2005

MERIT REVIEW & PEER EVALUATION REPORT

ADVANCED COMBUSTION ENGINE PROGRAM

Less dependence on foreign oil, and eventual transition to an emissions-free, petroleum-free vehicle

FreedomCAR and Vehicle Technologies Program

U.S. Department of Energy
Energy Efficiency and Renewable Energy
Bringing you a prosperous future where energy is clean, abundant, reliable, and affordable

FreedomCAR & Fuel Partnership

21st CENTURY TRUCK PARTNERSHIP

Department of Energy

Washington, DC 20585

October 5, 2005

Dear Colleague:

This document summarizes the comments provided by the Review Panel for the FY 2005 Department of Energy (DOE) Advanced Combustion Engine R&D Merit Review and Peer Evaluation Meeting, the "ACE Review," held on April 19-21, 2005 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) 2006. 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 2006.

The table below lists the projects discussed at the review and the major actions to be taken during the upcoming fiscal year. Panel member comments have been consolidated and are not attributed to individuals.

This review covers only national laboratory projects funded under the Advanced Combustion Engine Sub-Program 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	
Automotive HCCI Combustion Research (Richard Steeper, Sandia National Laboratories)	Continue project – Compare performance of different GDI injector types for HCCI; consider whether fuel volatility effects or kinetics should be addressed; present the limitations as well as the advantages of PDF method for this project in next review.
Automotive Low Temperature Diesel Combustion Research (Paul Miles, Sandia National Laboratories)	Continue project – Characterize CO reduction mechanisms and complete turbulent stress model assessment.
Characterization of Early Injection, Low Temperature HD Diesel Combustion Using Multiple Optical Diagnostics (Mark Musculus, Sandia National Laboratories)	Continue project – Investigate the relative importance of various in-cylinder conditions in emissions of unburned hydrocarbons; collect experimental data to support modeling done in collaboration with University of Wisconsin.
Developing Ultrafast Phase-Contrast Imaging of Diesel Injectors (Jin Wang, Argonne National Laboratory)	Work presented was not funded by FCVT. Will be considered for further development with FCVT support in FY 2007 if funding is available.
HCCI and Stratified Charge CI Engine Combustion Research (John Dec, Sandia National Laboratories)	Continue project – Investigate the potential of fuel with two-stage ignition to achieve higher power without knock. Investigate boundary-layer effects on heat-release rate in HCCI combustion.
High Efficiency Clean Combustion (HECC) in a Multi-Cylinder Diesel Engine (Robert Wagner, Oak Ridge National Laboratory)	Continue project – Characterize fueling and EGR parameters to expand the operating range of high efficiency clean combustion modes and improve transitions within and between combustion modes. Strengthen bridge to modeling and fundamental research.
Kinetic Modeling of Combustion of Practical Hydrocarbon Fuels (Charles Westbrook, Lawrence Livermore National Laboratory)	Continue project – Continue refining diesel fuel surrogate and low-temperature chemistry impacts on HCCI kinetics.
KIVA4 Development (David Torres, Los Alamos National Laboratory)	Continue project – Complete parallelization of KIVA-4; demonstrate a full engine cycle using multiple meshes; compare algebraic stress turbulence models to Paul Miles' experimental data.

Topic Title and Organization	FY 2005 Major Actions
Modeling of HCCI and PCCI Combustion Processes (Dan Flowers, Lawrence Livermore National Laboratory)	Continue project – Improve soot formation model by adding polycyclic aromatics; consider possible future approaches to enable model to run using typical computing capability.
Optimized Free Piston Engine Generator (Hans Aichlmayr, Sandia National Laboratories)	Continue project – Investigate coupling stability of opposed-piston design; optimize port-scavenged configuration with CFD modeling; improve estimates of fuel economy and emissions impact; seek industrial partner.
Recent Progress of X-Ray Fuel Spray Characterization at Argonne (Chris Powell, Argonne National Laboratory)	Continue project – Clarify connection between project results and improvement of combustion; expand collaboration with colleagues having expertise in fuel sprays.
Soot Formation at High EGR Low Temperature Conditions (Lyle Pickett, Sandia National Laboratories)	Continue project – Investigate effects of pre-ignition on combustion and soot formation of second-main injection; investigate the effect of boost on soot formation under high-EGR conditions.
Spark Assisted Low Temperature Combustion (Bruce Bunting, Oak Ridge National Laboratory)	Continue project – Further develop the understanding of controlled ignition assist to broaden HCCI operating range. Use nonlinear analysis to investigate combustion instabilities during transition to HCCI. Strengthen industrial collaboration.
The Direct Injection Hydrogen Engine-A Worthy Choice for Transportation Power (Steve Ciatti, Argonne National Laboratory)	Continue project – Use VisioScope measurements to attempt to identify timing and location of combustion non-homogeneities, with particular focus on high-speed, high-load operation.
Emission Control Devices for NOx and PM Control	
Advanced NOx Control for Diesel Engines (Darryl Herling, Pacific Northwest National Laboratory)	Discontinue project – Funds were not requested for the Off-Highway line and therefore no activities are planned for FY 2006.
Characterizing NOx Adsorber Regeneration and Desulfation (Shean Huff, Oak Ridge National Laboratory)	Continue project – Correlate reductant species with LNT performance for engine-based regeneration strategies. Refine regeneration strategies to improve fuel specific NOx reduction.
CLEERS Activities and Progress (Stuart Daw, Oak Ridge National Laboratory)	Continue project – Continue coordination of focus groups. Continue developing LNT kinetics data to support model development. Proceed with implementation of LNT standard protocol and its integration with aging and desulfation.
Development of an Advanced Automotive NOx Sensor (Larry Pederson, Pacific Northwest National Laboratory)	Project completed in FY 2005
Diesel Soot Filter Characterization and Modeling (Mark Stewart, Pacific Northwest National Laboratory)	Continue project – Emphasize tech transfer to industry.
Fundamental Studies of NOx Adsorber Materials (Chuck Peden, Pacific Northwest National Laboratory)	Continue project – Develop clear schedule and milestones for upcoming work. Increase supplier collaboration.
Fundamental Study of Lean NOx Trap Deactivation (Todd Toops, Oak Ridge National Laboratory)	Continue project – Characterize sulfur poisoning effects with respect to NOx conversion, surface species, and desulfation species, temperature and time. Correlate fuel penalty to desulfation parameters. Coordinate with related project at PNNL.
Hydrocarbon-Based DeNOx Catalysis using Diesel Fuels (Chris Marshall, Argonne National Laboratory)	Discontinue project – Program will pursue technical alternatives to CuZSM-5 at high C/N ratio exhaust mixtures that may have higher potential conversion efficiency.
Intra-channel Evolution of Carbon Monoxide & Its Implication on Regeneration of Lean NOx Traps (Jae Soon Choi, Oak Ridge National Laboratory)	Continue project – Apply techniques to a more realistic bench gas mix. Include NH_3 and N_2O. Consider this technique for DeSOx investigation.
Mechanisms of Sulfur Poisoning of NOx Adsorber Materials (Chuck Peden, Pacific Northwest National Laboratory)	Continue project – Clarify test methods and analytical approaches and edit down content in future presentations.

We are still considering the date and location for the FY 2006 ACE review and will follow-up with an email on this matter shortly. 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 2005 meeting.

Thank you for participating in the FY 2005 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 2006 review.

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Introduction

This report is a summary and analysis of comments from the Advisory Panel at the FY 2005 DOE National Laboratory Advanced Combustion Engine R&D Merit Review and Peer Evaluation, held April 19-21, 2005 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 2005 accomplishments and FY 2006 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
Rakesh Aneja	Detroit Diesel Corporation
Chinu Bhavsar	Ford Motor Company
Richard Blint	General Motors Corporation
Andre Boehman	Penn State University
Phil Bohl	Phil Bohl Services
Brian Bolton	Nissan Technical Center North America
Joseph Bonadies	Delphi Corporation
Matthew Brusstar	U.S. Environmental Protection Agency
Tytus Bulicz	International Truck and Engine Corporation
John Cavataio	Ford Motor Company
Karl Fiegenschuh	Ford Motor Company
David Foster	University of Wisconsin-Madison
Craig Haberger	Caterpillar, Inc.
Carl-Anders Hergart	General Motors Corporation
Jonathan Male	General Electric Company
Clark Midkiff	University of Alabama
Heinz Oelschlegel	DaimlerChrysler Corporation
Roy Primus	General Electric Corporation
Giorgio Rizzoni	Ohio State University
Anthony Rodman	Caterpillar, Inc.
Michael Royce	Albion Associates LLC
Peter Schihl	U.S. Army TARDEC
Walter Weissman	ExxonMobil
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 24 project presentations were given at the meeting, and a total of 359 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 2005 for the fourteen 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	*Automotive HCCI Combustion Research*: Dick Steeper, Sandia National Laboratories	3.42	3.26	3.26	3.00	3.26
9	*Automotive Low Temperature Diesel Combustion Research:* Paul Miles, Sandia National Laboratories	3.82	3.77	3.59	3.65	3.47
13	*Characterization of Early Injection, Low Temperature HD Diesel Combustion using Multiple Optical Diagnostics:* Mark Musculus, Sandia National Laboratories	3.75	3.45	3.40	3.50	3.45
17	*Developing Ultrafast Phase-Contrast Imaging of Diesel Injectors:* Jin Wang, Argonne National Laboratory	3.40	3.45	3.25	2.70	3.15
22	*HCCI and Stratified Charge CI Engine Combustion Research:* John Dec, Sandia National Laboratories	3.86	3.67	3.67	3.71	3.57
26	*High Efficiency Clean Combustion (HECC) in a Multi-Cylinder Diesel Engine:* Robert Wagner, Oak Ridge National Laboratory	3.17	3.00	3.00	3.06	2.94
30	*Kinetic Modeling of Combustion of Practical Hydrocarbon Fuels:* Charles Westbrook, Lawrence Livermore National Laboratory	3.65	3.65	3.47	3.18	3.29
34	*KIVA4 Development:* David Torres, Los Alamos National Laboratory	3.13	3.27	3.00	3.13	3.13
38	*Modeling of HCCI and PCCI Combustion Processes:* Dan Flowers, Lawrence Livermore National Laboratory	3.67	3.62	3.43	3.57	3.38
42	*Optimized Free Piston Engine Generator:* Hans Aichlmayr, Sandia National Laboratories	2.07	2.93	2.64	1.14	2.14
46	*Recent Progress of X-Ray Fuel Spray Characterization at Argonne:* Chris Powell, Argonne National Laboratory	3.14	3.24	3.00	3.52	3.29
51	*Soot Formation at High EGR Low Temperature Conditions:* Lyle Pickett, Sandia National Laboratories	3.88	3.71	3.82	3.71	3.65
54	*Spark Assisted Low-Temperature Combustion:* Bruce Bunting, Oak Ridge National Laboratory	3.39	3.15	3.15	2.62	3.23
57	*The Direct Injection Hydrogen Engine: A Worthy Choice for Transportation Power:* Steve Ciatti, Argonne National Laboratory	2.79	2.64	2.07	3.21	2.36
	Average Score for This Category	**3.40**	**3.37**	**3.23**	**3.17**	**3.20**

Overall Program Scores

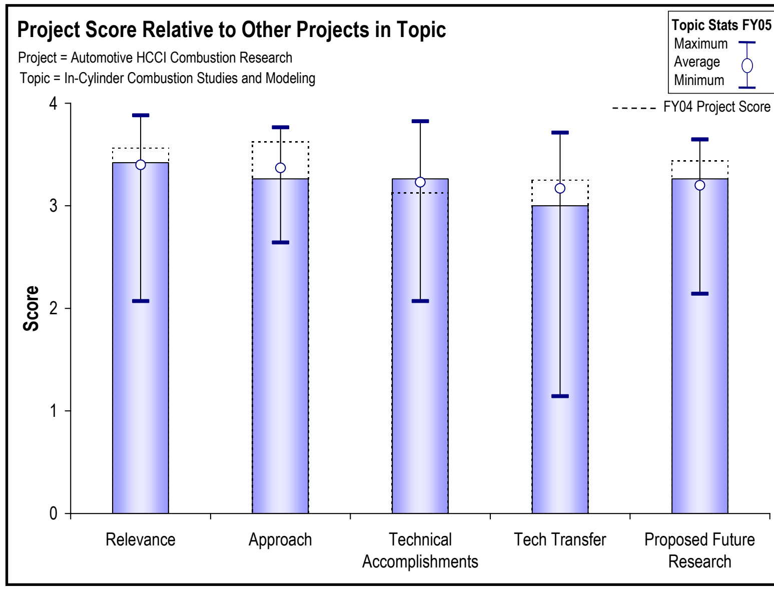
	Q1 Relevance Score	Q2 Approach Score	Q3 Technical Accomplishments Score	Q4 Tech Transfer Score	Q5 Future Research Score
Overall Program Average	3.36	3.34	3.14	3.14	3.13
Overall Program Maximum	3.88	3.77	3.82	3.86	3.65
Overall Program Minimum	2.07	2.64	2.07	1.14	2.14

In-Cylinder Combustion Studies and Modeling

Automotive HCCI Combustion Research, Dick Steeper of Sandia National Laboratories

Brief Summary of Project

The focus of this project is to understand the relationship between charge preparation and the resulting combustion and emissions performance in automotive HCCI[1] engines. The current work is implementation of stratified mixing to reduce emissions during low-load HCCI operation. An emissions bench has been acquired for the automotive HCCI laboratory, and the team continues to develop optical diagnostics for application in HCCI engines.



