projects in this category, along with the average, minimum, and maximum score for all projects in this report. The highest score in this category for each question is highlighted.

Summary of Scores for Projects in this Section

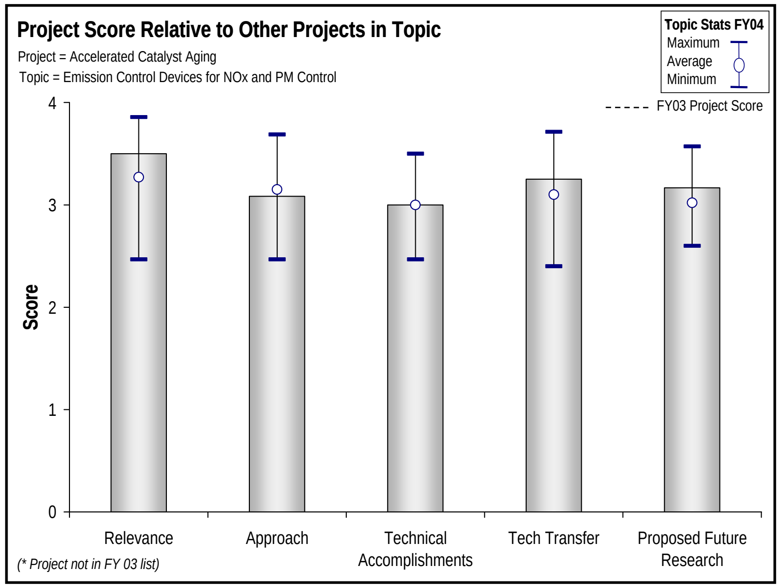
Page Number for Project Summary	Research Project Title	Q1 Relevance Score	Q2 Approach Score	Q3 Technical Accomplish-ments Score	Q4 Tech Transfer Score	Q5 Future Research Score
68	*Accelerated Catalyst Aging:* Bruce Bunting (Oak Ridge National Laboratory)	3.50	3.08	3.00	3.25	3.17
71	*Advanced NOx Control for Locomotive Engines:* Darryl Herling (Pacific Northwest National Laboratory)	3.06	2.78	2.83	2.61	2.78
75	*Bi-Functional Catalysts for the Selective Catalytic Reduction of NOx by Hydrocarbons:* Chris Marshall (Argonne National Laboratory)	2.47	2.47	2.47	2.40	2.60
79	*Characterizing NOx Adsorber Regeneration:* Shean Huff (Oak Ridge National Laboratory)	3.81	3.69	3.50	3.38	3.31
83	*CLEERS DPF Modeling:* George Muntean (Pacific Northwest National Laboratory)	3.36	3.29	3.14	3.43	3.14
86	*CLEERS Kinetics: Lean NOx Traps:* Stuart Daw (Oak Ridge National Laboratory)	3.86	3.50	3.15	3.71	3.57
89	*Dedicated Sulfur Trap for Diesel Emission Control:* David King (Pacific Northwest National Laboratory)	2.92	3.15	3.23	2.69	2.92
92	*Development of an Advanced Automotive NOx Sensor:* Larry Pederson (Pacific Northwest National Laboratory)	2.80	2.93	2.60	3.07	2.60
95	*Lean NOx Trap Chemical Behavior and Thermal Deactivation Effects:* Todd Toops (Oak Ridge National Laboratory)	3.47	3.33	3.13	3.20	3.07
98	*Mechanisms of Sulfur Poisoning of NOx Adsorber Materials:* Charles Peden (Pacific Northwest National Laboratory)	3.55	3.46	3.00	3.46	3.18
	Average Score for This Category	**3.28**	**3.17**	**3.01**	**3.12**	**3.03**

Overall Program Scores

	Q1 Relevance Score	Q2 Approach Score	Q3 Technical Accomplishments Score	Q4 Tech Transfer Score	Q5 Future Research Score
Overall Program Average	3.30	3.29	3.08	3.17	3.14
Overall Program Maximum	3.88	3.84	3.69	3.84	3.69
Overall Program Minimum	2.47	2.47	2.40	2.09	2.55

Emission Control Devices for NOx and PM Control

Accelerated Catalyst Aging, Bruce Bunting of Oak Ridge National Laboratory



Brief Summary of Project

In this project, accelerated aging of catalysts will be undertaken to determine effects of phosphorus and other contaminants on the materials for NOx adsorber catalysts. Thermal cycling effects will also be examined in this work.

Question 1: Relevance to overall DOE Objectives (Written responses from 8 of 12 reviewers)

Several people felt this is a key area and that an understanding of LNT aging and building protocols for effective accelerated aging is critical to implementation of LNT technology. One person felt the group has a strong understanding of catalyst durability issues. One reviewer commented that the important objectives of LNT are addressed. This reviewer added that accelerated test cycles under lab conditions could be a cost-effective method to improve development, but the main question is how realistic the test protocol is and how real driving conditions can be considered in laboratory testing. Another stated that the direction for this project is important for demonstrating the 120,000 mile durability for LNT devices, but to his knowledge, none of the industry is aggressively looking into the LNT durability at this point. The final reviewer commented that as soon as fuels are cleaned up, lubricating oils will have to be, too. He went on to say this work is “leading that charge” and with this understanding the ability to re-tune the engine for fuel efficiency and emissions becomes possible; hence this work ”does talk to the DOE's primary thrust.”

Question 2: Approach to performing the research and development (Written responses from 11 of 12 reviewers)

One of the reviewers felt the researchers had done a good background search, and have a plan to go forward. Another felt that the factors that affect aging have been well considered. He felt there seems to be a weakness in using the industrial experience in three-way catalysts to augment this study. Several reviewers commented that the engine used for generating diesel exhaust is not representative of today’s engines or the next generation of diesel engines. One reviewer felt that to better understand the deactivation mechanism, a sulfur poisoning/regeneration process needs to be included in the aging protocol. One person commented that the researchers are actively canvassing other DOE and industrial labs for input, as demonstrated from the program’s originating from Diesel Crosscut. He felt the close knit of the phosphorus work with PNNL's sulfur work is beneficial to DOE and the industrial sector as a whole. One reviewer commented that there seems to be no detailed analysis of engine- and field- aged samples before the studies. He felt it is positive that interviews were conducted with OEMs and suppliers. He was concerned that rich conditions by the burner without engine measures is strange, and will mean a huge exotherm in the DOC, and wondered if this gives comparable results. He was also concerned whether ZDDP incorporated in lube and sprayed into manifold gives realistic results. According to him, the task is extremely challenging and it is very difficult to develop representative accelerated test cycles under well defined lab conditions. Another reviewer was concerned that lean/rich aging temperatures much above 800°C are not representative of controlled desulfation temperatures and wondered if there was a plan to perform rapid aging tests with phosphorus.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 10 of 12 reviewers)

Several respondents acknowledged that the project has been active for a year, with work well underway and most of this time spent on information gathering and project planning and that the group has a sound approach that includes practical concerns of real failures and issues. One person criticized the lack of real new results and the addition of ZDDP as unrealistic and unlikely to give comparable results. He wondered whether phosphorus poisoning gives comparable results to ZDDP. Another questioned how this work is tied into the CLEERS on LNT. One reviewer stated that the differences in phosphorus compounds observed on diesel soot are informative. In comparing with result from engine-aged samples, he said, it may be helpful to define a suitable way to include phosphorus in the aging process. One reviewer felt that there was a nice balance of testing and detailed analysis of the samples to produce relevant results, addressing the fundamental scientific questions. He added that linking the accelerated aging studies through mechanistic understanding to field-tested samples is a bold endeavor and will yield extremely useful information. The final reviewer observed that lean-rich cycling during aging is a major concern—this echoes some of the observations in late 1980s with three-way catalyst aging. Allied Signal had a severe aging process wherein they cut the fuel at high temperature to do a rapid rich-lean shift, which led to severe catalyst deactivation.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 8 of 12 reviewers)

Overall, reviewer opinions were high in this category, with comments including: ample collaboration and industry input; several quality partners; good connection to resources outside ORNL; and working with aftertreatment and energy suppliers. One reviewer commented that there is strong inter-DOE lab work here (ORNL & PNNL with Diesel Cross Cut), and a strong portfolio of industrial partners and universities. Reviewers felt that next year it would be good to see more dissemination of this work at meetings and in the open literature. Another cautioned that significant input from catalyst suppliers and OEMs is required. It is positive that interviews were made at the beginning of the project, but results were not presented (but may have already been discussed last year). The final comment was that there was good information gathering, but not a good use of background knowledge on 3-way catalysis aging.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 8 of 12 reviewers)

There were many positive comments on the project stating that there is a clear plan going forward. One reviewer said it appears a lot of planning and thought went into this program and this modest-size program is well positioned for work in the coming year. Also, the comparison to field samples is extremely important and increases the relevance of the study. One reviewer felt that developing an accelerated aging protocol that reasonably represents the "field" NAC deactivation process is extremely valuable and that the principal investigator may want to consider this as an objective for this study. Another commented that the plan is to extend studies and observations, and verify aging mechanisms through materials characterization. This plan is the right strategy as evidenced by the aging work done on three-way catalysts, which used a similar array of techniques. One person suggested that OEMs should supply a couple of engine- or field- aged samples for detailed analysis. The final commenter felt that this project is weak on sulfur poisoning, but addresses very well the phosphorus issues that have been neglected up to this point.

Specific Strengths and Weaknesses (Written responses from 10 of 12 reviewers)

- Specific Strengths
  - The set-up with a small engine is excellent. It may allow agings to be carried out in a more efficient manner.
  - Approach is well constructed and can yield significant insights through the materials characterization.
  - Good use of multilab expertise.
  - They are investigating an important issue.
  - Short focused project with reasonable objectives.
  - Well thought out, structured program that addresses industrial needs and probes fundamental understanding.
  - Good planning.
  - Very good utilization of resources and facilities at ORNL.
- Specific Weaknesses
  - Perhaps the engine and its internal mechanisms of lube oil consumption, phosphorus release is limited in relevance to commercial engines. Unsure if this is the best choice of test engine.
  - Limited size project limits scope. Will results be representative?
  - Are the resources at the disposal of this program sufficient to enable reaching of the goals?
  - Engine test apparatus is not representative of modern / future engine exhaust stream. Phosphorus

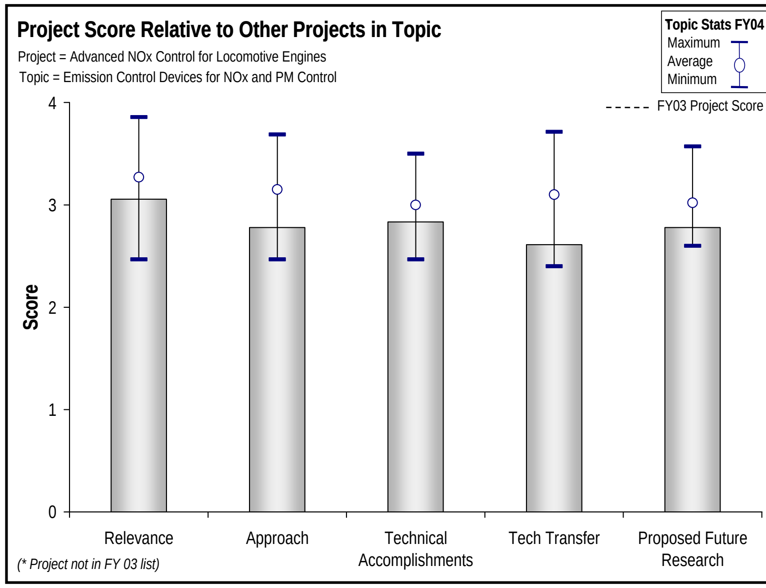
poisoning is a very complicated problem.
  – Poor utilization of known 3-way catalyst aging phenomenon.

<u>Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 9 of 12 reviewers)</u>

- It seem that a "representative" aging cycle consists of:
  (1) lean/rich cycle for NOx regeneration
  (2) sulfur accumulation during regular operation conditions
  (3) high temperature rich excursion for desulfation.
  (4) high temperature exposure to assess the thermal durability
  (5) phosphorus poisoning.
- Should at some point transition to studies in other engine platforms to confirm the observations with the current setup.
- Look at phosphorus as a function of length down the LNT, rapid phosphorus, compare with field data.
- Expand work based on findings or keep expectations modest.
- It should be discussed whether additional funding should be leveraged for this project. The level of funding/resources from the industrial sector is not clear in this project—it might well be sufficient when this aspect is considered. Will introduction of different species of phosphorus be considered? The different areas of introduction may solely manipulate which daughter product of ZDDP is present and the catalyst has to contend with.
- Need to consider increasing the funding and upgrade the experimental setup. Otherwise, the project may not have the minimum critical mass for effective execution and may consider stopping it.
- Provide a plan for using industrial experience in 3-way aging to add to this program.

Emission Control Devices for NOx and PM Control

Advanced NOx Control for Locomotive Engines, Darryl Herling of Pacific Northwest National Laboratory



Brief Summary of Project

In this project, researchers are developing a lean-NOx hydrocarbon-SCR aftertreatment system for an off-road application (locomotive). The goal of this project is to develop a system that can achieve a 70% NOx reduction at moderately high exhaust flow rates. Hydrocarbon SCR is being developed for the locomotive industry due to reluctance of the industry to invest in urea infrastructure for urea-SCR catalysts. The team has demonstrated 70% NOx reduction in bench tests, and has strong leads on catalyst-reductant pairs.

Question 1: Relevance to overall DOE Objectives (Written responses from 15 of 18 reviewers)

Reviewers generally felt that this project is relevant to DOE objectives, if only loosely tied (one reviewer) to DOE's advanced combustion engine program. It was seen as narrowly focused (on the rail sector), but as having the potential to lead to a breakthrough in controlling emissions from high-sulfur fuels, and with possible eventual applicability to on-road trucks. It was praised as a significant effort in a new direction and in an area (non-road engine emissions) that has received relatively little attention. Three reviewers noted the potential contribution the project could make to air quality objectives, because rail locomotive NOx is a significant environmental burden, and because a retrofittable approach to its control that didn't require a separate reductant and imposed a moderate fuel economy penalty could contribute to reducing that burden. Two reviewers noted the desirability of fundamental work on alternatives to urea SCR. Four reviewers, on the other hand, expressed the view that urea SCR is a preferable approach to rail loco NOx control, and that chances of success would be improved if the CRADA partnership would reconsider it. Two reviewers pointed to the complexity of the project system, one of them contrasting it to that of urea SCR. Another expressed surprise that urea SCR had been rejected for rail application, to which it appeared well suited. Finally, one reviewer found the technology demands of the locomotive manufacturers to be "incredibly unrealistic," and while believing the project to be "appropriate," cautioned against allowing it to be driven by those unrealistic expectations.