Question 1: Relevance to overall DOE Objectives (Written responses from 11 of 19 reviewers)

The comments regarding the relevance of this work to overall DOE objectives showed that this project has high importance. One person commented that OEMs follow this work closely because HCCI-like engine technologies will most likely be implemented in the future. Another added that HCCI studies may enable next-generation engines to meet efficiency and emissions targets. Enhancing the understanding of HCCI combustion and stratified-charge CI combustion via fuel-air mixing metrics is useful for optimizing the design and control of advanced combustion processes and thus relevant to the broader DOE objectives, as one reviewer said. Someone pointed out that the empirical data comparison to predicted results is valuable. A reviewer mentioned that HCCI will become a very important technology for both SI and CI engines. This project is focused on optimization on both energy usage and reduced emissions, said a reviewer. Another stated that this work addresses charge stratification, which may be useful for HCCI combustion. One person thought that this work is important in understanding the impact of charge stratification on combustion. Another mentioned that the diagnostic techniques and methodologies represent an important tool assisting engineers in developing engines with optimized fuel/air mixing. A mention was made that this is long-term, high-risk research that will take several years and require patience to produce commercial returns. One reviewer questioned the effectiveness of the phi PDF obtained from of HCCI/stratified charge LIF images for emission prediction. He asked if it is understood how the noise associated with the LIF method—as demonstrated by "missing fuel"—affects the actual fidelity of PDF.

Question 2: Approach to performing the research and development (Written responses from 15 of 19 reviewers)

The comments regarding the approach were positive with a few suggestions for improvements. A reviewer stated that the project employs balanced multiple approaches that examine the injection and the emissions from the nucleus to exhaust and modeling. A comment was made that the instrumental technology has been developed in the past. Someone was especially impressed with the efforts of Dick Steeper to extract information from the experiments that can be directly accessed by the modeling efforts. One person mentioned that the researchers have developed an understanding of fuel-air mixture preparation and its relation to combustion performance. He said that they have also added emissions measurement capability with simultaneous LIF measurements, to understand and predict emissions formation. A reviewer complimented the nice approach of utilizing LIF diagnostics to characterize equivalence ratio PDFs and attempting to correlate equivalence ratio metrics and emissions. One reviewer mentioned that the parameter space is quite small, and so it is difficult to extrapolate these results to many common operating conditions. Another commented that further investigations of temperature dependency are required along with more detailed HC-emissions characterization for aftertreatment investigations (methane is hard to oxidize). Another reviewer stated that empirical testing results are most valuable to industry engineers. One comment was made that it is difficult to fault the approach. A question was raised as to whether the data are

[1] This report contains a number of technical acronyms which are referenced in Appendix D on page 105.

unique to a given engine or if they are universal. A suggestion for improving the emission modeling methodology was made, which included accounting for the mixing between different packages of various equivalence ratios. One person thought that this work involves an impressive integration of optical engine study results with a simpler modeling approach to post-process the data into meaningful conclusions. He felt that it is very relevant to the future issues for the DOE and also the industry. Another question was raised why PRF 50 was used, since this seems low (in terms of octane number) for an automotive application. A reviewer suggested that in this case, the two-stage ignition will be dominant, as shown in the data, whereas with a more typical automotive fuel there might not be much two-stage energy release. One person thought that this is a very interesting methodology with well-devised experiments and a creative approach. Another thought that this work is outstanding. Someone confirmed that the development of PDF for emission prediction appears to be the right approach. A comment was made to improve/clarify long-term strategies.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 12 of 19 reviewers)

Reviewers had numerous positive comments regarding the accomplishments and progress of this work. A reviewer thought there had been good progress on expanding analytical capabilities, and thought it was encouraging to see the introduction of a simple model and how close it fits to the data. Reasonable progress appears to have been made, in one reviewer's viewpoint. This reviewer thought it will be interesting to see how this technique applies to alternative charge preparation strategies. One reviewer thought that the effort to extract the PDFs from the experiments is an excellent accomplishment. Another pointed out that the emissions measurements are in place, PDF-based emissions prediction capability and LIF tracer capability have been developed, and a new diagnostic project is underway. He also mentioned the homogeneous database that was built, and that its ability has been tested to enable prediction of stratified combustion via the PDF approach. He suggested that the work is ignoring the hydrocarbon loss mechanisms that take place in engines, in that discrepancy between BDC hydrocarbon measurements and prediction is attributed to missed fuel mass in the cylinder, whereas the answer could simply be due to enhanced losses when injecting into the BDC (largest volume) condition where HC losses/emissions formation may be maximized (think of MIT review in SAE literature of HC emissions mechanisms in SI engines). One person mentioned that as an early work, this shows promise toward complementing other works in contributing to a more fundamental understanding of HCCI and partially-stratified HCCI. Another thought that the paper about LIF tracers was very good. He also stated that the PDF approach is interesting but temperature as a parameter is still missing. According to him, since HCCI is controlled by chemical kinetics, PDF influence is somehow overestimated. Another commented that it appears this work just got started; however, significant progress has been made already. A comment was made that the predicted emissions versus the measured data are reasonable at this stage of the game. One person stated that a lot has been accomplished over the past year. Another added that this is an excellent project, especially because the results are being post-processed into a meaningful model. He appreciated the simple assumptions that were made that allowed this post-processing effort to be incorporated into the study results. He suggested that the later work can apply more detailed models, or alternatively use engine testing for model verification. A comment was made that the data analysis was very good. Someone commended the laboratory setup and recommended future funding. However, he did mention that the technology path for movement toward commercial usefulness needs to be identified. A suggestion was made that characterization of injection parameters and injection strategy effects on fuel spray formation and mixing in HCCI or PCCI process—including diesel sprays—may be a much more effective application of PDF/LIF methodology.

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

Comments regarding the collaborations and technology transfer were generally positive. One reviewer mentioned significant information transfer; however, not at the level where there is direct project activity with an industrial partner. Another felt this research involves excellent collaboration and interaction, and that the MOU worked well in this regard. It was pointed out that there is a student visitor from the University of Michigan and that the researchers are working with Stanford and the University of Wisconsin. Frequent publications were also mentioned. A reviewer noted that there were solely collaborations with universities, but that there was excellent distribution of knowledge through education of students. A reviewer commented that it appears the coordination between this program and Sandia's is adequate to avoid duplication of effort, but at the same time there is perhaps not enough commonality between the two to provide more program coherence. A comment was made that the fuel used prohibits direct transfer to industry. It was also mentioned that the LIF tracer investigations are very helpful. One person stated that exchanges with the automotive OEMs in addition to the semi-annual ACE MOU meetings must continue. Someone thought that it is not clear how this data/methodology gets incorporated into modeling/design tools. According to him, the researchers should identify an analytical counterpart for capturing/utilizing this work. A suggestion was made to perhaps start with university partnering first, then partner with industry as technology becomes more commercial. It was not clear to one reviewer how closely this project is tied into industry. He did not see any OEMs listed. Another commented that direct and continuous involvement of industrial partners could enhance the project. A reviewer thought that reasonable collaboration between the National Laboratories and universities seems to exist, but that collaboration with other industry partners is not apparent, other than the technology exchange during such reviews.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 8 of 19 reviewers)

Reviewers made several suggestions regarding the future research. One reviewer encouraged the connection with analysis/modeling and hoped this methodology can be formulated into an analysis/design tool. A suggestion was made to continue characterizing the charge preparation, extend the PDF method, and perform simultaneous temperature and concentration measurements. The team should consider including the characterization of wall-wetting and fuel-oil dilution by developing correlations between optical diagnostics and global injection metrics, as one reviewer noted. One person commented that the PDFs produced to date seem to be primarily for homogenous charge conditions; therefore, developing the PDFs for stratified charge conditions should be a priority. Another thought that it is critical to compare NOx measurements in different zones with model predictions. Prediction of NOx emissions would be extremely useful, in one reviewer's mind, who noted that this might also show the breakdown between nitrogen-containing species. A suggestion was made to identify whether objective is truly HCCI, or is it quasi-HCCI (stratified charge). Someone mentioned that understanding of data variability as a function of different hardware and fuel type might be important.

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

- Specific Strengths
  - Very good researcher and a good engine design for obtaining this type of in-cylinder information.
  - Comprehensive and fundamental study of charge preparation, should lead to valuable insights. PDF method, if it proves to be robust, may be useful in control strategies.
  - Ties advanced analytical techniques on the dyno with modeling.
  - Good assumptions and hypothesis, excellent combustion understanding.
  - The imaging techniques for developing fuel-air PDFs are novel and useful in the case of HCCI (though maybe not in the case of partially-stratified fields).
  - Correlating optical diagnostics to global engine-out emissions via equivalence ratio PDFs.
  - LIF technique helps significantly in understanding the basics of HCCI.
  - Good tie-in/collaboration with other HCCI activities. Main value is for guidance of prediction methods.
  - They are improving understanding of inhomogeneity in HCCI engines.
  - Addressing problems of interest.
  - Good foresight relative to the application of the work for development.
  - Apart from applying novel optical diagnostics, the PI has gone one step further to try and make sense out of the data and propose a methodology enabling emissions to be predicted.
  - Using simple assumptions to post-process fundamental data into a coherent strategy that can later be validated or disapproved. A good model for other researchers to follow.
  - Using a simplistic model has demonstrated a surprising correlation with measured data. Rapidly demonstrated proof of concept.
  - Good researcher, good collaboration, good facilities, well thought out program that is willing to receive comments.
  - Good implementation of actual measurable HCCI combustion.
  - Supports other HCCI projects.
- Specific Weaknesses
  - Could use increased publications.
  - The assumption of the PDF approach that reaction occurs within discrete and independent packets is a serious weakness that needs to be tested thoroughly.
  - The assumption that each of these "bins" in the PDFs are isolated from one another would seem tenuous, except perhaps for some nearly HCCI conditions. Since the work seems focused on providing information

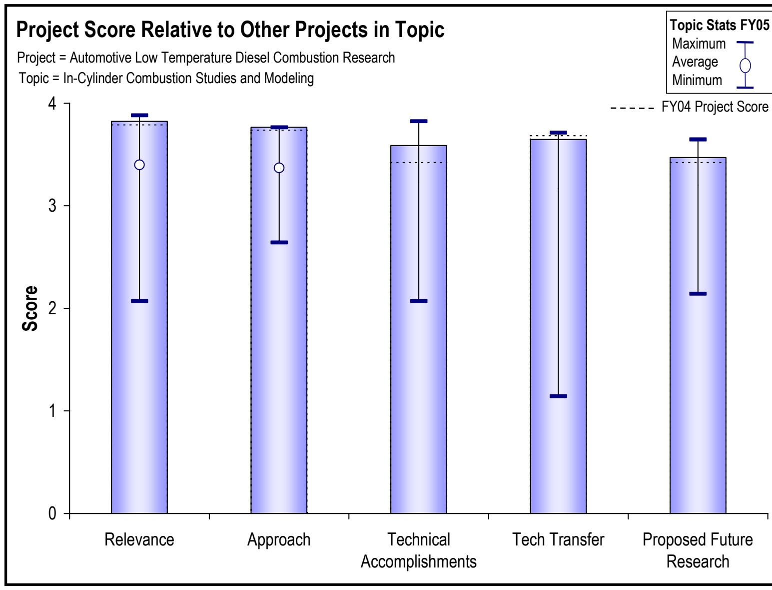
on partially-stratified combustion, this interaction must be understood, whether through additional data points, LIF images or (more likely) from KIVA.   Also, in order to extrapolate the fundamental mechanisms that this work attempts to explicate, a wider range of conditions must be explored.
- LIF technique with the fuel used prohibits direct transfer to engine application.
- Although their technique is useful, there are some significant limitations.
- Need the connection to modeling activities to capture/incorporate the data/methodology into analysis/design tools. I realize that this is planned but there is currently a gap, plus it is not clear what the modeling efforts will be.
- Equivalence ratio distribution is assumed to be frozen from the time of image capturing at 30 degrees BTDC.
- Although the results look very encouraging, it appears highly unlikely that the subsequent mixing has negligible impact on the distribution of equivalence ratios in the cylinder (how different would the predictions be had the image capture been at 40 degrees BTDC?).
- PDF method seemed overly simplistic and not meriting so much time.
- Need to do a better job of explaining overall technical goals and strategies.
- It seems that there is a significant amount of work from the current state to an actual engine. It is not clear what the critical variables are in this program   How much of this changes with minor changes in combustion geometry? It also seems that this work will be somewhat late in order to help the industry and DOE meet the efficiency and emissions goals.

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

- Would be advantageous to have an industrial collaborator.
- As mentioned, consider range of charge motion conditions to test the robustness of the assumptions in the PDF approach.
- In addition to effects of wall wetting and spray penetration, it would be useful to understand the role of fuel evaporation as well. Can the study be broadened to look at fuels of different volatility, and perhaps even a gaseous fuel? Also, in examining the effects of charge motion, the effects of a range of swirl numbers (quantified on a flow bench) would be useful—and perhaps more complementary to Sandia's work. Finally, given the relatively narrow focus of the study and the parameter space to be covered, NOx emissions might not add significantly to the work at this time, particularly if the concentration is to remain on low equivalence ratio operation.
- I would hope that the findings of this program supplement the results of the other optical engines at Sandia, and result in an overall emerging picture of HCCI and advanced combustion regimes.
- Include temperature dependency (kinetically controlled combustion); think about other fuels.
- Expand the speed/load range being investigated, define a specific program of charge preparation stratifies and present it to the AEC Working Group for review and approval.
- It is not clear to me how this approach works in the absence of test data on a given engine. I would like to see an explanation of how the emissions predictions can be made for an engine under design, i.e. no data available.
- Realizing that there are issues regarding Signal-to-Noise ratio etc, it would be helpful to have temperature data.
- My opinion is that valve timing manipulation (negative valve overlap, large overlap, CR changes, etc.) will be a critical component of any automotive HCCI application. Incorporating such scenarios into the research would increase its relevance.
- Lab techniques are quite good/advanced, but better collaboration is needed and technology strategic path should be identified.
- This program offers an opportunity to define ideal target equivalence ratio PDF. Analytical tools can be utilized to develop correlations between PDF maps and global in-cylinder calibration parameters. Coupled with experiments, the analytical tools can then possibly be used to identify optimal global engine calibration set-points without necessarily having to rely on predictive emissions models for advanced combustion regimes.

In-Cylinder Combustion Studies and Modeling

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



Brief Summary of Project

This project team is working to develop a fundamental understanding of low-temperature combustion regimes, identifying important physical processes and preferred parameter ranges for the system. In addition, the team is developing a quantitative predictive capability for low-temperature combustion by providing an experimental database to validate and improve submodels.

Question 1: Relevance to overall DOE Objectives (Written responses from 12 of 17 reviewers)

One reviewer stated that the project is focused on understanding and developing clean combustion systems, while another added that it is part of the "Grand Plan." One reviewer noted that the researchers are investigating important combustion regimes for light-duty engines. Another person felt that the project is relevant, although the stated goals were too vague. One person commented that this is a more applied study of practical diesel combustion, but has an opportunity to provide certain important contributions to the understanding of low-temperature diesel combustion. One of the reviewer commented that advanced injection timing and high EGR rates together with the proposed injection nozzle tip configuration are a very supportive means to investigate HCCI combustion. One reviewer noted the goal of developing a physical understanding of combustion and emissions formation, and improved models for the combustion process and engines, which should lead to key insights and capabilities to overcome barriers to advanced engine design. Another commented that low-temperature combustion regimes are a possible technology to achieve high engine efficiency with relatively low emissions. Research with optical and metal engines will help with engine design and combustion optimization. Development of predictive capabilities and a database for LTC regimes should also prove beneficial. One reviewer noted that this work is establishing significant building blocks relevant to combustion and the low-emission, high-thermal-efficiency goals. Another person felt that the project contributes to the fundamental understanding of mechanisms important in Low Temperature Combustion Concepts, in particular those involving early injections. The reviewer concluded by adding that this is well-synchronized with current industry trends. One reviewer commented that the combination of experimental and analytical investigations of fundamentals of various modes of diesel HCCI-like combustion and relevant emissions, fuel economy and load potential provides the most valuable information for developers of today's low emission in-cylinder combustion process. The final reviewer commented that this project is fundamental in nature and may lead toward improvement of the current understanding of low temperature combustion and also in the refinement of CFD turbulence sub-model. In particular, the marriage of optical engine measurements, metal engine experiments, and the multi-dimensional efforts are very productive for pushing the understanding of various combustion schemes.

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

Comments to this question were generally positive. One person simply stated that the research is very thorough, while another added that the project and the plan have all the right elements. Another person acknowledged the joint approach with simulation and optical engines. One reviewer added that the approach seems reasonable, although the team needs to be more specific and relate to goals. Another person noted that the approach is effective, with an attempt to analyze the system from various angles. One reviewer noted that the researchers are taking a comprehensive modeling and experimental approach. Another reviewer commented on the solid fundamental R&D, the accelerated data acquisition, the excellent collaboration and the quick integration into simulation tools, along with regular industry review. Another person added that SNL has combined its expertise in engine combustion R&D analytical capabilities in optical engines with key research institutions as partners to corroborate results with metal engines and to do analysis and modeling; a strong partnership. Another reviewer also felt that the approach is generally very good, but felt that it might be beneficial to spend more time on the metal engine experiments since such efforts are closer to real-world conditions that the optical engine experiments. Another person commented that the approach is reasonably conventional and straightforward, however gaining a fundamental understanding of emissions formation over the parameter space included, while important, may in some ways be reinventing the wheel. Another reviewer noted that the project is almost truly comprehensive approach to building understanding of in-bowl mixing controlled combustion through simultaneous metal engine/optical engine and CFD; the only part that that is missing are details of fuel spray mixing and its relation to in-bowl flow. The last reviewer commented that the researchers have used modeling capabilities and engine test capabilities to study low-temperature combustion regimes, considering that EGR, SOI, injection pressure and swirl provide consideration of charge motion, mixture preparation and thermal stratification on HCCI. The project is an excellent mixture of elementary and practical considerations within one project (e.g., considering both injector configuration and turbulence model development).

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

One reviewer felt that the researchers are developing a useful understanding of light-duty diesel combustion in unusual regimes. Another acknowledged the progress, but noted the group's difficulty in hardware procurement. Another reviewer commented on the evolving facilities by upgrading the injection system to consider a variety of nozzle configurations. They also noted the researchers added emissions instrumentation to an optical engine, contributed to the UW soot model development which now fits EGR influence on soot, supported development of low temperature heat release modeling in KIVA/CHEMKIN, and evaluated turbulence models to better fit turbulence and thereby turbulence-kinetics interactions in LTC, including the key observations which include the effect of swirl levels on CO emissions. Another reviewer also noted the nice job in using modeling to explain why high swirl leads to high CO. Another person added that the project has shown good individual accomplishments, but felt that the team needs to organize results along common, goal-oriented themes. They added that the presentation jumped around too much and perhaps put too much emphasis/concern on CO phenomena. One person noted that several potentially critical mechanisms in explaining emission trends in DI diesel engines have been identified (effect of swirl, and spray targeting etc). Another person felt that the results are interesting, but cover a comparatively limited range of load/speed to be considered too significant. One reviewer commented on the solid technical accomplishments with results that help understand effects of fuel spray on combustion. They felt that particularly noteworthy is the comprehensive research approach with results being corroborated between optical and metal engines, then having emissions analytically modeled and confirmed through experimentation. Another reviewer commented on the incredible results of a new turbulence model that is practical and can be incorporated into a tool including chemical kinetics, also noting the new KIVA applicable soot model, along with great insights into in-cylinder combustion. One reviewer noted that much progress has been made in determining potential combustion system parameter effects on overall engine performance. In particular, studies on swirl impact, injection timing, and EGR variance on fuel economy, NOx, and smoke have lead to generalized calibration charts for the engine in question that could be carefully extrapolated to other engines. The final reviewer commented that this program could be a good platform for understanding the basics of optimization of combustion bowl geometry—answering, for instance a question about what specific features would be required for LTC system.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 10 of 17 reviewers)

Several reviewers noted the group has good collaboration reported with several universities, other national labs and industry, also noting that the PI has assembled a team of some of the best labs and universities in the U.S. to do this research. One reviewer added that Paul displays superb interaction with both OEMs as well as the universities. Another added that the excellent coordination between the national lab, universities, and industry as demonstrated in the past and present through use of industrial know-how with engine hardware and national lab and university know how exploring the physics associated with various combustion control schemes. One person noted the detailed exchange of data and results ensured through one-by-one discussions. Several reviewers noted the group's participation in the AEC MOU group. One person added that it appears that all the right people are involved through the AEC MOU group, and that all the right people are receiving the information. The final reviewer commented that the collaboration contributes significantly to the chances of success of this project.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 7 of 17 reviewers)

Several reviewers felt the group has good plans to build on the base from prior years' research and concurred with the plan to change the engine hardware to more current technology levels by focusing on a common engine platform, such as the Fiat-GM 1.9L engine which may help to speed up the progress. One reviewer noted that a confusing aspect of the presentation is that it is unclear which test engine(s) from which the measured modeling results were obtained. Another reviewer noted that in general the future approach of including a high-swirl head and lower compression ratio combustion system should provide more fundamental insight into various combustion system control schemes. They added that within the future plans, the PI is moving onto a new engine and is was not clear if the future would also include metal engine experiments that are very crucial due to the realistic element such hardware brings to the project. One reviewer suggested continuing investigating the bulk flow effects on LTC. One reviewer felt that there was some lack of clarity as to how the nozzle library will be used in future work. The final reviewer commented that the future research proposed here seems to be a logical progression. I would like to see a focus on understanding higher speed and load emissions formation mechanisms, but it almost seems that the nozzle library is not consistent with the head and bowl choice to give a more fundamental understanding over a broad enough load/speed range.