Question 2: Approach to performing the research and development (Written responses from 15 of 18 reviewers)

About half the reviewers who commented expressed general approval of the approach employed in this project, one calling it excellent, two praising the test and work plans and others noting in particular the catalyst screening, reductant synthesis and combinatorial approaches, as well as the comprehensiveness of the overall approach. One reviewer predicted the project would motivate suppliers to develop fuel reformers useful in other aftertreatment systems. One mentioned the effective use of PNNL's core competencies. The complexity of the NOx control system again attracted further comment, however. One reviewer, in so noting, said the approach didn't seem based on a sound technical rationale. Another, while deeming the approach interesting technically, felt it unlikely to be practical in view of system packaging constraints. Control of the partial oxidation reactor output was also singled out as a major technical challenge, one that would be exacerbated by high fuel sulfur content. Two reviewers noted the system incorporates five separate processes to generate the NOx reductant. Each process potentially requires a different temperature and space velocity for optimum performance, one reviewer said, predicting a resultant cumulative fuel consumption penalty that would be unacceptable in practice. The other said significant further reactor engineering would be needed. Two reviewers urged alternative approaches be examined, including hydrogen SCR and others built on previous PNNL work (the example of non-thermal plasma was offered). One reviewer felt the flash distillation approach to generating raw material for reductant production was novel, and wanted more information on how that reductant compared to [whole] diesel fuel. But another pointed out that distillation of fuel light ends would alter the volatility and composition of the remaining fuel in ways known to affect its spray formation and sooting behaviors. Direct use of diesel fuel was a challenge one reviewer urged on the researchers, citing the early stage of the catalyst investigation. Finally, a reviewer cautioned that undesirable species could be produced over the catalyst.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 12 of 18 reviewers)

Three reviewers demurred on this question, citing the early stage of the project. One, however, opined that good progress had been shown in the project simulation studies. Two reviewers called the project's progress "good," in view of the time and effort expended to date. One noted that there was still a good deal of development required, specifically to identify the optimum selection of catalyst and reductant. Another credited the synergy between GE and PNNL for the results achieved to date, and the third said several techniques under investigation would "bear watching." The project was deemed "promising" by one reviewer, who said a closer look would be needed before an assessment of the likely viability of the approach could be made. Five reviewers pointed directly or indirectly to the volume of catalyst screening as a significant accomplishment; one called the catalyst selection process "very good," another said interaction with GE's "high throughput group" was very promising. Two reviewers qualified their praise of this aspect of the project, one by noting that improved powder catalyst samples from the combi-synthesis had not been shown to be scaleable to meaningful reactor volumes, and the other expressing concern that only those "hits" that supported what the reviewer called a "flawed approach" would receive adequate follow-up. Two reviewers singled out the reformer design and oxygenate synthesis reactor as a notable accomplishment, although one felt the former "unlikely to succeed."

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 17 of 18 reviewers)

Six comments reflected reviewers' belief that the project showed good collaboration, mainly between PNNL and GE; as two reviewers noted, GE is the sole industrial partner. Two comments cited the lack of catalyst developer involvment. Both noted that others had experience in this area, citing Engelhard's work with silver-alumina catalysts and reformer technology development and syngas production and conversion by others such as Catalytica and Hydrogen Source. Several comments suggested involving others in this CRADA - industry segments such as the marine diesel industry, national labs or industry consortia. One reviewer conceded that a rail locomotive project such as this might not engage the interest of vehicle or engine builders, and another found such interest "clearly absent." The latter added that there is not a clear need for exhaust aftertreatment in the rail sector. One reviewer found collaboration in this project to be lacking, since it appeared to consist primarily of one-way communication from locomotive manufacturers to PNNL. This reviewer regarded locomotive builders' expectations to be unrealistic and felt PNNL should provide them a clearer estimate of the maximum impact the technology is apt to have.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 14 of 18 reviewers)

Four reviewers regarded the proposed future research as "reasonable," "important," "well aligned with project goals," as having "good relevance to [the] application," and as addressing "many of the concerns expressed during the review." However, one reviewer called lean-NOx catalysis with hydrocarbon or primary fuel reductants "irrelevant for the advanced combustion engine program" in light of NOx trap developments. Another expressed doubt that the reformer work would be relevant outside the rail application. Yet another was "very doubtful" that the reformer would work, and recommended using the project's connection with GE to seek suitable catalysts for reductants readily producible from diesel fuel. This view was echoed by a reviewer who called for [presumably whole] diesel fuel to be used in future experiments, and for the likely fuel consumption penalty to be quantified. A "key objective," according to one reviewer, should be to tie the multiple chemical processes together in one demonstration unit. Concern over the technology choices of locomotive manufacturers was reiterated; urea SCR or carrying a suitable oxygenate (such as ethanol) on board were both suggested in lieu of the current project approach. Finally, one reviewer noted that no mention had been made of the start-up or other transient behaviors of the system, and found no indication that system design and scale-up effects had been considered. While the project focus had been on catalyst screening and reductant synthesis, this reviewer went on, system effects might prove an insurmountable obstacle, as had been the case with fuel reformers for fuel cell vehicles, largely abandoned by vehicle builders due to system integration barriers.

Specific Strengths and Weaknesses (Written responses from 15 of 18 reviewers)

- Specific Strengths
  - Good PNNL team, good collaboration with GE, good tie-in with locomotive industry.
  - Addresses a specific industry need.
  - Combinatorial chemistry, bench-scale reactor.
  - Interesting approach (distilling light hydrocarbons mentioned specifically); good to try something new; CRADA partner willing to go in a radically different direction from rest of industry.
  - High-volume catalyst screening increases chances of success.
  - Important subject, heretofore neglected.
  - PNNL well positioned to screen catalysts, reductants matching the application.
  - Good understanding of limitations and requirements of catalyst and its field application.
  - Latest tools and techniques applied.
  - Use of on-board reforming under steady-state conditions; may have synergies in other applications.
  - Pace of work; understanding of problem; good use of previous work' good screening techniques.
- Specific Weaknesses
  - System complexity.
  - High risk, with prospect of only modest payoff.
  - Reliance on technology that has received extensive prior investigation and development with only moderate success.
  - Lack of syngas technology company involvement.
  - Packaging, system integration will be difficult.
  - No significant weaknesses.
  - High risk, potentially high payoff, but likelihood of success is low.
  - Very challenging objective – putting reformer and active catalyst into high-sulfur environment.
  - Limited modeling and limited interaction with catalyst suppliers.
  - POX reaction is deactivated by coke formation; syngas-to-oxygenates reaction needs considerable work to be highly selective; hydrocarbon SCR unlikely to be effective at realistic monolith space velocities; HC slip must be controlled.
  - High carbon-to-oxygen ratios in feedgas will lead to failed catalysts.
  - Must control system to within a very narrow window; may be infeasible to produce oxygenate reductants at rates demanded by maximum NOx output rates.
  - Locomotive manufacturers' expectations are unrealistic.
  - Project offers an interim solution for diesel NOx reduction.
  - Little value, since much lean NOx reduction work has already been done for car/truck engine applications.
  - Investigators have not recognized requirements of rail diesel engines.

EMISSION CONTROL DEVICES

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 14 of 18 reviewers)

- Dump the POX reactor. Focus on finding new catalysts that work with onboard fuel.
- Do first-order calculations to show locomotive mfgrs the implications of their specifications for reformer size, energy losses, etc.
- Revise NOx reduction objective upwards – current goal is too low.
- Bring test conditions into line with requirements of real-world application (esp. space velocity – mentioned by 4 reviewers).
- Reconsider cost, space requirements and logistics of urea SCR.
- Program, if continued, should focus on application-specific tasks. For rail loco application, consider exhaust gas composition at specific throttle positions as basis for screening catalyst formulations, and matching diesel fuel reductant with lean NOx catalyst.
- If locomotive OEMs are willing to accept active aftertreatment, why lean NOx catalysis when LNTs make more sense?
- Consider alternatives to flash distillation for fuel preparation and evaluate tradeoffs. There may be more effective was to generate reductants.
- Determine maximum NOx reduction efficiency that could be achieved at theoretical maximum reformer output of oxygenates, compare to 70% target.
- Consider higher exhaust water vapor content. Is 6:1 C_1: NOx high enough? Is the 1.5% BSFC estimate

accurate? (seems low for lean NOx) Not sure funding is adequate to perform all development necessary to bring system to fruition.

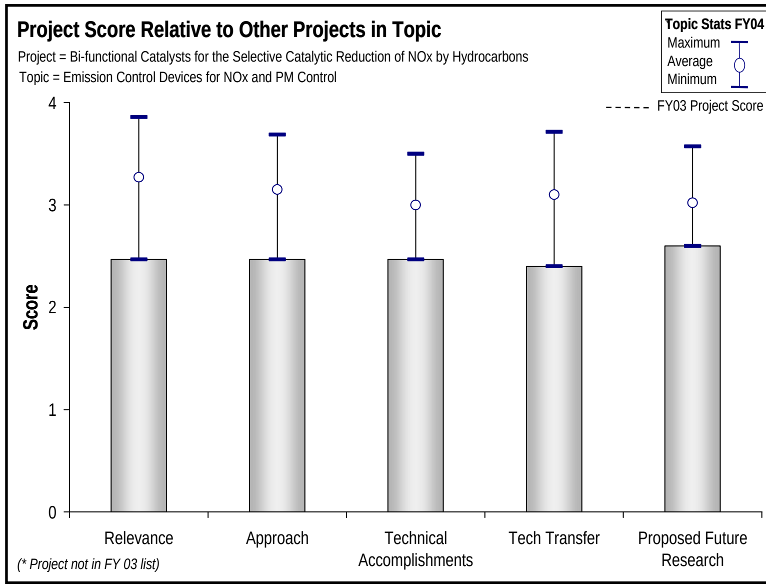
- Accelerate building of prototype reactor to assess start-up and transient response. How large will POX/syngas production/oxygenate production system have to be?
- Is there any modeling of locomotive to estimate required aftertreatment performance? Is there a relevant test schedule?

Emission Control Devices for NOx and PM Control

Bi-functional Catalysts for the Selective Catalytic Reduction of NOx by Hydrocarbons, Chris Marshall of Argonne National Laboratory

Brief Summary of Project

In this project, ANL seeks to develop bifunctional catalysts for the selective catalytic reduction of NOx using hydrocarbons, in order to improve catalyst activity and stability under wet conditions. To date, ANL has developed several novel bifunctional catalysts for hydrocarbon SCR and explored the catalyst behavior and mechanisms.



Question 1: Relevance to overall DOE Objectives (Written responses from 13 of 15 reviewers)

Five reviewers felt this project relevant to DOE objectives, three of them citing the criticality of NOx emission control and one expressing the view that the project could "facilitate the decoupling" of engine tuning for minimum emissions or for optimal efficiency. One also noted the lack of precious metal content in the catalysts under investigation as a "definite plus" and felt lean NOx catalysts could become important, particularly at high exhaust gas temperatures, as diesel combustion control improves. Another reviewer concurred, but noted that poor low-temperature performance would compromise the usefulness of the technology in light-duty vehicle applications. The specific objective of the project was not spelled out sufficiently clearly, in the opinion of a seventh reviewer, who also questioned whether hydrocarbon SCR has the potential to reduce NOx to the levels demanded by the 2010 standards. Other reviewers expressed skepticism concerning the relevance of the project. One called the NOx conversion levels "insufficient" to meet either light- or heavy-duty diesel standards. Another questioned whether industry would be receptive to the approach, even if it were successful. One other said the work "has limited ability" to solve the problem of NOx control. Two reviewers noted the considerable work that has been done in this area, one citing the "extensive" bi-functional catalyst research of Nakatsuji (Sakai Chemical Company), saying that better than 30 to 40% NOx reduction efficiency could not be expected at temperatures above 300 C. For that reason, he deemed this project's work to have only limited relevance, although such catalysts might be useful to assure compliance with applicable standards if combined with "excellent" engine-based NOx control measures. The other reviewer mentioning previous work said catalytic systems that function well in the presence of water vapor have been demonstrated, and that demonstrating thermal stability was the greater challenge. Indications that cerium-doped copper-ZSM-5 isn't durable even after 600 C treatment put it "far behind expectations," this reviewer concluded. The last reviewer also regarded the NOx conversion efficiency as "too low to be useful" for light-duty vehicles and perhaps also for heavy-duty vehicles.