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

- Specific Strengths
  - Breadth of scales in this project from practical fuel system configuration to turbulence modeling.
  - A basic understanding of the interaction of turbulent mixing and combustion should come from this research. The changes in hardware that are upcoming will also enhance the relevance of the results.
  - Cooperation between simulation and testing. Approach via advanced injection timing, EGR and swirl is essential.
  - All the "right" parties are involved in this project, and it ties in with other relevant people.
  - Paul is a good champion for what is needed in turbulence modeling.
  - The good collaboration with universities is beneficial to all involved.
  - SNL continues to build on its optical engine and combustion R&D strengths and to partner with universities which bring complementary expertise to the research plan.
  - Good use of modeling to rationalize experimental results and consideration of current model limitations.
  - Very experienced, enthusiastic PI, in-sync with current industry trends
  - Excellent diagnostic equipment available.
  - Good combination of experimental and modeling expertise aimed at automotive diesel engines. Clearly a major U.S. weakness compared to Europe/Asia.
  - The effective integration of experimental and modeling expertise.
  - Excellent experimental facilities and multi-dimensional modeling efforts.
- Specific Weaknesses
  - Emissions measurements are still limited. Seems to be no consideration of fuel effects in this study.
  - The physical understanding needed for more valid inputs into the combustion and spray models is lagging behind the experimental approach.
  - Since this investigation is not only limited to fundamental work, take-over to heavy duty industry may become difficult.
  - Need to do a better job of organizing/coordinating research along clearly specified objectives.
  - Potential lack of future metal engine experiments.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 6 of 17 reviewers)

- Consider even larger emissions measurement capabilities, since there is evidence of PAH emissions and aldehyde emissions from HCCI combustion under some operating conditions. Build into future work some consideration of how fuel properties may interact with LTC processes.
- Work on gaining a more basic understanding of the "air utilization" process in LTC to improve the state of the CFD models being used. It appears that more model validation will be needed to improve the spray-wall interaction models, and perhaps even in more basic spray models used.
- Instead of mixing parameters, homogeneity as the prime parameter is recommended.
- Develop collaboration with Andy McElroy's group at Sandia on effects of turbulence on molecular level mixing

time vs. reaction time effects for real fuel cases. First step is to determine when this needs to be considered in connecting kinetics with fluid dynamic models.

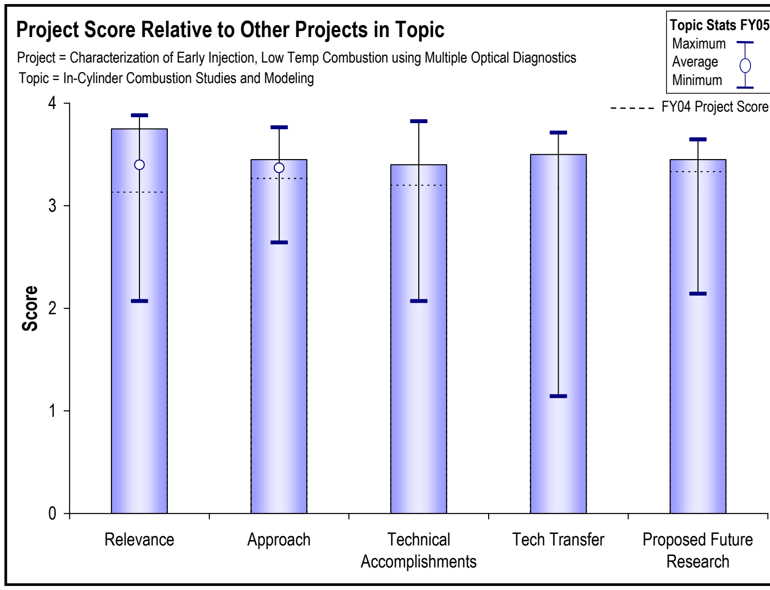
- Strive for assembling an extensive database on in-cylinder flows under various conditions that can be used in the development and testing/validation of turbulence models.
- Ensure that the future will include metal engine experiments.

In-Cylinder Combustion Studies and Modeling

Characterization of Early Injection, Low Temperature HD Diesel Combustion using Multiple Diagnostics, Mark Musculus of Sandia National Laboratories

Brief Summary of Project

The objectives of this project are to apply multiple laser/optical diagnostics to study spray, ignition, combustion, and pollutant formation processes for a low-temperature operating condition. In addition, a computer modeling collaboration has been initiated to improve predictive capabilities and enhance understanding of multiple low-temperature operating conditions.



Question 1: Relevance to overall DOE Objectives (Written responses from 14 of 20 reviewers)

One reviewer commented that this project represents great work and is extremely relevant, while another person added that it is highly relevant to meeting 2007/2010 diesel standards. One reviewer added that the effort has the potential of being highly relevant to DOE's overall objectives, provided it gets tied closer to Lyle Pickett's project. One person noted that the project is focused on understanding the clean combustion process. Another shared that we still have much to learn about diesel combustion and Sandia has been productive in addressing this need. One reviewer felt that this topic is the basis for all engine OEMs and was well done. They felt that Mark is an outstanding speaker who understands the material and does a great job of explaining combustion phenomenon as it applies for 2007-10. One person noted that characterizing the combustion characteristics of LTC fits very well with the DOE objective of developing combustion approaches that will intrinsically reduce the engine-out NOx. Another felt that extending the diesel combustion model and experimental techniques to low-temperature combustion is likely to provide substantial and valuable insights into advanced combustion, thus enabling engine development. One person stated that LTC will be very important to future clean, efficient engines, and this work promises significant information. Another reviewer commented that understanding the basic science of diesel combustion is critical to achieving maximum engine operating efficiency and minimizing emissions. Laser/optical analysis of spray, ignition and combustion operation in an engine provides an important tool that can help understand diesel combustion and emissions formation. Several others had comments along the same lines. One person felt that this optical study represents another fundamental element of the understanding of low-temperature diesel combustion. Another added that detailed analysis using different optical techniques simultaneously was well appreciated. Another reviewer commented that there seems to be a definite need for extension of Conceptual Spray Combustion Model to "unconventional" modes of diesel combustion such as PCCI combustion, and the integration of several laser diagnostics provide an effective tool for this type of investigation. The final reviewer commented that this is a very fundamental project that is aimed at understanding differences in spray formation between standard diesel-type combustion and low-temperature, early-injection-controlled combustion. They added that to date, a single operating condition was investigated that has resulted in the generation of possible fundamental spray formation issues, which is far removed from providing the community with tangible results that will aid in combustion system design.

Question 2: Approach to performing the research and development (Written responses from 16 of 20 reviewers)

One reviewer stated they felt the work was well planned and executed, while others noted the excellent experimental programs, while one noted the need to move toward more realistic conditions as possible. One person noted the good utilization of the available resources and another noted the good use of the conceptual diesel combustion model with reasonable extensions proposed. One reviewer commented on the outstanding application of proven methods to enhance our understanding, which also identifies the need to new tools via industry collaboration and expediting the tool development. One person noted that the work uses existing tools that built the conceptual model of diesel combustion and modeling to extend the model to LTC. Another person commented that the researchers are addressing important issues using good facilities and experience. One reviewer commented that SNL has a long history of effective and innovative use of optical and laser diagnostics to help increase the scientific understanding of diesel and HCCI combustion and this project continues to build on this experience; particularly interesting and thorough is the PI's use of numerous imaging techniques to characterize spray and ignition in the cylinder. One person added to this, saying that the employment of several different optical methods is somewhat unique and difficult to develop elsewhere, and as such, this approach represents an important contribution. Another commented that the technique of being able to simultaneously integrate the range of optical techniques to be able to gain a visual read of the structure of the combustion within the engine. This reviewer was uncomfortable that the research group did not describe a comprehensive approach to get the most information from this approach when it is not possible at this point to do parametric studies. One reviewer suggested setting priorities on key engine parameters to investigate based on speed and load, while another felt that the cutaway of the piston crevice area reduces the applicability; using a glass window or glass piston would overcome this issue. Another noted that the work preceded development of "conceptual models" by performing measurements at various EGR-rates, trying to understand the effects observed by Pickett. One person felt that it would be helpful if imaging diagnostics of diesel combustion process for moderately advanced single injection could be extended into investigation of effect of further advance of injection timing (up to 90°CA BTDC?) with different levels of fueling and injection pressure as well as different schemes of multiple injections including early pilot+main, pre-pilot+pilot+main and early pilot+main+post injection. The final reviewer commented that the optical measurement portion of this approach is excellent and provides much qualitative details of the spray formation and combustion processes. On the other hand, the experimental operating condition of the engine generated a number of questions concerning its practicality: for example, the engine speed and injection pressure could have been more representative of a realistic operating condition.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 15 of 20 reviewers)

One of the reviewers commented that the work is superb with lots of great information to build a fundamental understanding. Another person added that they appreciated Mark taking additional steps to combine significant results and creating a LTC mechanism that industry can first comprehend and then apply elsewhere; high value results. Another complimented the good resolution and consistent results helps understanding of the details of combustion. One reviewer noted accomplishments of the work included studying the early injection condition using conventional diesel hardware, noting that fuel injection penetrates deeper into the cylinder, seeing that cool flame heat release may serve to vaporize the rest of the fuel, and finding that soot starts to form where OH is not present. One person acknowledged that the project is still in its early days for results, and that soot formation understanding combined with fuel sprays is not firm yet—more R&D is planned with more depth. Another person suggested that the proposed (future) validation of computational models will add significantly to the accomplishments. One reviewer commented that the researchers have shown a very impressive set of data from optical engines, but need to quantify information relevant to achieving low soot and NOx and need to feed existing data into computer models. Another added that the researchers provided important results for LTC, and this provides understanding that is important for future clean, efficient engines. One reviewer felt that the research tem has developed an impressive suite of diagnostic techniques has been applied to the engine; however, there is more fundamental work to be done until an extension of Dec's conceptual model can be assembled. Another added that the measurements presented at this talk are impressive; it is especially helpful to be able to look at liquid phase, vapor phase and the oxidation phases simultaneously. One reviewer noted that the work shown demonstrates some important mechanisms for soot formation. However, they felt that the operating conditions picked and perhaps the compromise in the piston bowl to allow optical access leave some questions as to the relevance, e.g. the operating condition picked is not generally one where sooting is an issue; the rail pressure appears to be too high for this load and the effect of the bowl cutout on charge motion and local squish turbulence may confound the results shown. One person noted that the discovery of dual vortices as soot forming zones is an exciting discovery. One reviewer commented that using a combination of several optical and laser imaging techniques, SNL is able to provide photographic evidence of fuel spray, ignition, combustion, and soot formation which help the scientific community to better understand low temperature combustion which will help improve engine out emissions. The final reviewer commented that the progress to date is limited to a specific engine operating condition and thus it is difficult to make general conclusions especially concerning selection of the engine operating and boundary conditions.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 14 of 20 reviewers)

Several reviewers noted the group's participation in the Advanced Combustion Engine Working Group, which includes strong links to University and Industrial partners. Another reviewer noted that the collaboration extends outside the AEC Working Group. Others added that sharing information and collaborating on research is conducted in conjunction with universities (University of Wisconsin), auto OEMs and diesel engine manufacturers (Cummins, Detroit Diesel). Another reviewer added that the collaboration appears to be quite solid, and since the industrial partners are involved in the tasks and the work priorities, this reviewer would view this part of the program as quite successful. Others had similar comments including: the group is very well connected with the research community; Sandia is excellent at actively seeking industry collaboration and interaction; effective collaboration with industrial partners and combustion experts; the group is well connected to industry; improved modeling effort with the University; and it appears that certain industrial partner(s) are driving this project and thus collaboration exists. One reviewer suggested that more parameter studies with different bowl shapes, operating parameters, etc. could improve the transfer into the industrial research and development community. Other suggested that stronger coordination and more frequent communication with industry partners could possibly improve the operating conditions to be focused on.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 11 of 20 reviewers)

Several reviewers simply agreed that the plan was good, or excellent. One reviewer acknowledged the cooperation with simulation efforts and other combustion systems. One reviewer felt that the future direction appears to be reasonable, but they would have preferred to have more discussion as to the most effective way in which to extract the optimum information from the limited number of engine measurements that can be made. One of the reviewers noted that exploring other LTC, new diagnostics, and computer modeling will add considerably more useful information. One person suggested focusing the research on looking at a more realistic set of operating conditions and in understanding some of the sensitivities to such things affecting fuel penetration, including SOI. One person felt that in general the future plan is good, but probably should focus on revisiting a more realistic engine operating condition for assessing spray/combustion characteristics under low temperature operation. They also suggested extending Dec's conceptual model will require much additional test work and thus should be a lower priority versus exploring various injection strategies. One person suggested that a tool to look at unburned fuel would be great for looking at pre-mixed combustion, or also the high HC emissions from some advanced combustion techniques. Another person felt that the project can be improved given proper guidance. The final reviewer suggested the researchers consider other combustion/injection schemes, improve computer modeling strategies, and develop a new diagnostic for unburned fuel.

Specific Strengths and Weaknesses (Written responses from 16 of 20 reviewers)

- Specific Strengths
  - The combination of a laboratory with a wide range of optical instrumentation and a diverse range of expertise at Sandia makes this a major strength of this project.
  - Exceptional experimental capability and well constructed experimental approach.
  - The techniques used are outstanding, and represent a unique capability available for this research.
  - Simultaneous application of different optical measurement techniques.
  - Very well developed experimental facility and methodology.
  - Work is revealing unique insights with implications to future designs.
  - The facilities and experience are valuable and unique.
  - SNL has a long history of effective use of optical and laser diagnostics to help increase the scientific understanding of diesel and HCCI combustion. They have been highly innovative in their ability to instrument the single cylinder engine in so many ways and with so many different techniques to be able to observe fuel spray and combustion effects inside the engine from various perspectives. This project continues to build on this experience.
  - Great combination of planning, execution, experimental information combined with interpretation.
  - Good use of the conceptual diesel combustion model with reasonable extensions proposed. It will be important for spray and combustion models to be validated at this condition if optical experiments are precluded at high load.
  - Vast spectrum of optical measurement techniques available.

- Enthusiasm and desire to make the most out of the data.
- Momentum from years of previous activity to build on.
- Industry collaboration.
- Very talented critical mix of engine researchers at Sandia consistently delivers excellent results.
- Excellent diagnostic capabilities and optical engine testbed.
- The experimental tool and the analysis method used to understand the clean combustion process.
- Great facilities used to develop and refine basic understanding of diesel combustion types and emissions.
- Excellent experimental capability - great optical diagnostics.
-

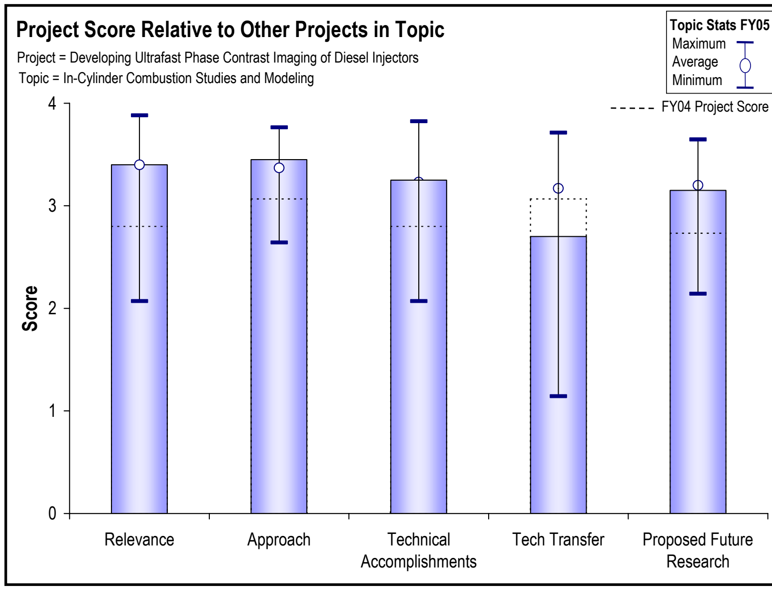
- <u>Specific Weaknesses</u>
  - There was not presented a clear set of engine conditions to study.
  - While the results, I believe, are still insightful, I think they could be improved by re-examining the baseline operating conditions used for the optical study.
  - Limited to optical accessible engines.
  - Limited set of experimental data.
  - Insufficient interaction with Pickett.
  - Need to do a better job of linking your results to the overall objectives of low NOx/soot.
  - What is the extent of combustion/fuel conversion efficiency?
  - Work hard to overcome limitations of optical engine; low pressure, piston cutout, simulated EGR, etc.
  - Lack of sufficient experimental evidence to develop a conceptual model; more effort should be spent on more realistic engine experiments.

<u>Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 10 of 20 reviewers)</u>

- Propose a comprehensive set of engine conditions that will provide the most effective range of engine conditions to be able to characterize the combustion mechanism.
- Expand study to consider a range of fuels: volatility, cetane number, oxygen content.
- Given the fundamental nature of the study, I believe that examining a wider range of boost, phi, SOI and ambient temperatures may be more significant than looking at different injection schemes (which may have less broad applicability).
- Avoid piston cut-out and use glass windows or glass piston. Apply typical operating conditions like boost pressure. Make parameter studies with different injection pressures, swirl variation, nozzle tip configurations, combustion systems, etc.
- This excellent program should be tightly coupled with the computational work done elsewhere. It appears that this is a future goal already, and that should be commended.
- Determine if simulations can reproduce findings on soot formation in vortices.
- Continue the work.
- Pursue the unburned fuel diagnostic and publish the results!
- Investigate the effects of varying the injection pressure and boost pressure.
- It would aid this research effort by adding more experimental effort in the low temperature combustion regime under realistic operating conditions.

In-Cylinder Combustion Studies and Modeling

Developing Ultrafast Phase-Contrast Imaging of Diesel Injectors, Jin Wang of Argonne National Laboratory



Brief Summary of Project

Researchers at Argonne are using ultrafast X-ray phase contrast imaging to see through the nozzle of an operating fuel injector. This shows the real-time motion of the fuel injector pintle during injection events, including longitudinal and transverse needle motion and cavitations after injection. This is being done in order to correlate in-nozzle dynamics with external spray characteristics.

Question 1: Relevance to overall DOE Objectives (Written responses from 17 of 20 reviewers)

A number of reviewers offered positive comments regarding this project's relevance, one noting that this work can significantly assist the development of fuel injectors and another stating that this work is outstanding work that will potentially enhance the understanding of spray dynamics. One reviewer stated simply that this was a nice basis for fundamental combustion and a nice tool. This tool may provide enlightenment to industry and researchers: the researchers have made excellent progress, have provided continuous development, and clearly understood some challenges ahead, but also knew how to have high potential benefits to all. A reviewer said that the program is highly relevant, and is probably the best opportunity for the U.S. to advance diesel injector technology. Another commented that this research is extremely relevant, and has a very good long-range vision of the problem, providing excellent data/information/insight into spray dynamics. Spray imaging at this level of resolution will have a significant impact on the engine technologies that are the focus of the DOE program, noted a reviewer, who said this work is going to impact the design of future injection nozzles. Development of advanced injectors and injector nozzles is becoming one of the most important issues in controlling low-emission in-cylinder diesel combustion, said another reviewer: Fast Phase Contrast Imaging provides unprecedented visualization of motion of internal components. Fuel spray research is fundamental to improving the efficiency and emissions from advanced diesel engines: thus, the subject area is highly relevant. The phase contrast technique may permit enhanced understanding of internal fluid mechanics of the injector to enable better design. It is important to understand fuel distribution inside the nozzle tip, noted a reviewer, who added that this fuel distribution is a valuable input not only for conventional diesel combustion (spray penetration) but also for the HCCI type of combustion for wall wetting issues at advanced injection timing. Understanding the basic science of combustion and developing a detailed knowledge of the operation of engine combustion system components is critical to achieving maximum engine operating efficiency and minimizing emissions. The X-ray imaging of injector operation in an engine provides an important new tool that can help understand operation of engine components with techniques not previously available. Finally, a reviewer said this was a very interesting technology that could lead to a breakthrough in fuel injectors.

Several suggestions were offered regarding the project relevance. One noted that understanding injector spray behavior and spray patterns is necessary, but only the first step in improving combustion. Enhancing the understanding of fundamental fuel spray characteristics is critical to advanced diesel combustion and engine development and is thus very relevant to overall DOE objectives, noted one reviewer. However, the benefit is likely to be significantly limited unless it would be possible to apply these advanced diagnostic techniques at operating conditions (e.g., injection pressures and ambient pressures) that are representative of typical diesel conditions. The work is a fundamental part of making some next-step improvements in engine out PM for clean diesel engines, noted a reviewer, but it was unclear that it can lend critical insight into the primary factors affecting engine-out emissions. The beginning and end of the injection process have been shown within the engine research community to have significant impact on emissions. Conventional optical techniques have been employed to study the early stages of the injection event but not with the resolution of this x-ray technique. Data presented are preliminary but future experimental activity should shed light onto the physics that are ultimately responsible for variances in emissions that are affected by the early stages of the injection event and in particular cavitation effects. Finally, a reviewer noted that if this is tied into combustion models it may show some benefits in the distant future.

Question 2: Approach to performing the research and development (Written responses from 15 of 20 reviewers)

Several reviewers were favorable toward the approach of the research and development, one noting that this was very good work and well done. A reviewer noted the very accurate, repeatable, and detailed analysis, while another highlighted the very impressive, clear presentation of the technology deployed. APS imaging provides innovative research into basic understanding of engine operation and combustion, said a reviewer. A reviewer noted the development of ultra-fast phase contrast imaging of diesel sprays in their comments. Phase contrast has provided new and useful information, said another reviewer. A reviewer felt the team was taking the appropriate steps to make progress against a long-range goal. The approach represents a highly unique visualization technique, said a reviewer, and the team has demonstrated improvements in the technique in a relatively short time frame. The approach appears to be well directed to answering the questions required, noted a final reviewer, who said that during the discussion it did sound as if the attainment of the goals was more important than preserving the integrity of the lenses.

Several reviewers had suggestions on improvements to be made, one noting that the presentation focused on the technique, not on the approach to meeting DOE's objectives. A reviewer said that it seems that technique still requires some refinement (unrobust x-ray detectors, x-ray filtering etc): as soon as these problems will be resolved, a more structured parametric study of cause/effect relationships of selected parameters should be undertaken (such as effect of needle wobble on nonuniformity of VCO sprays, effect of hole L/D on spray structure, etc). It was difficult for one reviewer to determine how this will be applied to future engine development: it is great capability, but how does it apply to the DOE's goals of reducing dependence on foreign oil? Overall the approach is very good, in one reviewer's opinion, but future efforts should consider duplicating real-world engine cylinder charge density and temperature: today it seems that reaching these boundary conditions is a challenge. The approach seems to be currently limited to conservative operating conditions, said another reviewer, who also noted the need to emphasize the specific plans /vision of how this work will influence the injector design process and combustion and emissions development. Lastly, a reviewer who said that this was excellent development of the tool towards practical application of a very interesting tool also asked the team to focus on comparison to existing state-of-the-art understanding of the fuel injection process.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 14 of 20 reviewers)

Technical accomplishments were generally felt to be good. One reviewer said that solid strides have been made in attaining the goals of the program. Others noted that significant progress has been made in the past year or that very good progress has been made to date. A reviewer commented on the outstanding development and use of tools, and another saw good progress so far and was looking forward to proposed plans to use APS to image fuel sprays in "real" engines. Excellent progress, said a reviewer who felt the work was much more exciting now that the test conditions are getting closer to real-life injectors. Most of the barriers are overcome, said another, and parameter studies can follow. Highlights of the work to one reviewer included the finding that the location of pintle is repeatable so that phase-locked imaging can be used to monitor transient (periodic) operations; the determination of the relationship between the spray dynamics and pintle position; and the ability to do single-shot imaging showing jet velocity and good correlation with visible light measurement. Finally, a reviewer said that the work described was that a technique has been developed, but how long it took was not discussed.

Suggestions on improvements were made by several reviewers. At the present stage of investigation, decoupling the effects of injector internal dynamics from effects of external ambient aerodynamic drag on spray formation definitely seems to be a good idea. In future investigations, however, interactions between those effects will have to be addressed since they may be (and probably are) co-dependent and understanding these relations can be very important for understanding of fundamentals of effective spray mixing. Another reviewer commented that this was very good work and the presented initial data set is hopefully a precursor to the future insight that will be developed through this study, and that next year will be an important stage for this project. It is reasonable to anticipate the generation of significant insight into the physics dictating spray formation during the initial stages of the injection event. Progress seems to be okay, said a reviewer who felt the project pace would need to be significantly accelerated to "diesel-like" conditions in order to assist in accomplishing the broader DOE objectives in the near-term. They are making good progress on measurements, commented another reviewer, but much work remains to affect DOE program technical barriers. Finally, a reviewer offered that this effort, particularly when combined with CFD and spray visualization techniques, represents an important contribution, but the results are somewhat sparse at this time.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 15 of 20 reviewers)

Several reviewers commented on the partnership with Bosch. One noted the partnership with Bosch on hardware and now personnel, and that an excellent level of collaboration with Bosch seems to be developing, as well as the ongoing collaboration with several other companies. Another noted that the team has a very good relationship with Bosch; further projects with automotive industry may follow. A final reviewer noted that so far, Bosch appears to be the only partner.