Question 2: Approach to performing the research and development (Written responses from 12 of 15 reviewers)

Two reviewers praised the approach employed in this project, one referring to it as a "good, systematic" one and the other noting it leveraged prior research in this area for stationary NOx sources, and that bi-functional zeolites offer additional flexibility and the potential to optimize catalyst performance. Six others offered qualified approval of the approach, suggesting modifications they felt would improve it. One believed a narrower focus to be worthwhile, and suggested two separate projects, one on diesel exhaust and the other on spark ignition (CNG) engine exhaust. Another expressed a desire to see further low-temperature testing and "some consideration" of adsorption effects. A third felt the synthesis of potential bi-functional catalytic materials for activity and efficiency optimization to be appropriate, but that real engine exhaust gas or a more representative surrogate stream would be preferable. This reviewer saw little linkage between reactor experiments and real engine conditions. The approach was regarded by two reviewers as either inadequately detailed or difficult to evaluate fairly. The latter suggested a literature survey be made of previous work in the area, if that had not been done heretofore. The second also noted the volume of previous work on hydrocarbon SCR, a technology, he said, that seemed to have been abandoned for lack of progress. This reviewer however felt that the ceria-stabilized bi-functional zeolite catalyst design could offer benefits. Three of the four remaining reviewers expressed the view that use of selected hydrocarbon reductants was less desirable than the use of diesel fuel. One suggested the thermal durability be addressed first, and noted that other hydrocarbon SCR catalysts had performed well using selected hydrocarbon reductants but poorly using diesel fuel, and that finding out if the ceria-stabilized copper-substituted zeolite behaved the same way should be given priority. Another said the project's limited work scope doesn't include the range of conditions encountered in a "real auto environment." The approach was described by two reviewers as lacking novelty; one said all the catalyst systems reported have been studied, the other concurred and added that the choice of reductants was unrealistic. That reviewer also noted that "very little effort" had been devoted to identifying the possible effects of NOx storage versus NOx reduction.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 13 of 15 reviewers)

The project was felt by five reviewers to be too new to permit ready evaluation of its accomplishments. One noted the previous work on stationary NOx sources and the fairly constant exhaust temperatures typical of such applications. Two other reviewers cited the stabilization of catalysts against moisture, the creation of reaction pathways promoting catalyst activity, the achievement of maximum activity in the 300°C range and the demonstration of bi-functional metal matrix conversion efficiency as project accomplishments. One of these reviewers said that to assess the accomplishments of this project, it would be necessary to know the complementary CRADAs being pursued on this subject. Another reviewer called the reverse formulation "interesting" (although the temperature window is "still too narrow") and one speculated that progress in synthesis might open the way to improved catalytic systems for hydrocarbon SCR. Other reviewers, however, said that no progress had been made in improving thermal durability, which the NOx conversion achieved to date was not "compelling," and that "negligible" new information had been developed. The hydrocarbon SCR approach, this last reviewer said, had been investigated by other national labs, with little progress toward high NOx conversion, leading to the programs' being replaced with urea SCR investigations which had been much more successful.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 11 of 15 reviewers)

One reviewer (of nine commenting) noted that a CRADA with Cummins is "in the works" if performance targets are met, and that discussions with catalyst manufacturers are ongoing. Another praised "good collaboration" with BP, but said more collaboration with an engine manufacturer was needed. Most reviewers who commented were more critical of industry and academic collaboration in this project. Three noted that there is only a single industry partner (BP), and one of them termed BP's participation "indirect," since it is through a related program. Two other reviewers also commented on Cummins' participation, both noting that the company clearly wished to collaborate only if the work began to show promise. One of these reviewers felt it "understandable" that the CRADA targets had not been disclosed, but found the presentation lacking any indication of the probability these goals could be achieved. Two reviewers called for more industry involvement to guide the work and to provide timely feedback to minimize duplication of work. BP's sponsorship of the program puzzled one reviewer who felt it "more important" that there was no participation by the Manufacturers of Emission Controls Association (MECA). One of the reviewers previously mentioned said it was unclear if there was collaboration with universities and other national labs, and whether there had been publications or presentations beyond mention of a patent application.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 13 of 15 reviewers)

Four reviewers applauded the proposed future research as "solid steps for early screening of catalyst leads," and as "well thought out." Two of them specifically praised the plan to investigate hydrogen and carbon monoxide as reductants. One said these species were more likely to be produced than specific hydrocarbons and the other said they would help to circumvent the sensitivity of the catalysts to hydrocarbon type. Other comments were more critical, and several of them offered suggestions for revised future work plans. The suggestion that the project be more narrowly focused and divided into two separate projects (one on diesel NOx control, the other on CNG spark ignition engines) was reiterated. One reviewer expressed doubt that the strategy would yield sufficient NOx conversion or temperature range to be useful. One reviewer called for an immediate end to work on "model hydrocarbons" and a switch to diesel fuel, saying "nothing else is of practical importance." Another agreed, calling the selection of reductants "poor," and saying the emphasis on dry, rather than wet, catalyst feedgas "artificial and [of] no clear value for the work." Two reviewers called for "intermediate milestones for a multi-year program" and "better-established performance goals linked to a time frame." Issues including high-temperature durability, sulfur tolerance, hydrocarbon type sensitivity and coke formation should be addressed, in the opinion of one reviewer. Among the other suggestions offered by two reviewers for approaching future work were more emphasis on sulfur poisoning, phosphorus poisoning, coking effects, the effect of additional hydrocarbon use on fuel consumption, expansion of the temperature range investigated from 300 to 350°C to 300-550°C, higher exhaust oxygen content of approximately 8% (this was termed "critical") and "realistic experimental conditions" with periodic engine tests to check the validity of NOx reduction claims. Finally, one reviewer felt the technology might be useful in some applications, but pointed out that close-coupled catalysts upstream of the bi-functional catalyst would be required, resulting in the addition of a dosing system, which would pose its own "significant problems, mainly at low temperatures."

Specific Strengths and Weaknesses (Written responses from 14 of 15 reviewers)

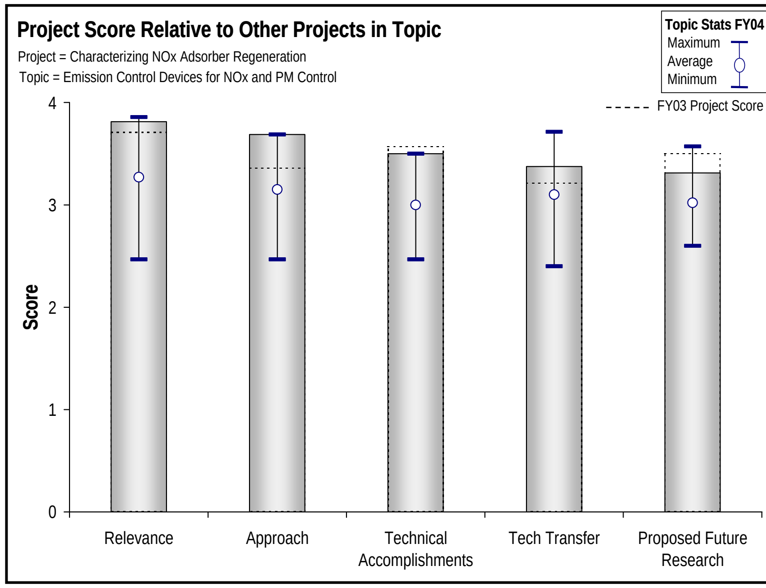
- Specific Strengths
  - Provides competition for NOx adsorbers. Suggest keeping up this activity.
  - Catalyst development is fairly mature and showing promising results.
  - Good catalyst development. Water-activated catalyst.
  - Rapidly progressing, with good leverage of prior research. Demonstrated stability in presence of water, in fact with need for water.
  - Concept avoids regeneration and usual engine operating conditions.
  - Catalyst combinations.
  - Lean NOx catalysts shown to be activated by water, which has been a major problem for these catalyst systems Fairly good collaboration with BP and work that has gone to the stationary power area is a definite bonus.
  - Interesting bifunctional catalyst approach using "nano" particles. But similar results can be obtained with more classical approach to catalyst preparation.
  - Synthesis of new materials. In specific, the coating of zeolite with a metal oxide.
  - None precious metal based catalyst is a possible means for affordable product, if the efficiency is more than 70% at reasonable size (space velocity).
  - Bi-functional metal oxides seem promising to fulfill the conflicting requirements of higher conversion efficiencies at lower temperatures.
- Specific Weaknesses
  - Temperature range of catalyst too narrow.
  - Catalyst appears to have severe sensitivity to type of HC reductant species. This may require an impractical need for specific types of HC's (e.g., olefins) in the exhaust.
  - The project needs to be tied to EPA requirements. No catalyst performance goals.
  - Need to look at nitrogen balance in detail with particular attention to nitrogen-containing hydrocarbons. Need to re-examine work with SO_2 and the return of activity to catalyst upon removing SO_2 from stream.
  - Catalyst efficiency is relatively low and needs reactive hydrocarbons.
  - Previous work has been done in this area.
  - Needs collaboration from a catalyst company to make sure that this project moves from the laboratory to industry.
  - Stated goal of 70% conversion at a space velocity of 30,000 is insufficient. HD applications with catalyst volume of twice engine displacement will have space velocity of 150,000 at not-to-exceed points.
  - For 2010 applications, any system must operate in a system with a particulate filter. Therefore, a system with only 550C durability is unacceptable. This temperature durability limitation is typical of all Zeolite-based HC-SCR systems, and is why the HC-SCR concept is no longer a prime candidate for future emission control.
  - Poor selection of reductants, emphasis on dry versus wet feeds which is artificial and no clear value for the work.
  - This work has not shown potential for achieving 70% NOx reduction.
  - Reactor experiements are fine but the researchers need to improve the test conditions and selection of test parameters. For example, exhaust gas composition and temperatures shall be more acceptable (similar to engine like conditions.) The reductants shall be diesel like fuel rather than primary fuels.
  - Use of specific HC species as the reductant. Adsorption and desorption is a potential problem under transient conditions. Reminds me of the NTP catalysts. Should avoid repeating this type of performance.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 12 of 15 reviewers)

- Stop funding or set specific short term performance criteria necessary to continue the project.
- Stop DOE funding unless strong OEM support occurs.
- Need to get practical diesel exhaust results soon to continue to show potential relevance to real-world diesel applications. Work to tune the catalyst to be less sensitive to HC type. Expand the study of poisons and aging that would take place in a diesel vehicle.
- Can this technology compete with ammonia SCR(90% NOx reduction) in terms of required NOx reduction for 2007 or 2010 and cost to operate?
- Need to examine SO_2 species downstream of catalyst. Increased production of SO_3 due to external oxidation catalyst could be troubling. Coating of these zeolites on a monolith would be extremely interesting particularly examining the stability of the coated catalyst to water, SO_2 and thermal/vibrational cycling. Probing the registration of ceria on different zeolites might aid in the coating of the wider pore materials.
- They need to use diesel fuel as the reductant instead of reactive hydrocarbons.
- Try to make it more relevant to real cycles.

Emission Control Devices for NOx and PM Control

Characterizing NOx Adsorber Regeneration, Shean Huff of Oak Ridge National Laboratory



Brief Summary of Project

The main objectives of this project are to characterize hydrogen, carbon monoxide, and hydrocarbon emissions from a small diesel engine, and to characterize candidate NOx adsorbers for performance and degradation for use with this engine. Additionally, the project team seeks to develop a stronger link between bench and full-scale system evaluations. The project team has been examining several regeneration strategies for the candidate NOx adsorbers and how the choice of strategy affects exhaust emissions.

Question 1: Relevance to overall DOE Objectives (Written responses from 11 of 16 reviewers)

Reviewers had generally positive things to say about the relevance of this project to DOE objectives. One noted that LNT regeneration is a prime-path technology. Another felt it was a critical endeavor to meet advanced emissions requirements and to lower the fuel penalty for the 2010 diesel emissions strategy. Others said it was an excellent coverage of needed characterization, and that the program (which is looking at many aspects of engine/aftertreatment integration) is obtaining important system performance characterization that can feed CLEERS modeling. The opinion was expressed that the work was outstanding and relevant to the important lean-NOx trap subject. One reviewer continued by saying that developing the direct relation between the engine controls and the aftertreatment response fits in well with DOE's goal of engine design to improve emission control and fuel economy. The team is working to develop a better understanding how NOx adsorbers operate under realistic conditions but at a fundamental level, noted one reviewer. A reviewer felt the work was interesting and that there seemed to be opportunities to make the work relevant to aftertreatment challenges. Identification of species concentrations will help to assess the performance of NOx adsorber and further optimize of regeneration, which is quite relevant to the advanced combustion engine program. A reviewer noted, though, that the focus of the project could be improved by defining the goals more precisely, as the project is very complex.

Question 2: Approach to performing the research and development (Written responses from 13 of 16 reviewers)

The approach of the principal investigators generally met with the approval of the reviewers. One reviewer said that directly addressing last year's reviewer comments demonstrates clarity in the purpose of the project. The breadth of analyses to address the key chemical species and their evolution is extremely thorough, this reviewer continued, and the frank presentation of the need for engine replacement (with additional details in the appendix) was greatly appreciated and further demonstrated the vigor of the research. Another approved of the realistic testing with engine and injection controls, and their effect on the emission system. Other researchers approved of the tools used (noting that ORNL is using all available tools and integrating them for better understanding of results at a detailed level) and the sound, systematic approach in which many aspects appear to have been considered. The use of sophisticated analytical tools to link calibrations, emissions, and catalytic controls was noted. These thoughts were echoed by another reviewer who noted that this project is both well focused and utilizes the range of analysis tools developed by the DOE (e.g.; SpaciMS and LII laser soot detection) to approach this problem. Another reviewer went further, saying the approach was excellent and that the combination of engine operation know-how with catalyst knowledge will result in outstanding results in the future and a successful project. The large, diverse team and excellent facilities supporting the investigation were also mentioned by a reviewer. Several reviewers mentioned the selection of injection strategies for regeneration, noting that there are strategies worth considering beyond the ones used in the project: more industry interaction would make these choices more effective. Another reviewer felt that some simulation in parallel to the testing would add substantial value to the project, and asked if the CLEERS connection was sufficient in this regard. Finally, one reviewer said that the technical approaches were well defined and the lab has excellent experimental facilities to carry out the stated tasks.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 9 of 16 reviewers)

Several reviewers offered positive comments about the information being collected in the project, noting that the results are readily helpful (and relevant) to industry R&D efforts and relevant to meeting DOE goals: considering a variety of fuels was felt to be valuable in this regard. One reviewer felt little could be improved in the accomplishments to date. Another said that good progress is being made in understanding the effects of injection method on LNT efficiencies. Some progress is being made, said one reviewer, and it is hard to tell where this will lead but very encouraging opportunities are seen. One reviewer noted that this project is well focused and utilizes the range of analysis tools developed by the DOE (e.g.; SpaciMS and LII laser soot detection) to approach this problem. Aspects of the accomplishments highlighted by reviewers included the development of a desulfation strategy; expansion of the project to tie into CLEERS; development of two strategies to achieve intermittent rich conditions for regeneration; and provision of detailed characterization of the engine-out, DOC-out and NOx adsorber-out species (including real-time PM); and consideration of the impact of fuel composition on results. In addition, reviewers noted the detailed engine strategies for rich transient operation coupled with characterization of $CO/H_2/HC/PM$ as a function of control strategy, with these strategies being correlated with NOx conversion. Real-time analysis of soot generation and hydrogen consumption provides unique insight into special performance characteristics, noted one reviewer. One reviewer felt that a weakness is the selection of injection strategies, and that more interaction with industry would make those choices more effective. Another said that limited catalyst samples (types) may limit the applicability of results. Finally, a reviewer noted that since the test setup and test procedures were well developed, one would expect to see more data (for example, post-injection variables such as start of injection and duration of injection).