Other comments from the reviewers included that good relationships are developing with visual test results that will lead to advanced fluid injection models. A reviewer said that the current research builds on a solid base of past research done by research partners. Another said that the team has established both interest and support from industrial partners and universities. Another said that it was encouraging that Professor Lee's group is being included: this reviewer thought together with the ANL team they will be very effective.

Others had suggestions on improvements to collaborative efforts. One reviewer noted that collaboration appears adequate to produce quality results in the early stage of this effort, but a sustained program should include closer work with more industrial partners. This reviewer wanted to see a greater connection between the CFD results and the experiments--right now, they seem somewhat independent. Another offered that collaboration is limited to one university but this arrangement probably is sufficient for this type of effort: in the future, fuel system suppliers should become partners to fully leverage the insight generated within this project. No industrial partners were listed, said another reviewer who stated that the project, if it goes forward, must tie in with an injector manufacturer and the AEC MOU team. Another reviewer asked similarly if there was work with any industrial partner. One commented that coordination has been limited, but should improve as more data is collected. A reviewer felt there was little indication within this talk that there was significant technology transfer to industry; however, from Chris Powell's talk this reviewer suspected that this information is being well communicated, but the reviewer did not get that information from this talk. A reviewer said that the team needs to improve the collaborations or do a better job of explaining collaboration in your presentation. Finally, a reviewer said it is not apparent what the specific outcome of the various collaborations has been.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 14 of 20 reviewers)

Comments were mixed on the future research aspect. One reviewer noted that the team had a very good plan for the future, while another was eagerly anticipating future research into imaging of sprays in a combustion chamber. A reviewer felt that the improvement of efficiency of technique looks promising; application of parameter variation recommended. Another reviewer offered that this project seems to be headed in the correct direction. This is a hard technology to implement and the group is working well to overcome those hurdles. Especially relevant is imaging the flow right at the front or within the nozzle, which was felt by this reviewer to be very important. Also it was quite interesting that the group could show the resolution of "spray" close to the nozzle exit and to show that it does not image as a distribution of drops. The technique is useful, said a reviewer, and the issue will be applying it to diminish barriers. The nozzle imaging has demonstrated relevance to the transient development of the spray structure, and the single-shot work also represents an important step forward, in the opinion of a reviewer.

Other comments included that future plans are generally good, but it would be nice to see more of a focus on developing experiments that include diesel like boundary conditions. Upgrading equipment is important for developing more capability to perform these experiments and so is computational analysis as an aid in developing understanding of the governing physics, but such tasks should represent realistic boundary conditions. The overall plan seems to be directionally consistent with the broader objectives, noted a reviewer who said it would help if the specific plan and vision of how this data would be applied to spray modeling improvement/combustion enhancement could be emphasized. This reviewer was not sure how this effort is coordinated with Powell's work. There are very many options, said one reviewer, all of which are relevant: the difficulty will be in the prioritization. It was not clear to this reviewer how the priority is being set for the follow-on tasks. Another reviewer said that no real work plan was presented. The future work was not clear to another reviewer, who asked that the team focus on benchmarking new findings against available data and methods where applicable. A reviewer suggested that it would be good if expertise from diesel injector manufacturers could be consulted to guide research. Stay on track, said a reviewer, who suggested the team get more industry involvement: special dedicated open house and discussions encouraged. A reviewer suggested continuing development of phase contrast tomography and single-shot phase contrast imaging. Finally, a reviewer asked if the simultaneous analysis of structure of sprays from multi-orifice nozzle (both VCO and micro-sac) could be accommodated in future work.

Specific Strengths and Weaknesses (Written responses from 17 of 20 reviewers)

- Specific Strengths
  - The home of the APS source is the correct place to do this project. It is clear that all of the expertise to solve many of the problems that come up in these unique problems are here. This group is very good about solving these tough problems.
  - The APS is a unique facility. The technique appears to have great potential to assist combustion research if utilized correctly.
  - In-situ measurements can shed light on internal behavior of the injector and lead to improved designs.
  - Phase contrast.
  - Detailed analysis of spray formation and boundaries for simulation can be generated inside the nozzle even at very high injection pressures.
  - The unique physical insights provided by this technology can help with the understanding of important primary and secondary effects in sprays. The facilities and techniques developed here represent a valuable resource.
  - Methodology, quality of results.
  - Good scientific approach.
  - They are obtaining new information that should lead to improved understanding of the injection process.
  - Use of the APS for X-ray imaging is an excellent example of applications for government research using tools that are unavailable to industry to help achieve goals for improved engine efficiency and reduced emissions that industry and DOE jointly share.
  - Excellent utilization of the unique capabilities at ANL to acquire extremely valuable data.
  - A novel technique for peeking inside a production-type of injector nozzle has been developed
  - The technique enables nozzles to be investigated very quickly.
  - Good team is assembled. Very good progress finding better ways to apply the APS tool to fuel injectors.
  - Unique, powerful technique of imaging flow within injector, which will probably lead to opportunities to improve injector design and evaluate injector performance that no other technique can offer.
  - Incredible experimental technique for addressing near injector spray behavior.
  - It provides innovative & new method to understand spray behavior
  - Unique technology application; Opportunity to improve understanding of injector motion and near-nozzle sprays.
  - Great opportunity to provide data for CFD model validation.
  - Excellent capability of ANL X-ray capabilities of the Advanced Photon Source demonstrated.
- Specific Weaknesses
  - None as long as they continue to push the environments to more engine-like conditions.
  - This is a hard project and it requires significant work to overcome the substantial technical challenges.
  - Limitation to truly periodic behavior.
  - Only applicable at ANL due to required high X-ray power.
  - No combustion partners, e.g. SNL Combustion Lab. or engine manufacturers. No real plan.
  - Too narrowly focused. Expensive service work for Bosch.
  - Much work is necessary to analyze the information and result in knowledge that will improve engines.
  - Funding?
  - Status of verification/benchmarking to current state-of-the-art optical visualization or transient CFD simulation.
  - Please be very clear regarding the limitations and unknowns in the current results and methods. Is there

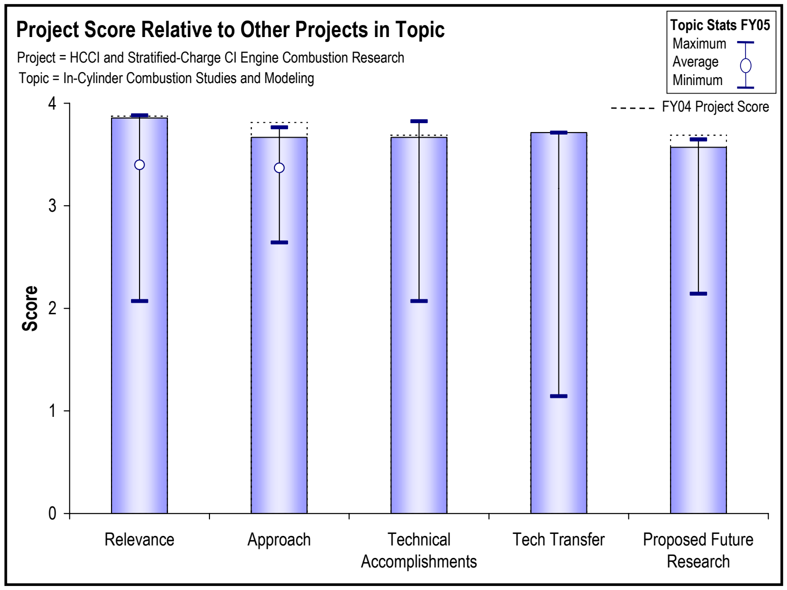
still a dopant required in the fuel? Is this still a significant contribution to the total fuel? Many advances have occurred, but I am not sure the status of the method. This can be fixed by your presentation.
- Difficult to relate how this relates to the DOE objectives: seems more like basic science. Information was not tied into models or engine results. Excellent basic information that will take a significant amount of time to be utilized by industry through models etc. Many interactions can influence the diesel engine combustion.
- Potential lack of capability to conduct real world, diesel-like experiments.
- Need increased emphasis on drawing quantitative conclusions on the results obtained.
- Not sure if/how the results are being specifically utilized either for spray modeling enhancement and/or injector design.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 14 of 20 reviewers)

- Please make sure that we know that you are working on modern supplier injectors.
- See if you could consider in-use effects on injector behavior, such as effects of coke, gum, varnish or lacquer development on injector parts to see how coking affects pintle and spray behavior.
- I believe the single-shot imaging needs to represent an important area of concentration for this work to understand the near-field spray structure. Also, the behavior at the end of the spray event, both inside the nozzle and in the flow field, may be quite significant to the formation of PM and HC emissions. It may be worthwhile to map the temporal evolution of the entire spray event with single-shot techniques.
- Parameter studies with different injection parameters and different injection systems recommended.
- No need to change the work scope - the project is focused and the methodology is excellent.
- Join the AEC MOU group. Define, with them, a viable, cohesive work plan that includes actual combustion work.
- Show improvement relevance to DOE goals. Drop if budget tight.
- Keep up the good work.
- It is questionable whether this is the appropriate forum for presenting new project proposals. Whereas the presented material certainly has a lot of potential to comprise a highly interesting project, this event was intended to review existing projects and not proposals.
- This represents a new capability. Extensive effort should be invested in comparison to previous methods. Opportunity and verification of the new APS method, better understanding of how their new technique modifies the current understanding. How well do the new results correlate to the existing reference information. Compare APS results to glass/quartz injector models and to detailed simulation models.
- Excellent research!
- Possibly could be used as diagnostics and checks for model development. It would seem that everything will change with temperature, pressures, swirl, multiple injections etc. As this capability develops some critical questions should be developed for this system to assist in answering.
- Focus future experiments on pushing toward diesel like boundary conditions, i.e. charge density and temperature.
- Need to migrate to operating conditions representative of typical diesel operation.
- Need specific plan and vision of how this project results in improved spray sub-models, injector design enhancements and combustion development.

In-Cylinder Combustion Studies and Modeling

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



Brief Summary of Project

The objective of this project is to provide the fundamental understanding required to overcome technical barriers to development of practical HCCI engines. Specifically, the team has developed a combination of metal and optical engines to investigate HCCI fundamentals, and has also developed modeling capabilities both internal to Sandia and external at other facilities.

Question 1: Relevance to overall DOE Objectives (Written responses from 16 of 21 reviewers)

The reviews were all positive to this question. One person agrees that the project is focused on ICE goals, and is very good. Clear and concise focus on goals that directly advance DOE's objectives of fuel efficiency and emissions reduction, said a second reviewer. The project aims to enhance the fundamental understanding of HCCI, said a reviewer, specifically with respect to technical barriers to HCCI application and is relevant to DOE's overall objectives of advanced combustion development. Another added that the work was a well-stated argument of relevance. Another reviewer commented on the excellent focus and that the project is extremely relevant. Another commented that the research seeks to understand the fundamental physical and chemical processes underlying HCCI. Another acknowledged that the project is highly relevant and focused on developing a clean efficient engine system. One reviewer noted that the work here represents a high level of technical leadership in one of the most critical areas of engine combustion technology. One reviewer noted the valuable results including: mixing, stratification, thermal stratification factors, rate of pressure rise, and peak pressure. Another added that the researchers are addressing important issues for HCCI and SCCI engines. Another reviewer added that this project is very fundamental and addresses in-cylinder phenomena that may lead toward expansion of HCCI or near-HCCI engine operation. One reviewer acknowledged that the work is gauged towards extending HCCI to higher loads and under transients can help overcome barriers. Another added that the understanding the HCCI combustion and the relevance of homogeneity is a key issue. One reviewer applauded the excellent work towards characterization of gasoline HCCI combustion and "knobs" to control it, but felt that there is some uncertainty as to how difficult precise control of thermo-stratification will be in a real engine. Another acknowledged the significant effort that is leading to a key understanding of combustion in this area with the cross-functional approach. The final reviewer commented that these engine technologies are crucial for reducing the engine-out NOx in order for the present NOx aftertreatment technologies to reduce the NOx in the exhaust to Tier II levels.

Question 2: Approach to performing the research and development (Written responses from 16 of 21 reviewers)

All comments to this question were positive. Several reviewers noted the very well-formulated, methodical, systematic and thorough approach that is providing very clean data. The overall approach is comprehensive and systematic, said a reviewer who also noted that the dual test-beds (optical and metal), coupled with modeling offer the unique opportunity to characterize and understand a range of "dimensions" related to HCCI and stratified charge combustion. Another noted the good measurements and careful analysis. Another reviewer simply stated that the work shows an excellent, integrated test/simulation approach. One reviewer noted that the important questions are being addressed in systematic fashion. Another person commented on the well-explained, multi-faceted approach toward developing a practical HCCI engine. Another noted the effective approach with good utilization to the available resources and expertise. Another reviewer commented that the approach, as always, has been good; especially the combination of the engine work and fairly simple modeling to do an approximately parallel estimation of the kinetic effect of the combustion along with the actual measurements. One reviewer commented on the very thorough and effective simultaneous coupling between modeling and experiment within one project, one feature of the approach that seems to be less evident in diesel combustion work. The reviewer cautioned that the use of cylinder wall cooling may be adverse to fuel economy. Another commented on the simplified 4 to 9 zone modeling that helps but may not explain all issues; further detailed simulation efforts are required: temperature and pressure dependency should be studied. Mixing after start of combustion is negligible since chemical kinetics is significantly faster. Several reviewers were pleased by the approach of using a metal engine to do parametric studies followed with the optical engine work. One reviewer highlighted the balanced approach of using optical and metal engines, with experimentation and theory. The final reviewer commented that the combination of metal and optical engine experiments has been valuable in assessing thermal stratification; it might be helpful to revisit projected heat transfer effects on peak pressure rise rate since a bulk of the conclusions are based on modeling efforts that tend not to predict actual in-cylinder heat transfer rates well.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 17 of 21 reviewers)

All comments to this question were positive. One reviewer felt that the work was very well planned and executed project. Good progress overall, said a reviewer who felt that the results on the impact of thermal stratification on HCCI combustion characteristics are fairly detailed. Others just commented on the excellent work and presentation that was easy to follow, comprehend, and had sound conclusions. One reviewer noted that the progress of work commensurate with general goals of the project. Another added that this activity is consistently productive, offering insight into the problem. One person commented that the researchers have shown good solid results as we have come to expect, adding that there is nothing revolutionary in the results. One person felt that the program is continuously making progress in the direction of interest, while another added that the project is providing a good understanding of HCCI process, but, there is still a lot more work to be done. Another noted that the areas of research have provided interesting results, but progress toward a viable HCCI engine concept has been slow. Another person commented that the research has generated some important insight into the processes critical to the operation, and load extension of an engine operating in the HCCI-regime. One reviewer commented on the good combustion insights for mixture control-NOx versus thermal stratification, and that he agreed that lower CR testing should be next. Another added that much progress has been made in addressing the impact of stratification on heat release, pressure rise, and peak cylinder pressure along with establishing equivalence ratio bounds on pressure rise threshold with gasoline-like fuels. Another added to this, noting the excellent review of progress, good explanation of effects and potential of thermal stratification for achieving higher load which shows sensitivity to barriers to commercialization/practical applications. Another added that using chemiluminescence was used to investigate stratification effects. They also noted the multi-zone model development, thermal stratification for high load HCCI, and the fuel composition study. Very good results, said another; focus on EGR and variable valve actuation recommended (instead of wall temperature and compression ratio). The final reviewer commented on the outstanding progress is being made in areas where others have made contributions, but has advanced to a degree to contribute unique insight into future aftertreatment and health effects considerations.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 17 of 21 reviewers)

Several reviewers noted the excellent interaction, collaboration, and integration of highly specialized and talented teams with Universities, engine manufacturers, and with the other laboratories. One reviewer simply stated that the work was fine as always, suggesting no major changes. Another agreed, stating that there they could not fault the work. Another person noted the many partnerships and information exchange efforts. One person stated they were very pleased to see this data used by LLNL. In addition, another felt there was good interaction with Cummins, International, and GM on hardware, plus work with universities on modeling, diagnostics, and instrumentation. Another commented that the cooperation with International seems to be interesting. A reviewer pointed out that the project seems to have a fair bit of general interaction with other stakeholders as part of the ACE working group, and specific collaborations with a few industry partners, university partners and National Laboratory partners are also apparent. Several specific, industrial, government and academic collaborations were noted by a reviewer, who said that a broader memorandum of understanding with a large group of companies is also a great means of knowledge dissemination, and that the team is demonstrating solid technology sharing through publications and conferences. One reviewer commented that the technical papers and presentations have been very good. Another noted that the results are further demonstration of technical leadership. The final reviewer commented on the “always valuable insights from John” for combustion/emissions.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 12 of 21 reviewers)

One reviewer said that the PI clearly articulates what he has done and where he is going. Another person simply stated that the researcher showed a good continuation plan. They have many plans to investigate different areas. Futurei work with Stanford will yield an interesting tool, said a reviewer, who suggested that the team drive to more industrial testing conditions to aid in transfer of knowledge. The proposed future work seems relevant and builds upon past progress, a reviewer said, but the team should consider prioritizing means to achieve thermal stratification based on feasibility in potential production engine configurations. Another person said that they look forward to seeing the results of this work, as John does an excellent job of building upon previous results and planning very logical extensions. Another reviewer noted that the aspects of the future research stated here represent a potential to contribute significantly to the fundamental understanding of HCCI/partially stratified CI combustion. One person encouraged more chemiluminescence of cooling effects and mixing, asked that the team study compression ratio effects on combustion and thermal efficiency, and noted that the team had added variable valve timing: all these efforts will deepen the understanding of how to improve HCCI. One reviewer felt that the lower R_c makes sense, I'm looking forward to the VVA results. Another added that if focus is VVA and not wall temperature/compression ratio modification, this helps a lot in the development of HCCI combustion. The last reviewer marked down his score based on the plan to "complete the fabrication and shakedown testing" of an International VVA system.

Specific Strengths and Weaknesses (Written responses from 17 of 21 reviewers)

- Specific Strengths
  - Very strong PI and a good engine laboratory. Also a good collaboration with LLNL for the modeling.
  - Combination of metal and optical engines with modeling is providing significant insights. Excellent mix of techniques and excellent overall work.
  - The main strength of the work is its outstanding relevance to HCCI research being done by others in industry and in other research labs. This is enhanced by the extensive collaboration and coordination with other groups working in this area. The fundamental understanding gained through this work makes a significant contribution in the understanding needed to provide controllable HCCI operation in a vehicle application.
  - Comprehensive - The dual test-beds (optical and metal) coupled with combustion modeling provide a unique opportunity to comprehensively characterize the fundamentals of advanced combustion regimes.
  - Variable valve actuation gives this investigation a new boost.
  - John's work compliments that of Dick Steeper.
  - The use of both the optical and metal engines is a real strength.
  - Combination of engine tests and optical studies continuing to provide unique insights on critical factors affecting HCCI.
  - They have obtained many interesting results and significantly improved understanding of HCCI engines.
  - Very nice combination of experiments, analysis and good sound engineering reasoning.
  - Excellent experimental data.
  - Thorough analysis.
  - Good use of simple models.
  - Well-designed experiments (numerical as well as real).
  - This program is very good!
  - Excellent understanding by PI of objectives and how to reach them.
  - Excellent utilization of the currently available resources.
  - Iterative approach checked by models.
  - Excellent probing tools to examine evolution of fuel and combustion events in cylinder. The data is fused with the theoretical modeling very well.
  - Excellent experimental facility combining practical metal and optical engines that is critical for developing understanding of in-cylinder HCCI-like combustion.
  - Expand the operating range of HCCI operation.
- Specific Weaknesses
  - More transfer with multi-zone modeling simulation recommended.
  - They have made little progress toward a practical HCCI or SCCI engine.
  - The ways in which the various proposed strategies for expanding the HCCI operating range (retarded

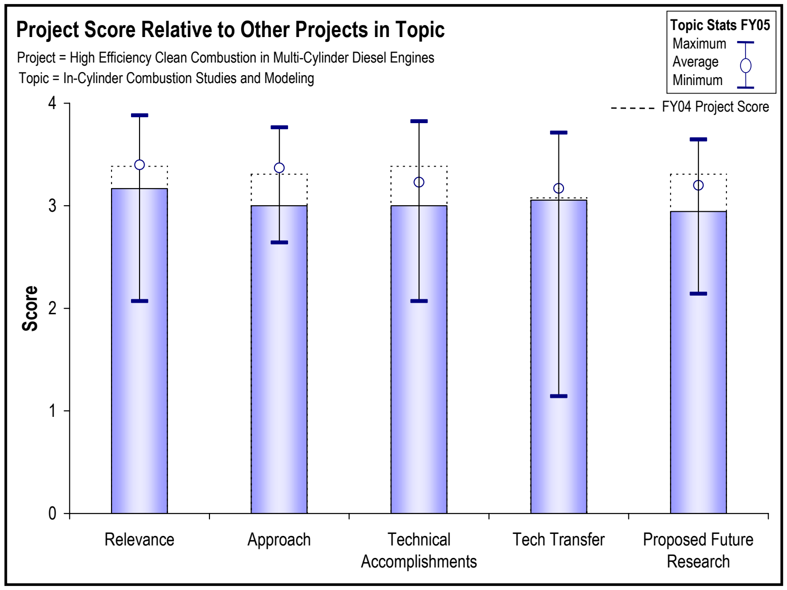
injection timing, thermal stratification etc.) affect fuel economy and combustion stability could be better elucidated.
  - None, only issue is that can one control the heat transfer in the real world or will this be a major problem for the HCCI type of engines?
  - Not much emphasis on transient control.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 13 of 21 reviewers)

- Continue as in the past.
- Did not see any mention of interaction of the charge stratification and cooling with transient operation. In other words, could efforts to utilize thermal stratification cause problems during transients?
- It would be instructive to see a direct connection made with the effects of thermal/concentration stratification seen in "real" multi-cylinder applications. Looking at the extreme cases, while instructive in demonstrated isolated effects, may not fully clarify the combined effects observed in a multi-cylinder engine. Also, further work is needed to be able to characterize speciated emissions over a reasonable range of engine operating conditions, consistent with those anticipated for advanced hybrid vehicles (the most plausible
- Use of VVA instead of wall temperatures (not feasible in automotive applications) and reduction of compression ratio (this was conducted by several researchers already but no variable compression ratio engine survived in the market). Use of commonly available fuels helps.
- Don't waste time getting the VVA system to "work." The valve opening events of VVA can be simulated in other ways. From personal experience, getting a VVA mechanism to work properly can be a full time development program on its own. Leave that to International. They should do the "donkey work" and produce a "turn key" system for SNL.
- Make it a priority to get the VVA-system operable. Don't lose sight of the big picture!
- Increase priority for study of fuel effects.
- Keep up the good work.
- Try to avoid going in too many directions at once.
- Future experimental work in gasoline HCCI combustion should include some level validation of steady state findings in transient mode of engine operation.
- Revisit the heat transfer modeling efforts as noted above.
- Consider quantifying the impact of thermal stratification and combustion retard on thermal efficiency.
- Continue the project; Do additional work on understanding transient issues.