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 10 of 16 reviewers)

A reviewer saw the linkage to industry applications and thought that this is a promising area of work. Another noted that the principal investigators were working with CLEERS, LEP and an unidentified MECA partner, also noted by a reviewer who felt the group had a regular "reality check" with CLEERS and LEP groups and a very interesting link to Sandia (Peter Witze) for in-situ transient PM measurement. A reviewer saw good collaboration with industry but thought there is limited university participation. One reviewer would like to have such an institute close to Stuttgart. Finally, a reviewer noted that more interaction with industry would be better. The catch-22 with this criticism (in this reviewer's mind) is that industry considers their injection/engine control strategies very proprietary, so a way must be developed to evaluate those strategies without compromising the competitive edge each company believes it possesses based on its engine control strategy.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 10 of 16 reviewers)

Reviewers offered numerous suggestions for improving the relevance of the proposed future research. Suggestions included the addition of simulation within the core program; the addition of a second catalyst to determine if results hold for different systems; focusing of additional efforts on desulfation strategies and NOx adsorber durability following desulfation; expansion of temperatures considered; further examination of low-temperature combustion with regeneration and the soot/NOx tradeoff; coordination with the CLEERS LNT group; consideration of other injection strategies for regeneration; and increases in the industrial input to the project. A reviewer felt it was important to emphasize low-temperature (200^{o}C) regeneration as a critical area of development. Reviewers offered positive comments about the research plan, noting that it was good to focus on the needs of industry and that the project will give fruitful knowledge for LNT applications. One reviewer said that the approach seems quite straightforward and is appropriate for the proposed future research.

Specific Strengths and Weaknesses (Written responses from 15 of 16 reviewers)

- Specific Strengths
  - Excellent experimental capabilities.
  - Excellent experimental facilities and tools to carry out characterization of NOx adsorbers and exhaust HC chemistry.

- Capabilities of the team, facilities available for the work.
- Solid team and process.
- Combines engine, bench & basic core competencies available at ORNL. Excellent team. The frame of work is within the practical domain of engine operation, albeit fairly fundamental.
- Systems approach to understanding emission reduction. Use of mass spec at various positions within the LNT.
- Unique collaboration between control strategy efforts and transient emission characterization.
- Strong interaction with LEP.
- Excellent utilization of one-of-a-kind instrumentation. Thoughtful selection of areas to investigate such as desulfation and effects of fuel components. Also coordination with CLEERS enhances the impact of the work.
- Chemical speciation capability and SpaciMS set-ups are excellent. This facility should be able to generate extremely useful information in understanding the NAC transient behavior.
- SpaciMS is an extremely useful tool. Its use in observing NOx and SOx concentrations down the catalyst length can be a useful experiment on how big (aspect ratio of catalyst) needs to be to achieve the required performance.
- Extremely detailed analysis of the evolution of species in the stream and interaction with surfaces.
- This work is providing very useful information on NOx trap regeneration.
- Applying the latest tools in a fully integrated engine/aftertreatment system - detailed speciation helps understanding.
- Basic understanding of the effects of various reductants on NOx conversion efficiency using engines. Excellent application of tools (Spaci- MS) showing the effect of hydrogen on NOx adsorber performance.

- Specific Weaknesses
  - Because the scope of the study is so broad, there seem to be many fundamental questions that are not being addressed - For instance, why were the PM emissions during regeneration so much lower for the Post 80 strategy than the extended main injection? Is there an optimum timing for the post injection to maximize the composition of the HCs in the exhaust and increase the rate of regeneration?
  - End of LNT regeneration strategy could be improved to reduce HC slip.
  - Limited to one catalyst type: do these results hold true for different catalyst formulations?
  - How does this system hold up as a function of time? Indication of an engine problem but did not describe in detail. How do these results compare to reactor data? Will there be models or equations that can be delivered to industry from this project?
  - Important to perform multiple sulfation/desulfation cycles prior to catalyst evaluation.
  - Do not use OEM-GDI off-the-shelf catalysts, because these have been optimized for hot stoichiometric operation rather than diesel NOx-adsorber conditions.
  - Progress is slow.

EMISSION CONTROL DEVICES

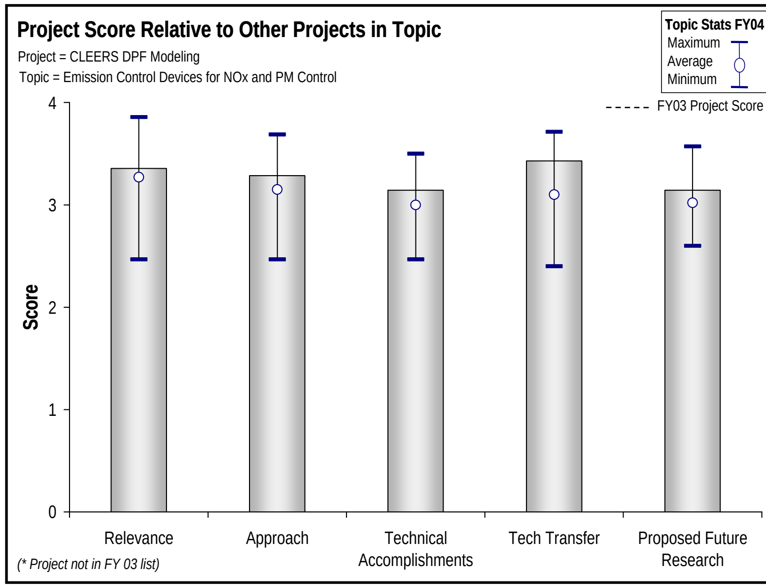
Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 12 of 16 reviewers)

- Provide more detailed information during NOx regeneration phase. [For example,] does NOx release first from the front part and get reduced at the back of the catalyst?
- It would be extremely valuable to examine the sulfation/desulfation behavior. Does sulfur deposit on the front and migrate to the back? During desulfation, will sulfur released from the front re-adsorb on the back?
- Is H_2S formed directly, or is it actually from the SO_2 released from the catalyst that further reacts with reductants at the back of the catalyst?
- Information on unregulated compounds, such as NH_3, N_2O, H_2S, SO_2, during regeneration is valuable as well.
- Look for ways to spin off smaller investigations to pinpoint questions that the main program cannot address due to limits on time, personnel and access to facilities.
- Discuss the experimental approach to desulfation. Calculate the effect on BSFC for each strategy (delayed and post).
- Could use a more detailed plan for future work with clear ties into the remaining technical barriers and estimated timeline of deliverables in the drive to market.
- The number of possible experimental combinations in this work is so large, that it is difficult to imagine in what direction to aim this very good effort. Is there an experimental plan, design-of-experiments-based or otherwise, that can guide these experiments to provide specific answers in response to the stated goals? I think that there is - it would be nice to outline the big picture next time. This project needs more funding.

- They need to also look at adding EGR to get to rich conditions for NOx trap regeneration instead of increasing fueling.
- Keep improving the industry connections.
- Add simulation of flow, macro-device boundary conditions, etc. Correlate the results statistically.
- Optimize NOx conversion for minimum HC slip.
- Important to evaluate at HD not-to-exceed point to demonstrate space velocity limitations on this technology.
- Project is on a good way.
- Better selection of injection strategies and more evaluation of the effects of EGR on the engine out compositions.
- Tests with switching the placement of catalysts (NOx adsorber followed by DOC to retain higher H_2 peaks for NOx regeneration).

Emission Control Devices for NOx and PM Control

CLEERS DPF Modeling, George Muntean of Pacific Northwest National Laboratory



Brief Summary of Project

The overall goal of CLEERS is to promote development of improved computational tools for simulating realistic full-system performance of lean-burn engines and the associated emissions control systems. In this project, PNNL has developed a full-flow single particle deposition model and a PDE-based continuum soot cake model, and has also developed a single channel experimental technique for validation of models.

Question 1: Relevance to overall DOE Objectives (Written responses from 9 of 14 reviewers)

Several reviewers commented that DPFs are essential for advanced combustion engines to meet the 2007 emissions regulations and must develop further to be practically implemented, particularly with regard to understanding how and when to regenerate. One person added that DPF is central to the PM reduction objective, and thus assessing the loading characteristics and PM deposition modeling is quite relevant. He went on to say the CLEERS DPF effort seeks to develop better modeling targeted at development of first-principal understanding of the fundamental processes of soot collection on and within the filter media as soot is filtered, the filter cake forms and filter regeneration as soot burns off via modeling in "real" systems. Another agreed, stating that the CLEERS structure focuses work on desired objectives. Another reviewer went on to say that CLEERS could be a good tool for soot/filter studies and that this is clearly an area of considerable interest. Another reviewer added that due to the fact that the back-pressure signal cannot be used as a clear signal for the mass of soot inside the trap a soot-loading model must be developed to avoid uncontrolled regenerations. Another questioned how the overnight effect can be projected. There was also a question of whether the morphology of soot cake is influenced by the C-NO_2 reaction. Nothing was mentioned in the talk, but the reviewer wondered if this was perhaps addressed by earlier work.

Question 2: Approach to performing the research and development (Written responses from 10 of 14 reviewers)

One reviewer commented that this is a very good approach but it appears that there are many more years of modeling left to do to incorporate many more important factors that affect DPF technology, and he questioned whether the addition of oxidation data (discussed after the presentation) can be done in a suitable timeframe to be of interest to OEMs. He added that validation of the models is critical; it appears to be great modeling, but is it accurate? Another reviewer agreed and added that the model needs to be validated with actual filters, which is included in future work. Another reviewer had the opinion that the experimental basis must be increased by mainly catalytic reactions. The CRT function must be integrated, either by data from literature (for example work done by Professors Gilot and Mulhouse), or better by their own experiments, which should be not a major problem for PNNL (in this reviewer's opinion). Second, a model for thermal regenerations including the not-yet-finalized regeneration process must be considered. Others added that soot cake filtration is the dominant filtration mechanism/medium for today's diesel particulate filters; this approach is clarifying the factors that influence this filtration mechanism. However, another reviewer said that a simple 1-D model to describe particle deposition process is questionable. It is not clearly defined what relevant parameters from experimental data would be compared to the results from analytical work. The approach toward a more practical way and not going too much in the details is positive which will give the engineer a tool for development in a realistic time frame. They concluded that the principal investigator has a very good scientific overview from literature. One reviewer stated that the work started with continuum soot cake modeling and then went back to look at how particle deposition impacts cake formation. They commented that the researchers have not yet considered how soot collects on a partially regenerated filter. Others said that the work had an innovative strategy by trying to resolve the permeability of the filtered material, and had a solid approach to soot modeling. Another person stated that CLEERS is evolving to build a nice collaborative organization where individual organizations are working on their core competencies. Better understanding of the nature of soot deposited in a DPF would be useful to develop durable, efficient devices.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 11 of 14 reviewers)

One reviewer commented that this project appears to gather other researchers' work, and summarizes this in a usable explanation for industry and other researchers, which is a very acceptable goal. Another reviewer agreed, stating that the team has had good accomplishments in two years of work. Another person simply stated "great progress on developing the models." One person said that there has been a lot of progress getting the organization set up, and now each sub team is working towards a joint industry/national laboratory objective and database. Another reviewer thought that good progress towards objectives has been made, although many challenges still remain. One reviewer thought that important steps toward understanding the particle deposition process and the soot cake filtration, structure, and growth process have been made. Another agreed, stating that the researcher made significant model extensions over Konstandopolous' model, at what appears to be a significant increase in computational time. Another reviewer commented that the 1D modeling work seems progressing well, but they were concerned that was no mention about 3D modeling work. It is unclear if the results are a significant improvement over those obtained with the more simplified model. The final reviewer said that the work is very challenging and SAE indicates increasing activities, therefore future work progress can be expected. The basis of their own experimental data should be increased mainly in the catalytic or thermal reactions which is essential for "cake permeability".

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 11 of 14 reviewers)

One reviewer again stressed that the work appears to gather other researchers' work, and summarizes it in a usable explanation for industry and other researchers; a very acceptable goal. One reviewer noted that there is a broad based and active team, but would benefit by having better representation of filter manufacturers. Another reviewer noted that there has been a lot of progress getting the organization set up, and now each sub team is working towards a joint industry/national laboratory objective and database. One reviewer thought that many activities appear involved and the tools developed here will require some work by outside users. Several reviewers thought that there was a good connection to industry through the CLEERS Program and the program is driven by CLEERS focus group; however one person suggested that the focus group needs to be more applications oriented. Another reviewer commented that transfer to industry is assured by philosophy of DOE projects. A fruitful collaboration with the key players in DPF modeling like Konstandopoulos is difficult or impossible, but PNNL will make significant progress in the near future. One reviewer questioned why International was not included in the partners list and provided Alan Karkkainen as a contact (708-865-3406 or a.karkkainen@nav-international.com).

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 8 of 14 reviewers)

One reviewer commented that there is a very good plan and tough tasks ahead. Another agreed, adding the direction appears good, although there are still many questions. To be useful, this work must proceed quickly. One person commented that the future direction is primarily driven by monthly conference calls with the CLEERS partners. Another commented that it would be interesting to determine if the walls are shielded due to other cell walls and how this alters the soot deposition along the length of the channel. Also there should be some work on other soot filter media, i.e. comparison of cordierite to SiC to a composite media. This effort would provide guidance in the development of advanced filters with lower back pressure. Another reviewer thought that the single channel experiment to measure soot deposition is an interesting idea that may help to validate model. However, it is unclear if this same system without appropriate exit channel constraints will be applicable to regeneration experiments, given comments about importance of back diffusion. Another person simply stated that the relevant problems and targets are mentioned. The final reviewer suggested that regeneration is a higher priority issue than the soot cake filtration. The reviewer agreed that characterizing the soot cake is an important first step, but moving more quickly to the study of regeneration, partial regeneration and "patchy" regeneration is a must.

Specific Strengths and Weaknesses (Written responses from 13 of 14 reviewers)

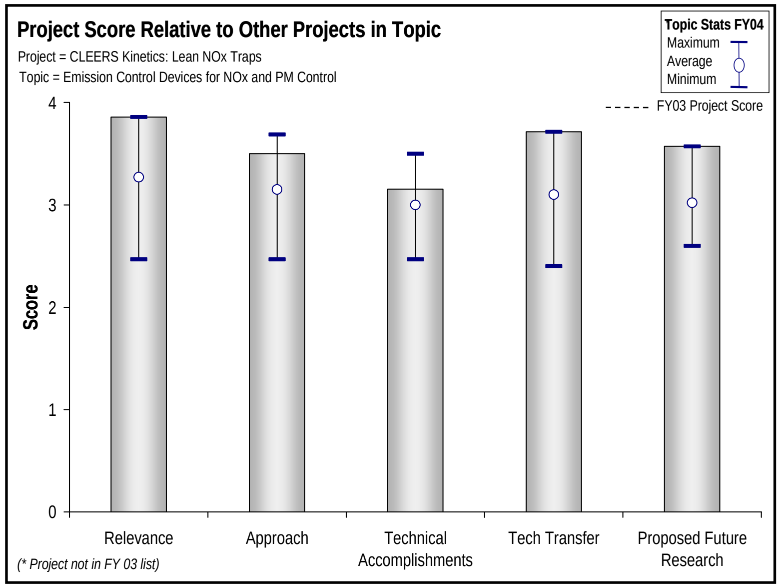
- Specific Strengths
  - The mixture of levels of approach, starting very fundamental and looking to link to practical simulation, with validation via single-channel experiments.
  - Very detailed models, good computing facilities.
  - Comprehensive approach to studying DPF loading.
  - Solid work in a field of great interest.
  - CLEERS is evolving to build a nice collaborative organization where individual organizations are working on their core competencies. Better understanding of the nature of soot deposited in a DPF would be useful to develop durable, efficient devices.
  - Program goes from basic modeling to the development of information and models that are useful to the industry. Approach used is innovative and demonstrates good understanding of the literature and the areas that require further investigation.
  - Claimed to have a fundamental, first principles, soot loading model.
  - Claimed to be able to calculate how soot density and permeability vary with increasing soot loading, although no data was shown.
  - The practical approach which gives a tool for development in a relatively short time frame.
  - Good research team with an industrial background.
  - Directly applicable to near future products, therefore, it's useful work for industry.
  - Driven by CLEERS goals—modeling shall enable better understanding of PM loading and efficiency characteristics.
- Specific Weaknesses
  - Needs more experimental data to validate models.
  - Should have filter media manufacturers involved in the team.
  - Models not validated.
  - Speed of progress needs to be watched. Diesel particulate will not wait for implementation benefits.
  - Slow pace!
  - All of the aftertreatment and engine technology is competitive by nature - so finding ways to share needed data without scaring paranoid industry folks and keeping this win- win for all participants is challenging.
  - Scope needs to be expanded to include aged soot and also a look at the soot oxidation rates.
  - Lack of model validation, even for soot loading on clean filter.
  - It appears that modeling of soot regeneration has not yet started. It is unclear how oxidation kinetics will be obtained.
  - Own experimental basis should be increased.
  - Not enough work on regeneration, definition of regeneration and the related effects on pressure drop.
  - Need to strengthen technology transfer to industry involving both MECA and EMA members.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 10 of 14 reviewers)

- All models for oxidation using thermal source and catalytic source.
- Add a filter media company.
- Increase the effort on the validation work.
- Please investigate other filter types than EX type, such as Corning CO or RC filter types to look at the effect of filter morphology.
- They need to devote more effort to studying ash deposition since it is a major limitation to DPF life.
- Good future efforts on oxidation and effects of ash on the experiments.
- Extend soot loading model to case of catalyzed DPF.
- In Q&A session made an interesting comment about back diffusion of NO_2. Use this and oxidation kinetics to calculate NOx turnover on catalyzed DPF.
- Increase focus on regeneration both in the research and with the focus group.
- Keep in the program. Need to consider kinetics.
- Need to speed up the development and validation of single channel modeling efforts.

Emission Control Devices for NOx and PM Control

CLEERS Kinetics: Lean NOx Traps, Stuart Daw of Oak Ridge National Laboratory



Brief Summary of Project

This project, a component of the CLEERS project, seeks to develop and consolidate information about chemistry and rates of key reaction steps for lean-NOx trap sorbent materials, to develop tools for LNT performance modeling, and to use the tools to identify sources of inefficiency and potential solutions.

Question 1: Relevance to overall DOE Objectives (Written responses from 11 of 14 reviewers)

Reviewers were generally positive about the relevance of this CLEERS work. Among the comments were that the CLEERS structure provides “linkage to high-level goals,” and that this was “more good CLEERS work” (specifically, fundamental work that is useful to lean NOx traps). Comments were also provided to the effect that the current effort is a prime path for the diesel community in 2010 and beyond to meet the emissions levels for NOx. Others said that the program was extremely relevant and is one of the key technologies for 2010 heavy-duty diesels, that the program had a good focus and will help LNT development, and that improvement of LNT is critical to making this technology a viable solution. A reviewer summarized the objective of the program as correlating fundamental chemistry to device functionality and efficiency with the goal of developing potential NOx-trap solutions to lean NOx control. A reviewer said that the program goals and work scope are very “object oriented” and are well within the objectives of the advanced combustion engine program. Another reviewer noted that CLEERS seeks to improve efficiency and lower emissions from diesel engines and provide the means of incorporating more sophisticated simulation within vehicle control systems. A reviewer said that there are two parts to this work: the overall CLEERS modeling coordination and the focus on LNT aftertreatment technology. Both of these, he said, are key to the DOE goal of enabling light duty diesel powertrains into the US consumer market. A reviewer pointed out that the work provides a tool for a possible valuable contribution to advance the state of the art of aftertreatment. Finally, a reviewer said that the large ammonia peaks were unexpected.

Question 2: Approach to performing the research and development (Written responses from 10 of 14 reviewers)

As with the relevance question, reviewers offered positive comments regarding the approach of the work. One noted that this was a good approach that will result in a tool appropriate for engineers in their application work. This reviewer continued, saying that global models can be very helpful, but the problem is also that for the application of a given catalytic system, experimental data must be worked out for every specific catalyst. Nevertheless, this is a first, necessary approach. It would be interesting if microkinetics are also considered in future work. Another reviewer said that development of elementary chemical and physical phenomena, moving to modeling and then to comparison of bench and engine tests provides the scientific foundation necessary to achieve the objectives. A reviewer stated that the project had a good plan and execution, and that the model seems to do a good job of understanding trap phenomena. The work complements other activities, and is evolving to be a significant building block in the technology development pursuit of the DOE-FCVT, in the opinion of a reviewer. This approach is well focused on supplier provided devices and engine manufacturer/supplier input on modeling the devices, said another. Finally, a reviewer pointed out that there was a good progression of analytical work, bench tests, and engine data to develop the model set.

Some reviewers focused on certain aspects of the research. One noted that using model catalysts, lab reactor protocols have been defined that allow results to be fit to fundamental reaction models. Another pointed out that the bench-flow reactor followed by engine tests and global modeling provide comprehensive data on the LNT, and that this was a well thought-out approach.

Suggestions for improving the research included looking at the global effects of desulfation. Another suggestion was to ensure that the pre-history of the catalyst should be well-defined, as it significantly affects the testing results.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 12 of 14 reviewers)

Reviewers had generally positive opinions of this aspect of the research, but offered areas for improvement as well. One stated that the reduction of NOx is a difficult technical challenge. The project is making significant progress in the understanding of these key questions. However, it is not clear that the information and the solutions will be available in time for the industry. Another reviewer said that the team has made good progress this year, with some issues understood and progress on others. "Good progress made toward 2004 goals," said another reviewer, who noted the good fit of model to empirical data. Another reviewer went into more detail, saying that the LNT modeling has not yet had an impact on the industry, but that the workshop organization has had very good impact on industrial communication. LNT experimental work is well done and provides a good public focal point for making measurements that the engine manufacturers consider too confidential to share. A reviewer said the work was well done, and with the analytical equipment in hand, good progress in the future can be expected. One reviewer felt that the modeling is not keeping up with the experimental work. A reviewer was expecting to see information from model predictions.

Several reviewers focused on key aspects of the research. The upgraded lab reactor with a state-of-the-art fast analytical package was singled out by several reviewers. Also highlighted were the definition of a standard test protocol and the development of a global kinetic model that reproduces bench and dyno results. One reviewer emphasized the great piece of information on the sulfate effect on NOx conversion, which can guide engine control development in terms of regeneration frequency, air-fuel ratio control, and regeneration duration. The data, though, seem to be incomplete—sulfur effect is clearly demonstrated by temperature and space velocity is not. A reviewer noted that the team reported many accomplishments that include bench reactor data with model sorbents and engine-dyno data. A global model seems to be a better tool guiding these experiments.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 11 of 14 reviewers)

The interaction of the project team with CLEERS members, the other CLEERS sub-groups, and other national labs was noted by several reviewers. This interaction with the CLEERS group was felt to directly link this work to the comprehensive list of industrial partners with a variety of interests (although one reviewer asked if the industrial partners listed were providing input to the approach and direction). One reviewer said that interactions were very good from a CLEERS workshop level and experimental level, but that LNT modeling has not been very well propagated. "Excellent evolution of CLEERS," said another. One said DOE crosscut team and LNT focus group provide guidance from all OEMs, the LNT supplier group provides catalyst insights, and national lab partners provide fundamental chemistry and analytical capabilities. Finally, a reviewer expressed the opinion that International should be part of the focus group, and that CLEERS should continue to have workshop, at least twice a year.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 11 of 14 reviewers)

Some reviewers felt the future approach was good, saying that the group had a very good understanding of the process and the weaknesses of the work so far, and future plans were good. The future plans are very logical sequences towards fulfilling the overall goal of understanding and optimizing LNT, said a reviewer. A reviewer singled out the fact that many missing items are recognized by the team , such as equivalence of HC and H_2/CO at temperatures above 350°C, and O_2 storage effect (competition with stored NOx for available reductants). One reviewer simply asked the team to keep pressing on, while another said that all the research was very good except the propagation of the LNT modeling code. Reviewers focused on the plans to develop a standard test protocol and to relate global and micro-scale models, and the focus on kinetics and mass transfer limitations. Finally, one reviewer said that although the approach appears sound, the progress appears slow.

Reviewers offered several suggestions on improving the future research. First was, the researchers should consider how aging and sulfation affect the testing data on which the model is based: a model based on data generated on fresh catalyst might provide misleading information. Second, microkinetics and models based on detailed chemistry and physics separated from transport phenomena would be interesting, since ORNL seems to have impressive capabilities.

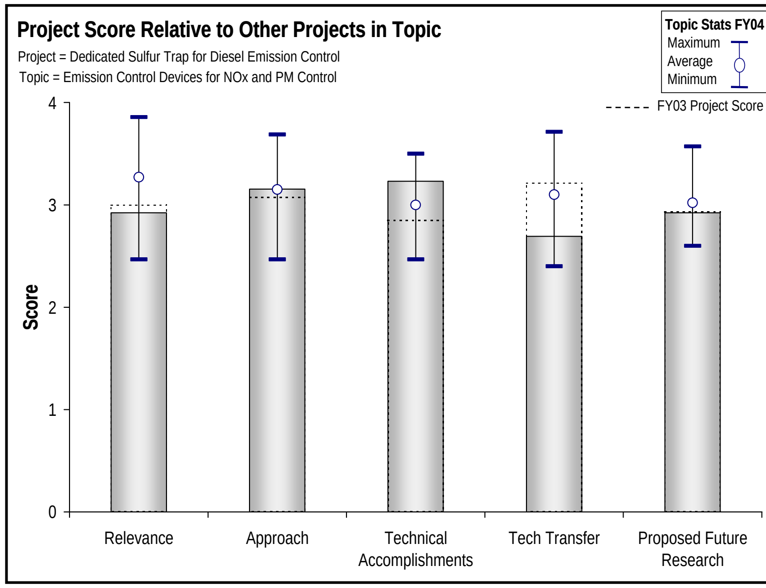
Specific Strengths and Weaknesses (Written responses from 10 of 14 reviewers)

- Specific Strengths
  - Access to experience and instrumentation capabilities within ORNL from other LNT work, linkage through the CLEERS structure to lab, industry and university partners. Vision of the program - starting with fundamentals to get the science right and thereby have a robust model.
  - Very well planned and coordinated work.
  - Good plan and focused investigation.
  - Excellent work in laboratory validation of models. Developing basic understanding of the NOx adsorber catalysts and what controls the system. Developing transport functions for the various species. Excellent teaching.
  - Starting to correlate results with engine tests.
  - Recognized that NH_3 and N_2O by-products need to be incorporated into kinetic models.
  - Very good combination of lab reactor, engine measurements and industry coordination.
  - Unique approach to the LNT. Good interaction with industry with Ron Graves' leadership.
  - Unique facilities, expertise and support from CLEERS partners.
  - Once a representative model is developed, parametric experiments using the model will be a great aid in improving the LNT technology.
- Specific Weaknesses
  - My only concern is the rate of progress. Will this be done fast enough to influence designs considered for vehicles?
  - The number of features that need to be addressed to develop a truly robust LNT model that includes variation in regeneration process, aging, etc., seems beyond the scale of the project as structured. This program should be expanded by providing more support so that more of the key technology issues can be addressed, perhaps by building a separate, complementary program that focuses on aging alone or on development of an elementary reaction model for LNTs.
  - Some elements of the trap formation are not understood.
  - Have not yet grasped that preconditioning is critical to results. An aging model is also required.
  - Chemical kinetics are not enough. Understanding transport phenomena within washcoat is also important.
  - Low emphasis on developing the modeling codes for public use.
  - Probably regenerating too rich, generating more NH_3 than N_2.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 9 of 14 reviewers)

- Incorporate the impact of the type of regen process (e.g., "Post 80" or "DEM") in the regeneration model.
- Work on the necessity of other HC in your models. Look at the competitive adsorption of other HC.
- Can future work be linked to reductant delivery methods? Eventually, it will be important to assess the effectiveness of different reductant delivery strategies.
- Continue to refine model and correlations.
- Understand critical performance limitations as a function of sulfate.
- SV effects have not yet been studied. This is critical for HD NTE emissions!
- Move away from model catalysts to more fully formulated systems.
- Excellent work.
- ORNL should provide an approach to develop the LNT code into a documented, user-friendly code for outside use.
- Need to accelerate the rate of progress to help industry assess LNT maturity towards 2010 emissions targets by May 2005.
- Consider a method to determine the end of LNT regeneration, without over-regeneration.

Dedicated Sulfur Trap for Diesel Emission Control, David King of Pacific Northwest National Laboratory



Brief Summary of Project

The goal of this project is to develop a high-capacity, low-cost sulfur trap to protect lean NOx traps from sulfur contamination. The trap is envisioned to be replaceable at reasonable maintenance intervals (approximately 30,000 miles), and will be compatible with the lean-rich cycling operation of lean NOx traps.

Question 1: Relevance to overall DOE Objectives (Written responses from 11 of 13 reviewers)

One reviewer stated that diesel fuel sulfur is a barrier to emissions control, and fuel sulfur may adversely impact aftertreatment even after ultra-low-sulfur fuels are available. Another reviewer commented that sulfur traps are a technology that needs a breakthrough; this "high-risk work might just provide that breakthrough." One reviewer cautioned that the target SOx trap space velocity and performance need to be clearly defined. An in-line SOx trap would protect advanced aftertreatment devices and enable meeting 2007-2010 standards. Another person commented that SOx traps are critical for current NOx trap technology durability. Another went further to say that this may in fact be an area that is under-appreciated by the DOE. This technology can benefit areas outside diesel emission control (from the jam industry to coal fired boilers). Several reviewers said that protection of the NOx trap is important (assuming NOx traps are the first choice), although many technical issues exist in making this a practical approach. A sulfur trap for the vehicle lifetime, or at least for a certain time (30,000 miles), could be important in case a desulfation strategy fails in real applications. However, two reviewers added that servicing parts is not a good concept. The objective is to protect the NOx-trap so that it can meet the durability requirements. Two reviewers stated that there is an assumption that EPA will allow servicing of the exhaust system at maintenance intervals, and followed with the question of whether EPA would, in fact, accept such a practice.

Question 2: Approach to performing the research and development (Written responses from 10 of 13 reviewers)

Several reviewers stated that the work took an interesting approach, noted that the sulfur trapping properties analyzed in this study are appropriate, and said that cryptomelane was an interesting material. Development of the material to form a high-capacity, low-cost sulfur trap that is compatible with lean/rich cycling was noted by a reviewer as an important advance. The mechanical property of the storage materials seems to be critical to allow the results of the work to further move toward applications. The current material changes its chemical composition after sulfur storage. It was suggested that questions such as how to fix the material in the exhaust stream need to be considered. One person commented on the method that was developed for SOx uptake quantification with a flow reactor system to identify adsorber/absorber materials. One person suggested considering washcoat adhesion after a very large weight gain of the material as a function of sulfur storage. One person noted that the work readily addresses prior-year reviewer comments, has a clear research plan, and showed a thorough analysis of the materials and insightful mechanistic experiments. Another reviewer noted that the approach has been primarily chemical in nature, and that a number of other technical issues must be addressed as a system. A SOx trap is a heat sink in the system and must be placed in front of the NOx adsorber.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 8 of 13 reviewers)

One reviewer had positive comments about the work that developed manganese-based SOx traps that appear to operate with high sulfur removal efficiency. However, there is a need (noted a reviewer) to check performance at high space velocities, conditions typical of heavy-duty not-to-exceed conditions. Due to transport issues, this high space velocity testing should be performed on coated monoliths. Other reviewers commented that there is a need to extend operation to lower temperatures and to high space velocities. Cryptomelane is a promising sorbent material that can achieve good SO_2 uptake, including at 60,000 1/h and 250°C, but it needs more in-depth testing. One reviewer was concerned that the breakthrough capacity at low sulfur concentration is very high, although he went on to further comment "Promising!" Another reviewer stated that the gas chromatograph analysis of SOx is not trivial at all, and that the cryptomelane materials are extremely novel with enormous SOx uptake with key selectivity, which gives these materials a clear competitive advantage. Another noted that there was good progress, a wide range of data collected, and a good job of NOx trap protection.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 8 of 13 reviewers)

Two reviewers noted the CRADA with Caterpillar. Others commented that this area is weak, and suggested that the project could use more interaction with other industries, universities, and other DOE labs. The project team should clarify if the information is being presented at meetings and in journals, said a reviewer. Another noted the very limited scope right now, but as the project is modest, this is not unexpected, he said.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 9 of 13 reviewers)

One reviewer noted that if a sulfur trap is coupled with a NOx trap, it is likely the sulfur trap will be exposed to rich pulses much-richer than had been used in the study, which leads to the question of whether stored sulfur would be released from the material during rich excursions. Another commented, "the future looks promising, several opportunities appear possible, and real-world experience will be needed." Others noted that the essential work packages are addressed and that the researchers recognized the importance of testing on monoliths at low temperature. Another reviewer noted that the researchers need to quantify performance at lower temperature, perform more lean-rich cycling, and suggested moving to monolith form and testing at Caterpillar. The researchers should perform tandem studies with other aftertreatment studies, suggested a reviewer. Another person noted the thrust to put the material on a monolith, fiber or foam is critical in the development of a product. A brief table on spillover benefits of this technology would be useful. One reviewer reinforced the point that developing an aggressive industrial partner may be the necessary next step.

Specific Strengths and Weaknesses (Written responses from 10 of 13 reviewers)

- Specific Strengths
  - Identified a material that seems to meet the project objectives.
  - Great material.
  - Cryptomelane has advantages over most competitive MgO alternative due to markedly better performance in the presence of water.
  - This project has been very successful.
  - Good approach. Novel material evaluation. No precious metals.
  - Good work in the chemistry.
  - SO_2/SO_3 analysis method that allows SOx breakthrough measurement at 100 ppb.
  - Material development.
- Specific Weaknesses
  - The material is damaged by reducing conditions (however, practical LNT regeneration cycles may not hurt the material). Material is not sufficiently active below 300 C.
  - No washcoat adhesion information to date.
  - Not enough details on the regeneration aspects (this may be due to proprietary nature of work).
  - Trap still needs development.
  - It appears that high temperature may have a significant effect on the SOx trapping capability. Limited work on structural capabilities of the material. Material will be in the hot zone of the exhaust, i.e., in front of the NOx system. It is also not clear if this will eliminate the regeneration of the NOx trap.
  - Not applicable to LD applications that have cold start requirements, since SOx-trap is a heat sink and will inhibit warm-up of downstream NOx-trap.
  - All work done at low space velocity on powder samples.
  - $MgSO_4$ water solubility may be an issue if dissolution forms water during shutdown which would lead to transport onto downstream NOx trap.

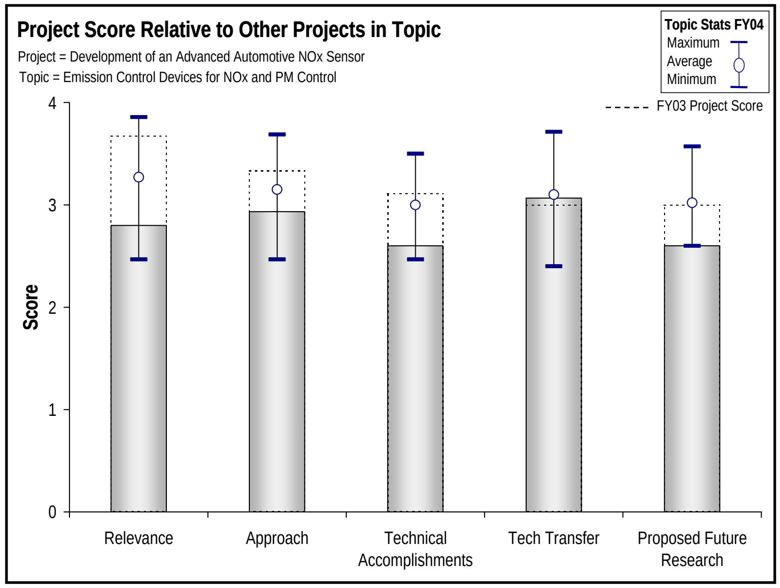
– Thermal durability under forced filter cleaning conditions may be an important system limitation.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 8 of 13 reviewers)

- Work to improve the low temperature capability. With the lack of activity below 300°C, a vehicle at extended idle could release large amounts of SO_2 to the other aftertreatment components and this SO_2 trap would be of no use. Also, should do calculations to translate the present experiment's packed bed tests to supporting the material on a monolith. How much monolith volume is needed, what type of cell density will be needed to provide sufficient contact area?
- A brief table on spillover benefits of this technology to other applications would be useful. This looks like real traction with this novel system. Thermal and vibrational cycling on the absorber on the monolith would clearly demonstrate the robust nature of the system and enhance confidence in a drive of a product to market. A time line with key deliverables on the advance to market and discussion with an industrial partner interested in manufacture of the product would be beneficial (or just a plan for this avenue).
- The investigation of onboard regeneration, as suggested by the researcher, should be pursued.
- Complete work and evaluate real world opportunities.
- Need to think about it as a system, including disposal issues and service issues for a SOx trap. Also need to answer the question of the structural stability of the material and the temperature capability: 500°C may be too low for many applications.
- Test on monoliths at exhaust flow rates of not-to-exceed conditions, based on high space velocity SOx breakthrough, recalculate size of S-trap and determine practicality.
- Keep the program after revising the target application such as space velocity, SO_2 trap capacity, and performance targets so that the target results will be feasible for practical use.

Emission Control Devices for NOx and PM Control

Development of an Advanced Automotive NOx Sensor, Larry Pederson of Pacific Northwest National Laboratory



Brief Summary of Project

In this project, the PNNL team is developing an electrochemical NOx sensor to meet performance targets for sensitivity, range, accuracy/resolution, transient response, cross-sensitivity, lifetime, and cost. The NOx sensor will be needed to monitor combustion processes and emission control effectiveness for future systems.

Question 1: Relevance to overall DOE Objectives (Written responses from 12 of 15 reviewers)

There was general agreement among reviewers that this project is relevant to the DOE program. Many reviewers agreed that a NOx sensor for real-time feedback control of NOx control systems is a significant need as an enabling technology for low emissions, advanced combustion engines. The development of a reliable, low-cost, and durable sensor would be helpful to overall DOE program objectives. However, while the need for the sensor is great, some reviewers questioned whether this project is actually making progress or contributing toward that goal. One reviewer commented that the objectives of this CRADA were not explained specifically enough. Others stated that NOx sensors are already available in the marketplace, thus, the author did not make the case that this work is contributing to NOx sensor designs or that it fits into the overall DOE objectives. Further, since Delphi is a direct beneficiary of the research, Delphi should be shouldering all of the project costs at this point (in this reviewer's opinion). Finally, one commenter recommended that the researcher provide more emphasis on the impact of closed-loop control on fuel efficiency to improve the context of the presentation. For instance, fuel savings calculations for tight engine operation around an emission standard would help drive home this impact.

Question 2: Approach to performing the research and development (Written responses from 9 of 15 reviewers)

One reviewer stated that the approach is very good, high quality, and essentially "leap frogs" current sensor technologies. Positive responses were provided regarding the development of a robust, sensitive, and accurate NOx sensor. The project builds on several years of related work. The development of performance criteria with Delphi was positively viewed. However, several reviewers stated their uncertainty with the specific objectives of the project (i.e., what is in and out of scope) and as a result, whether the project was on target. One reviewer commented that the approach seems rather "Edisonian" in that it is still in the screening process. Another reviewer expressed his belief that the project employs a "pretty standard approach" for an oxygen sensor, and that similar approaches are being used by foreign NOx sensor suppliers. The approach is essentially targeted for addressing oxygen pump performance and sensing electrodes, but experiments were completed entirely on model gases, not realistic exhaust gases or conditions. Another reviewer questioned why the project still seems to be focused on the same design when the design does not seem to be accomplishing the intended goals. Water and carbon dioxide effects are summarized, but little evidence is presented to support these conclusions. Based on an anticipated project completion at the end of 2005, field testing and process capability might be useful if allowed under the agreement with Delphi. Also, the research should include cross-sensitivity to ammonia (a significant deficiency in current sensors) and should be more inclusive of sulfur effects.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 10 of 15 reviewers)

The responses to this question were mixed. Some reviewers stated that the project is making significant progress in a difficult research area. For instance, results of La(Sr)CrO_3 electrode were reported from the parametric studies using different variables. However, the majority of comments indicated uncertainty concerning the accomplishments and progress of this project without more knowledge about the research pathway and plan. The project has done a good job of highlighting challenges, but is it breaking new ground. One response offered that the project has demonstrated NOx sensor performance sensitivity to oxygen partial pressure, which raises questions as to the practicality of the device if oxygen levels must be controlled. Given the current research plan, it is uncertain whether an improved or practical sensor can be realized by the end of the project. Other reviewers raised concerns on whether the accomplishments of this project are significant, and whether the current work complements the Delphi product. While the project has compared base metal oxides as replacements for noble metal electrodes showing the potential for use in the oxygen roughing cell, this will have little use as the sensing electrode. Finally, one reviewer intimated that some repeatability and probe variability studies produced with the same composition and electronics would add value to the research.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 12 of 15 reviewers)

Comments concerning the project's collaboration efforts were generally positive. The project appears to have Delphi as a close working partner for the research. Having such a viable industrial partner is an excellent leverage of government funding. However, some reviewers expressed concern that the project may be very useful to Delphi, but the rest of industry may not receive the full benefits of the work, at least not right away. For this reason, additional diesel industry partnering may be warranted. A few reviewers raised concerns about a lack of interaction with other DOE laboratories and universities. There was also no evidence of publications or presentations resulting from the research to aid in technology transfer efforts.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 6 of 15 reviewers)

While one reviewer deemed the work very relevant to the current status of NOx control systems, another stated that it was unclear how the future research plan serves to overcome the technical barriers in achieving a practical sensor. One reviewer commented that the work appears to repeat proprietary work being done by competing sensor companies. While the future work seems focused on increasing selectivity and sensitivity for NOx, the sensor applications are very limited and thus this focus may not be warranted in addressing it practical use. Other recommendations for future research included studies of sulfur effects (although there does not seem to be enough time left in the project for these studies) and investigations within the "real" rich-lean diesel exhaust regime.

Specific Strengths and Weaknesses (Written responses from 12 of 15 reviewers)

- Specific Strengths
  - A good team with Delphi and PNNL.
  - Solid, interesting work.
  - Electrochemical and materials background of PNNL.
  - Detailed mechanistic work with probing of molecular species by mass spectroscopy is quite impressive. The introduction of the gold to de-sensitize electrode surface is interesting (I assume details on the optimum alloy composition, preparation and diffusion have previously been presented).
  - Using Delphi's expertise in sensor design.
  - Effective collaboration with the industrial partner.
  - The cooperation between Delphi and PNNL appears to be exceptionally good.
  - Expertise on materials and facilities.
- Specific Weaknesses
  - Not enough effort to demonstrate sensor viability under real operational conditions (short rich transients with very high CO/HC levels).
  - Must consider ammonia cross sensitivity if used on currently available NOx aftertreatment (LNT/SCR).
  - Not clear how this work is being integrated into the DOE objectives of lower emissions and improved fuel economy. The program is of major interest to the industry; however, this should have been clearer in the presentation. Perhaps there should be some university interactions in this program.
  - This project does not appear to be going anywhere. This was the most difficult project to evaluate because we cannot see the big picture.
  - Relevance of this work to the development of a practical NOx sensor.
  - The project does not provide any additional value to the technology or our understanding of NOx sensors that are commercially available or being developed elsewhere.

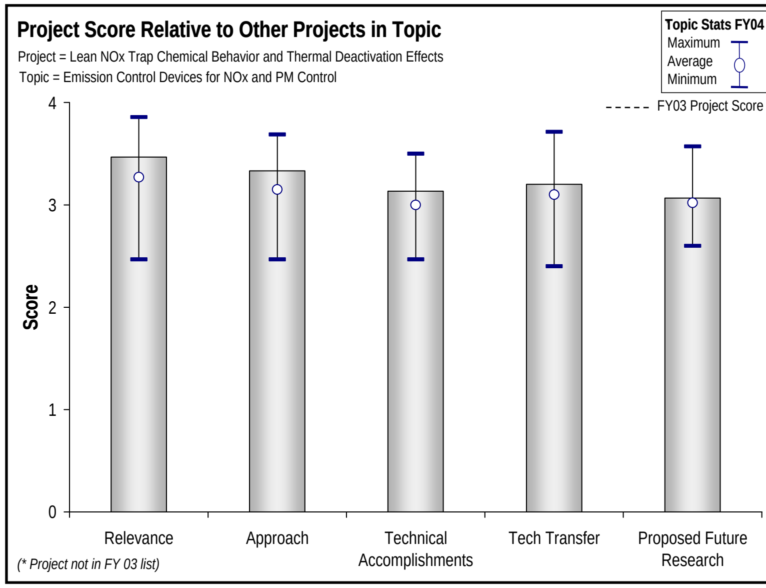
Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 6 of 15 reviewers)

- Clarify the specific barriers to creation of the sensor and their relation to the experiments performed during the project and the results produced.
- Will the standard amperometric sensor work for 2010 NOx emission levels? Measurements of about 0.2 μA/50 ppm NOx were shown. It is likely NOx levels will be less than 10 ppm over the measured emission cycles. Please perform some calculations to see if this type of sensor is viable in a 2010 application.
- Are there any plans to test with streams that are closer to real applications containing soluble organic fraction and particulates? A statement on the critical requirements to go to the market might be used. Currently, does the unit meet the cost requirements for introduction into the market? Are there plans for significant testing time on stream?
- Need to further explore potential interferences in exhaust (CO, HC, SO_2), especially the very high CO/HC levels found in rich diesel exhaust.
- Need to check for interference from NH_3 and N_2O formed under short rich transients.
- Check equivalence of signal from NO and NO_2.
- The value of this work needs to be analyzed based on the prototype NOx sensors being introduced into the market place.
- Since the program is expected to end by FY 2005, it would be good to see whether the group can test and validate the performance of this sensor on a real engine application.

Lean NOx Trap Chemical Behavior and Thermal Deactivation Effects, Todd Toops of Oak Ridge National Laboratory

Brief Summary of Project

The ORNL project team for this research is determining the chemical storage behavior of model catalyst materials at temperatures between 150°C and 400°C. Additionally, regeneration behavior is to be examined, and thermal deactivation effects are to be inspected. This project uses two model catalysts ($PtKAl_2O_3$ and $PtBaAl_2O_3$).



Question 1: Relevance to overall DOE Objectives (Written responses from 11 of 15 reviewers)

Five reviewers' comments underscored the importance they attach to the fundamental nature of the project's investigations. All affirmed the necessity of a detailed understanding of the mechanisms of adsorption, reduction, sulfur poisoning and thermal ageing in lean NOx traps, which one said have the greatest potential to reduce lean-burn engine NOx emissions to regulated levels. Reviewers were likewise generally agreed that the reported work is relevant to DOE objectives and useful in increasing understanding of basic chemical mechanisms. One reviewer termed the project "directly applicable" to the objective of maintaining engine performance while meeting emissions standards. Another anticipated that "good information" can be gleaned from the ORNL work, and called for "more complete analysis" in thermal deactivation investigation. One reviewer, however, did not feel the presentation adequately showed how "this data leads to improved mechanisms."

Question 2: Approach to performing the research and development (Written responses from 12 of 15 reviewers)

There was broad approval among the reviewers of the approach employed in this project. One termed it "solid" and another "very good." Others identified for specific praise: the DRIFTS work; the linkage to related projects at ONRL; its equipment and tools; the use of argon in nitrogen detection; analysis of intermediate species on the catalyst; and the project's combination of detailed speciation with integrated engine and aftertreatment. Five reviewers directly or indirectly raised the question of whether results from work with powder catalysts would be fully representative of results with monolithic catalyst "bricks." Three of those reviewers specifically recommended that the project validate results from catalyst powder tests on monoliths. One mentioned employing an "integral reactor," and one recommended that LNTs be obtained from one or more automotive catalyst suppliers. The latter predicted that results would be found to differ, due in part to the influence of particle size in both precious metal and alkali oxide catalysts on adsorption, regeneration and ageing rates. (This reviewer surmised that experimental catalysts from project partner EmeraChem would be found to have larger particle sizes and different washcoats from automotive catalysts, which also contain cerium oxides capable of storing oxygen.) The third reviewer recommended correlating the powder catalyst results of this project with work done elsewhere on monoliths. A reviewer also questioned whether, in view of the continuing development of LNTs, the model catalyst used here is representative of the current state of the art. This reviewer urged that catalyst morphology changes induced by ageing be tied into the investigation. One reviewer questioned remarks made in the presentation appendix, saying they were inconsistent with other published data, which typically show that desulfating potassium-based catalysts is very difficult. This reviewer also urged special attention be given to achieving a complete sulfur balance during experimental desulfations.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 12 of 15 reviewers)

One reviewer felt it too early to assess the project's accomplishments, but said the technical and analytical system provided a basis for successful work. Others implicitly agreed, expressing optimism at the promise of future work and the value of anticipated results. One reviewer said progress so far had been good in light of the available budget. The "good, detailed understanding of mechanisms" was an accomplishment cited by one reviewer, who looked forward to presentation of sulfur data. Two mentioned development of the PF/DRIFTS reactor, one the study of the low-temperature behavior of the potassium-based catalyst, and one the development of instrumentation for the project studies. The mechanistic insights developed into NOx storage via a barium peroxide intermediate and the correlation of NOx reduction with hydrogen disappearance were accomplishments noted by one reviewer. Two other reviewers mentioned, respectively, the number of catalyst materials and operating conditions that had been investigated, and the demonstration of LNT thermal deactivation. Finally, one reviewer expressed appreciation for the appendices to the presentation.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 11 of 15 reviewers)

Five comments reflected reviewers' belief that the project showed particularly good collaboration with the CLEERS focus project. One reviewer believed this, in turn, led to significant industry interaction. A second expressed the view that CLEERS has successfully promoted strong collaboration among national labs and various levels of industry. Two other reviewers urged that the researchers [continue to] transfer the data developed in this project to CLEERS and to ensure the CLEERS LNT focus group remained engaged in the project. Project interfaces with EmeraChem were noted in two comments, and with MECA in one.

Suggestions for improving and increasing collaboration included three comments encouraging additional input from catalyst suppliers, including a direct collaboration with such a company in measurement and modeling. Also suggested were collaboration with an engine builder, with other industrial partners (unspecified) and with universities, the last being considered particularly appropriate in light of the detailed, mechanistic investigations undertaken in this project. Two reviewers felt the project had been effective in reporting results in the literature.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 11 of 15 reviewers)

Two reviewers felt, respectively, that the proposed future work covered "the relevant points," and that the new reactor would help advance that work. Another said identification of competing species on trap surfaces when SO2 was introduced would be "extremely important," and a fourth said the same of "sulfur effects," washcoated substrates and thermal deactivation. There was another comment expressing interest in the addition of sulfur effects to future work. Four comments recommended particular areas for future investigation, including 1) a transition to monolith catalysts, 2) obtaining and testing an automotive supplier-produced LNT and collaborating directly with an industry LNT modeling effort, 3) evaluating the low-temperature storage behavior of a barium-based catalyst, and 4) examining storage kinetics, particularly during the early storage phase. The reviewer based the last suggestion on the fact that an LNT would have to achieve better than 90% efficiency, which means that "only storage sites responsible for early-phase storage" are used.

Specific Strengths and Weaknesses (Written responses from 12 of 15 reviewers)

- Specific Strengths
  - Powerful tool to understand catalyst operation.
  - Tremendous experimental capability – provides key insights.
  - DRIFTS work.
  - Detailed mechanistic experiments extract key intermediates and kinetics of trapping and conversion at catalyst surfaces.
  - Solid research team, good equipment.
  - Good basic results on catalyst systems aid understanding of fundamental behavior.
  - Actual measurement of N_2 formation.
  - Analytical system, highly structured approach.
  - Ageing and low-temperature studies.
  - ORNL has very good range of experimental and modeling work – a major strength.
- Specific Weaknesses
  - Limitation to pre-competitive materials – development of these continues. Thermal deactivation of materials without advanced stabilizers, promoters may not be representative.
  - Groundwork shows clearly in results, but additional follow-through needed to bring same to fruition. (If

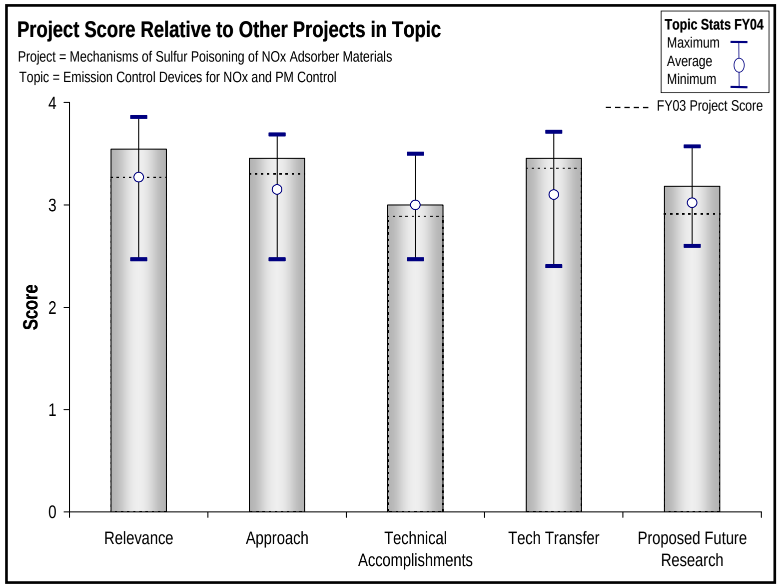
industry partners don't want this information disclosed, PI should make same clear.)
  - Need "fully formulated" catalysts to test, or catalysts nearly fully formulated.
  - Regeneration work with saturated catalyst has little meaning for real-world application, where periodic reduction will occur at a small fraction of NOx saturation.
  - Oxygen storage of model catalysts may not be typical of production automotive catalysts.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 9 of 15 reviewers)

- To more fully understand thermal deactivation mechanism, perform morphological examination in concert with thermal deactivation tests.
- XPS (or other surface material composition analysis) would be useful during sulfur effects studies. (such measurements helped understanding of three-way catalyst deactivation and development of accelerated ageing protocols for TWCs.)
- Would it be possible, perhaps through collaborations, to employ complementary probing techniques (e.g., metal NMR, DR-UV-vis, classic isotope labeling followed by IR or XANES/EXAFS) in conjunction with IR experiments?
- Perform more complete analysis of thermally deactivated materials.
- Drive to use monoliths instead of powders will be very important.
- Clearly laid-out plan to collaborate with outside modeling experts would help.
- Develop collaborative measurement/modeling project with a supplier or engine builder.
- Question of possible interactions with stabilizers, binders in alumina and interactions with platinum and potassium will assume greater importance when transition to monoliths is made.
- Evaluate powders representative of commercial catalysts..
- Measure potassium remaining on catalyst after 900°C treatment.
- If nitrate formation is not limiting at low temperatures, why is there no NO_2 slip prior to saturation?
- If N_2 formation isn't observed below 250°C, what is nitrogen-containing product of storage/release reaction?
- Complete sulfur balance, especially in case of potassium-based catalyst. Need to know what's going in and what's coming out.

Emission Control Devices for NOx and PM Control

Mechanisms of Sulfur Poisoning of NOx Adsorber Materials, Charles Peden of Pacific Northwest National Laboratory



Brief Summary of Project

The focus of this work is on identifying and understanding the degradation mechanisms of NOx adsorber materials with respect to high-temperature operation and sulfur poisoning. The team is developing an understanding of the mechanisms and applying this to new formulations, and is developing protocols and tools for failure analysis of used catalysts.

Question 1: Relevance to overall DOE Objectives (Written responses from 8 of 11 reviewers)

A reviewer commented that the project has the right focus for development of LNT technology. The collaboration with a major catalyst supplier and Cummins is promising for the work. One person thought that this fundamental understanding of sulfur poisoning of materials is an important function for the DOE to lead. Another reviewer agreed, adding that understanding the poisoning of NOx adsorber materials is critical to implementation of LNT systems and therefore is critical to advanced combustion engine development. Another added that the objective of understanding deactivation mechanisms (thermal and sulfur poisoning) of NOx adsorbers is key to development of a durable product. The final comment was that this work is directly applicable to low-NOx engines and maintaining engine efficiency, and is focused on a critical problem - the degradation of NOx adsorber catalysts. Another reviewer simply stated that this is very relevant and timely work.

Question 2: Approach to performing the research and development (Written responses from 9 of 11 reviewers)

One reviewer felt that the approach is good but that it needs to mimic real-life exhaust gas environments a bit better. One person simply stated that there is a solid team and technical approach. Another person noted that the group utilized characterization tools available at PNNL to study catalyst properties of both model and "real." Another reviewer commented that the group has taken an excellent approach and has included a catalyst company, national laboratory, and engine evaluation. He went on to add that the group has also developed protocols for failure analysis for used catalysts. The researchers started with model and representative catalysts as well as home-grown materials. The researchers are doing a detailed examination of the materials, including structural and chemical analyses of surfaces of as-received, sulfated and thermally aged samples. Reviewers felt that the researchers have taken a very good approach which includes the essential deactivation assessment techniques. It also includes "representative" samples with enhancements that would not be present in the model systems, so insights will be more relevant to the field. Another reviewer thought the work was very practically oriented, which leads to information directly applicable to products. The researchers used extremely thorough probing of the surfaces with an array of complementary techniques. It is clear that there is a lot of work here that cannot be discussed due to proprietary issues. The results show classic development of structure-reactivity models. The final reviewer commented that good analytical capabilities are available in the project. The reactions between storage materials and washcoats (among other factors) are reported and have often been shown elsewhere, so the presented results are not new. Model catalysts with presented weaknesses are only a little bit helpful, but the analysis and the presentation of these proprietary results are obviously not allowed. This makes it difficult to give a fair evaluation. The 1-minute switching time between lean and rich in the test rig is not realistic (2-5 seconds is normal depending on the depth of Lambda); the 1:4 ratio gives unrealistic results, therefore the experimental test set-up must be improved.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 8 of 11 reviewers)

One reviewer commented that the work characterized the various samples in a new reactor and with a broad range of techniques. The team observed $BaAl_2O_4$ formation at higher temperature for the model catalyst. Another commented that the results demonstrated severe thermal deactivation of both model and "real" catalysts, although the fully formulated catalyst was "better." One person was impressed by the results, stating that the project investigators developed copious results in a relatively short time, which was very impressive work in less than one year. One reviewer said that it appears that the team had investigated the more representative LNT and was unfortunately not willing to show it, so this reviewer assumed good progress was made. Several reviewers commented that it is difficult to assess the progress due to CRADA protection of confidential work.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 9 of 11 reviewers)

One reviewer noted the close collaboration with Johnson Matthey and Cummins, including regularly scheduled progress meetings. Another added that this type of collaboration with catalyst manufacturers is difficult and that this was good work. Another felt that the team had taken a well balanced approach, including a national laboratory, catalyst supplier and engine company. A reviewer added he presumes valuable results will be achieved in the project, but cannot be presented here. The final comment was that the research team readily disseminates practical/experimental advice/details to the scientific community within the confines of proprietary information control, although clarification of presentations and publications would be useful.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 7 of 11 reviewers)

One of the reviewers commented that the group will perform thermal and sulfur poisoning of the Johnson Matthey catalysts, however, given that the presentation omitted details on the Johnson Matthey "representative" catalysts, it appeared to this reviewer that this future work will not be publicly available. He expressed concern that the lessons learned will not be available to the general community. Another felt that the detailed milestone schedule with CRADA partners sounded like a structured and focused path forward. The detailed mechanistic work with Johnson Matthey is something he looks forward to hearing about next year. Another person added that these types of projects are well addressed and will help to improve LNT development. Several reviewers commented that it is difficult to judge the milestones due to the CRADA.

Specific Strengths and Weaknesses (Written responses from 10 of 11 reviewers)

- Specific Strengths
  - Use of the broad spectrum of material, chemical and performance measures of deactivation of the LNT catalyst, which provides the opportunity to understand the physical and chemical aspects of the aging processes.
  - Good collaboration with Johnson Matthey. PNNL analytic tools and catalyst expertise.
  - The breadth and depth of the work is remarkable. From mechanisms to detailed molecular structures to new test protocols.
  - They seem to have useful tools to study these catalysts.
  - Strong engine/catalyst partnership.
  - Excellent tools, excellent technical approach using model and improved catalysts. Systematic method of developing understanding of the aging of the catalyst samples.
  - Close cooperation between OEM, catalyst manufacturer and National Lab.
  - Use of both model and fully formulated catalyst.
  - Strong integration with industrial partners.
- Specific Weaknesses
  - Aging in air for thermal pretreatment. Why not include a more complex and realistic aging process that includes periodic exposure to rich conditions to incorporate the impact of regeneration? An example of such aging techniques was that of Allied Signal in aging of three-way catalysts, where they used a high temperature + "rich-fuel cut" cycle process where they would run hot and swing stoichiometry. This could devastate a catalyst and provide very rapid aging.
  - The differences between the model catalyst and the representative catalyst do make you wonder is this the best model system that could be used?

– Limited value beyond Cummins
– Difficult to access due to CRADA protection.
– Experimental test set up is poor. Lean/rich cycling timing must be improved. Present status is not realistic.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 6 of 11 reviewers)

- Extend the thermal aging of the catalyst to include high temperature lean/rich cycling to increase the severity of the aging conditions.
- The kinetics of thermal deactivation need to include the realistic amounts of water at operating temperatures.
- Comparison to samples in the field with known histories will be extremely useful in the probing and repetition of deactivation processes in the lab.
- The aging exo to the testing apparatus is nice since it allows more parallel processing, which made me think is this possible in my work.
- May want to consider methods of lowering the overall cost of the system, effect of platinum on the results.

ADVANCED COMBUSTION ENGINE R&D MERIT REVIEW AND PEER EVALUATION

Evaluation Form **May 2004**

TOPIC: ______________________________

PRESENTER: ______________________________

REVIEWER NAME: ______________________________

Using the following criteria, please rate the **work** presented in the context of the program objectives. Please provide **specific** comments to support your evaluation.

1. Relevance to overall DOE objectives.

Numeric rating (circle one below)
4 = Outstanding, the project is sharply focused on one or more key technical barriers to development of clean, efficient CIDI engines.
3 = Good, most aspects of the project will contribute to significant progress in overcoming these barriers.
2 = Fair, some aspects of the project may lead to progress in overcoming some barriers.
1 = Poor, the project is very unlikely to make significant contributions to overcoming the barriers.

Specific comments

2. Approach to performing the research and development

Numeric rating (circle one below)
4 = Outstanding, it is difficult for the approach to be improved significantly.
3 = Good, the approach is generally well thought out and effective, but could be improved in a few areas.
2 = Fair, the approach has significant weaknesses.
1 = Poor, the approach is not responsive to the project objectives.

Specific comments

3. Technical Accomplishments and Progress toward project and DOE goals

Numeric rating (circle one below)
4 = Outstanding, the project has made excellent progress toward overcoming one or more key CIDI program technical barriers; progress to date suggests that the barrier(s) will be overcome.
3 = Good, the project has shown significant progress toward overcoming barriers.
2 = Fair, the project has shown a modest amount of progress in overcoming barriers, and the overall rate of progress has been slow.
1 = Poor, the project has demonstrated little or no progress toward overcoming the barriers.

Specific comments

4. Technology Transfer/Collaborations with industry, universities, and other laboratories

Numeric rating (circle one below)
4 = Outstanding, close coordination with other institutions is in place; industrial partners are full participants.
3 = Good, some coordination exists; full coordination could be accomplished fairly quickly.
2 = Fair, some coordination exists; full coordination would take significant time and effort to initiate.
1 = Poor, most or all of the work is done at the Lab with little outside interaction.

Specific comments

5. Approach to and Relevance of Proposed Future Research

Numeric rating (circle one below)
4 = Outstanding, future work plan builds on past progress and is sharply focused on one or more key CIDI program technical barriers.
3 = Good, future work plan builds on past progress and generally addresses removing or diminishing barriers in a reasonable timeframe.
2 = Fair, future work plan may lead to improvements, but should be better focused on removing or diminishing key barriers within a reasonable time period.
1 = Poor, future work plan has little relevance or benefit toward eliminating barriers.

Specific comments

6. Specific Strengths of This Research

7. Specific Weaknesses of This Research

8. Specific Recommendations or Additions/Deletions to Work Scope

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Acronym	*Definition*
A/F	Air/fuel ratio
AHRR	Average Heat Release Rate
ANL	Argonne National Laboratory
APS	Advanced Photon Source
CA	Crank Angle
CDPF	Catalyzed Diesel Particulate Filter
CFD	Computational Fluid Dynamics
CHAD	Computational Hydrodynamics for Advanced Design
CHEMKIN	Chemical Kinetics software
CI	Compression Ignition
CIDI	Compression Ignition Direct Injection
CLEERS	Crosscut Lean Exhaust Emission Reduction Simulation
CO	Carbon monoxide
CR	Compression Ratio
CRADA	Cooperative Research and Development Agreement
CR-FIE	Common Rail Fuel Injection Equipment
DDC	Detroit Diesel Corporation
DECSE	Diesel Emission Control-Sulfur Effects
DME	Dimethyl ether
DOC	Diesel oxidation catalyst
DOE	U.S. Department of Energy
DPF	Diesel particulate filter
DRIFTS	Diffuse Reflectance Infrared Fourier Transform Spectroscopy
EERE	DOE Office of Energy Efficiency and Renewable Energy
EGR	Exhaust Gas Recirculation
ELS	Elastic Light Scattering
EPA	U.S. Environmental Protection Agency
FTP	Federal Test Procedure
FY	Fiscal year
HC	Hydrocarbons
HCCI	Homogeneous Charge Compression Ignition
HD	Heavy-duty
HDD	Heavy-duty Diesel
HSDI	High Speed Direct Injection
ICEM	Computational fluid dynamic software company
IVC	Inlet Valve Closing
KIVA	Modeling code developed at Los Alamos
LANL	Los Alamos National Laboratory
LD	Light-duty
LDRD	Laboratory Directed Research and Development
LEP	Low-Emission Partnership
LES	Large Eddy Simulation
LIBS	Laser Induced Breakdown Spectroscopy
LID	Laser Induced Desorption
LIDELS	Laser Induced Desorption with Elastic Light Scattering
LIF	Laser Induced Fluorescence

Acronym	*Definition*
LII	Laser Induced Incandescence
LLNL	Lawrence Livermore National Laboratory
LNT	Lean NOx Trap
LTC	Low-Temperature Combustion
MECA	Manufacturers of Emission Controls Association
MK	Modulated Kinetics
MOU	Memorandum of Understanding
NOx	Oxides of nitrogen
NSF	National Science Foundation
OEM	Original Equipment Manufacturer
ORNL	Oak Ridge National Laboratory
PCCI	Premixed Charge Compression Ignition
PDF	Probability Density Function
PI	Principal Investigator
PLIF	Planar Laser-Induced Fluorescence
PM	Particulate matter
PNNL	Pacific Northwest National Laboratory
R&D	Research and Development
RCM	Rapid Compression Machine
RPECS	Rapid Prototyping Engine Control System
SAE	Society of Automotive Engineers
SCCI	Stratified Charge Compression Ignition
SCR	Selective Catalytic Reduction
SI	Spark ignition
SNL	Sandia National Laboratories
SOF	Soluble Organic Fraction
SpaciMS	Spacially Resolved Capillary Inlet MS
SV	Space Velocity
TARDEC	U.S. Army Tank Automotive Research, Development, & Engineering Center
TEOM	Tapered Element Oscillating Microbalance
UNIBUS	Uniform Bulky Combustion System
USCAR	U.S. Council for Automotive Research
UW	University of Wisconsin
UW/ERC	University of Wisconsin Engine Research Center
VVA	Variable Valve Actuation
WSU	Wayne State University
XRD	X-Ray Diffraction
ZDDP	Zinc dialkyldithiophosphate

A Strong Energy Portfolio for a Strong America

Energy efficiency and clean, renewable energy will mean a stronger economy, a cleaner environment, and greater energy independence for America. By investing in technology breakthroughs today, our nation can look forward to a more resilient economy and secure future.

Far-reaching technology changes will be essential to America's energy future. Working with a wide array of state, community, industry, and university partners, the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy invests in a portfolio of energy technologies that will:

- Conserve energy in the residential, commercial, industrial, government, and transportation sectors
- Increase and diversify energy supply, with a focus on renewable domestic sources
- Upgrade our national energy infrastructure
- Facilitate the emergence of hydrogen technologies as vital new "energy carriers."

The Opportunities

Biomass Program
Using domestic, plant-derived resources to meet our fuel, power, and chemical needs

Building Technologies Program
Homes, schools, and businesses that use less energy, cost less to operate, and ultimately, generate as much power as they use

Distributed Energy & Electric Reliability Program
A more reliable energy infrastructure and reduced need for new power plants

Federal Energy Management Program
Leading by example, saving energy and taxpayer dollars in federal facilities

FreedomCAR & Vehicle Technologies Program
Less dependence on foreign oil, and eventual transition to an emissions-free, petroleum-free vehicle

Geothermal Technologies Program
Tapping the Earth's energy to meet our heat and power needs

Hydrogen, Fuel Cells & Infrastructure Technologies Program
Paving the way toward a hydrogen economy and net-zero carbon energy future

Industrial Technologies Program
Boosting the productivity and competitiveness of U.S. industry through improvements in energy and environmental performance

Solar Energy Technology Program
Utilizing the sun's natural energy to generate electricity and provide water and space heating

Weatherization & Intergovernmental Program
Accelerating the use of today's best energy-efficient and renewable technologies in homes, communities, and businesses

Wind & Hydropower Technologies Program
Harnessing America's abundant natural resources for clean power generation

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