In-Cylinder Combustion Studies and Modeling

High Efficiency Clean Combustion (HECC) in a Multi-Cylinder Diesel Engine, Robert Wagner of Oak Ridge National Laboratory



Brief Summary of Project

This project is investigating high-efficiency clean combustion as a means to improve engine efficiency through improved combustion efficiency and through reduced performance requirements for aftertreatment systems. This project is being undertaken on a multi-cylinder platform, and efforts are being taken to develop methods and strategies for management of HECC operation.

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

Several reviewers offered positive comments regarding this project's relevance. One said that HECC and LTC combustion are important areas for research, while two other reviewers said that the project was clearly relevant to DOE's high-efficiency, clean combustion goals. The project seeks to develop high-efficiency, clean combustion processes, said another reviewer, and is thus directly relevant to the overall DOE objectives. A reviewer noted that the project is focused on developing a clean high-efficiency combustion system. A reviewer said that improving efficiency while reducing requirements on aftertreatment equipment is a key component of developing advanced engines. Another stated that finding ways to expand the HECC envelope is a "key" need. A reviewer highlighted that the demonstrated results of HECC emissions and BSFC within the investigated range of load/rpm map generally confirm current state of experience existing in industry. The approach is well in-line with the kind of strategies many diesel OEMs are looking into currently, said another reviewer who continued by saying that the research would benefit significantly from a closer interaction with the industry partners. A reviewer felt it was relevant to make a note of unregulated emissions levels. This is another project that focuses on heavy premixed burn combustion at light load, said a reviewer. It provides another data point supporting use of this type of combustion strategy under portions of the engine map for reducing NOx and PM.

Several reviewers offered other comments. One said that the project offered reasonable value, but the reviewer was not sure of anything new here. Another said that the project seems to be feeling its way into an important area of technology, but seems to lack enough awareness of work being done by others to get up to speed and make a significant contribution. One item that a reviewer had difficulty with was the definition of HECC and how HECC is different from other combustion approaches: this reviewer said that if he had a better understanding of this, then the relevance score he provided might be higher. Finally, a reviewer said that these were important investigations, but HECC is difficult to run in a stable operation.

Question 2: Approach to performing the research and development (Written responses from 12 of 18 reviewers)

Several suggestions were provided regarding the research approach. A reviewer said that the approach was good overall, while another said the approach is practical and effective within the available resources. One suggested that the team members are obtaining useful data, but need to conduct more analysis. Another reviewer highlighted the team's approach of operating the engine in alternate combustion modes, understanding the thermodynamics of the engine operation and doing detailed chemical analyses, as well as using high EGR rate and injection strategy control. One reviewer said that the approach seems reasonable to address the objectives of the project. The experimental test-bed and the nature of the experiments chosen provide an opportunity to bridge the gap between some of the more fundamental diagnostic work conducted elsewhere and the typical industry development effort. Another suggested that the approach is sound (adding large amounts of EGR and advancing timing in order to force premixed dominated combustion operation.) More time could be spent wringing out details of overall engine system management to explain cooling and in-cylinder effects on both emissions and fuel consumption. Another said that the team has done a decent job of describing the experimental approach and motivations for the technical choices and has provided good detail on experiments, but needs to do a better job of explaining the HECC regime.

A reviewer offered the suggestion that if the intention is to use an existing engine platform to investigate a new combustion system, then it has limited potential to make a contribution. If a new engine configuration is to be investigated, then it is not clear from the work presented what that configuration should be. Further, the load/speed range under consideration is not of prime significance to most engine manufacturers, and it is unclear why one would want to transition in/out of HECC. Another noted that low-pressure EGR is interesting in terms of fundamental research but not for practical applications, and that the efficiency study was very interesting. A reviewer offered suggestions on several areas that could be improved: speed-load point weighting procedure, noise measurements, and control of mode transitions (especially the HECC to OEM configuration transition). A reviewer said that trying to achieve the fundamental understanding of HECC is confounded by having a multi-cylinder engine. Issues such as unknown air-EGR mixture temperature, etc., also confound acquiring a fundamental understanding due to cylinder-to-cylinder interactions. Finally, a reviewer offered that, although it may be a way of presenting the data, it seems that aggressive transitions between “low load” HECC modes and “high load/high speed” conventional diesel combustion regions are not well investigated—illustrated transitions are between the modes of combustion at fixed operating points which carry limited practical application.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 11 of 18 reviewers)

Several reviewers spoke about the good progress toward goals, one noting that the team is making progress toward good combustion at lower loads at all speeds and another stating that reasonable progress has been made. This project has demonstrated (in the eyes of one reviewer) that the combustion concept does work at a few light load operating points—perhaps expansion to other light load conditions would help validate this concept. A reviewer highlighted the addition of an improved control system, and the ability of the engine to operate in “HECC” at modest torque levels but as good or better BSFC and very low NOx. This reviewer also noted that HECC operation was shown to affect three of the five key light-duty engine operating conditions. A reviewer pointed out that it appears that this R&D is applicable to light-duty diesel (more so than heavy-duty), so it is recommended that the author make this statement more clear to the audience.

Several suggestions were provided. One reviewer said the team needs to do a better job of comparing ORNL results with those of other researchers. Another suggested an increased emphasis on identifying issues and developing resolution strategies related to transition among multi-mode combustion processes. More details about control procedure were requested by a reviewer: pressure transducer, engine-out emission, air management, and so on. This reviewer requested an acceleration of progress but acknowledged the difficulty in doing so. A very limited range of parameters has yet been explored, in one reviewer’s viewpoint, and the capabilities demonstrated thus far do not appear to represent a comprehensive strategy for addressing LD diesel emissions. Finally, a reviewer said that the author distinguished HECC from LTC: it seemed to this reviewer that they are the same (HECC is good LTC).

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 10 of 18 reviewers)

Some reviewers approved of the collaborative nature of this project: one noted that good cooperation with Ricardo and AVL was demonstrated, while another referred to the excellent ongoing collaborations. Interaction with national labs, universities, and industry is sufficient for this type of effort, said another reviewer. A reviewer said the collaborations were OK, but not much above what has already been discovered by industry.

Several reviewers suggested areas for improvement in collaboration. One said that the team has a good start on collaborations with industry and universities, but needs to develop more substantive collaboration with a few industrial and university partners. Another noted that some collaborations have been established with universities and SNL, but the interactions with industry need to be improved substantially. This was reflected in another’s comment that the project needs more collaboration with industrial partners, and in the comments of a reviewer who stated that a reasonable level of collaborations seems to exist among various stakeholders, but the project could benefit from increased participation from an industry partner. A reviewer suggested that the first and second law analyses may be more useful when exploring other parts of the load/speed map, and that collaboration with engine manufacturers would significantly improve the relevance and focus of this work. Finally a reviewer said that the presenter could be a little clearer on the amount and nature of the technical collaboration.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 7 of 18 reviewers)

Several reviewers provided input into the possible future research direction. One said that the work needs to be focused on modifying the engine to achieve HECC over a broader range. Another similarly suggested an increased emphasis on expanding the range of HECC operation and transitions among multi-mode combustion processes. A reviewer offered that the team could improve thermodynamic analysis, and examine injector configuration effects, injection strategy (mixed mode combustion) and fuel effects as enabling HECC. A reviewer suggested that the team needs to study injection effects more thoroughly instead of exploring fuel effects. A reviewer stated that the team needs to do a better job of elaborating future goals and paths toward achieving them, and identify clear goals and research programs to meet them. This was reflected in another comment that the future plan is not clear—it is generic in nature and hard to differentiate exact issues that will be addressed in the future. A final reviewer said that this was a key technique for further work.

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

- Specific Strengths
  - Relevant topic.
  - Excellent demonstration of HECC in a multicylinder engine.
  - Excellent engine system test mule.
  - Practical approach to developing HECC strategies. Project provides an opportunity to bridge the gap between fundamental characteristics of HECC operation and global in-cylinder engine calibration metrics.
  - The practical approach in analyzing the multi-cylinder system.
  - Good practical experimental setup capable of producing useful data relevant to practical engine improvement in the near-term.
  - Sophisticated experimental strategy permitting cutting-edge combustion studies.
  - This research could be used to evaluate and validate thermodynamic models of energy efficiency, to determine where efficiency gains can be made using an HECC-like approach, and at what cost. Also, the study of soot precursors in the exhaust over a range of intake oxygen concentrations has the potential for a significant contribution.
  - Detailed engine control for HECC combustion is one of the most challenging tasks. Results may be used for other HCCI combustion investigations, too.
  - ORNL has the analysis tools and expertise for the necessary multi-cylinder work on this topic.
  - They are investigating an important phenomenon and making some progress.
  - Good utilization of modeling in conjunction with the testing.
  - Characterization of soot precursors in O_2 depleted combustion.
- Specific Weaknesses
  - As yet, the thermodynamic analyses seem fairly primitive and do not provide particularly detailed insights as yet.
  - The HECC results demonstrated here are reasonably well understood by others. The engine concept does not seem to make a new contribution to the understanding of diesel emissions control, and does not seem to represent a coherent strategy for meeting regulatory standards. No aftertreatment requirements are proposed, and it is difficult to ascertain what the EGR and boost requirements will be to achieve the full implementation of this combustion system.
  - Due to the sensitivity of HECC on ambient and production tolerance parameters, a broader view for other HCCI combustion systems control needed.
  - Not all the "knobs" for combustion control are being investigated, e.g. variable valve timing and variable (switched) valve lift. A "standardized" common engine platform has its pitfalls–beware and consider carefully before implementing.
  - Work is confused and poorly focused.
  - They don't have a good understanding of the combustion in the engine.
  - One might argue that a national lab should focus more on fundamentals than on the optimization of a combustion system. It may be difficult for OEMs to provide guidance without revealing their own strategies. If the work aims at being more fundamental in its nature, it probably would have made more

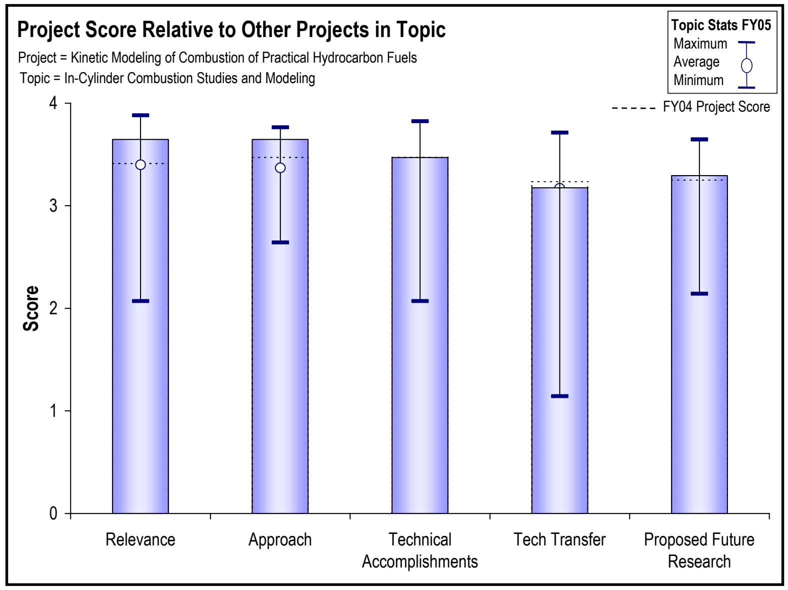
sense to use a single-cylinder engine. For example, in the multi-cylinder engine used here, the EGR-distribution to the various cylinders is likely non-uniform.
- I suspect/fear that some of the results may be rather specific to your particular setup (this is a common problem not limited to this project).
- Need to work to find universally applicable, or at least broadly applicable information.
- Work seems to be focusing more on answering the question "can pre-2000 MY LD diesel combustion systems be re-tuned to meet EPA FTP75 Bin 8 - Bin 5 requirements" versus "how can such a combustion system needs to be optimized to meet these requirements?"
- Did not define whether HC increase would be an issue. Emissions are measured as a total of NOx + HC. Actually emissions increased for many of the operating points. Perhaps these can be removed via an oxidation catalyst but it is unclear what the exhaust temperature is for this engine with all the EGR. Temperatures going into the turbo were very high: difficult to get to high BMEP effort.
- This effort seems to be lacking a strong analytical ingredient; the experimental effort is very good but could use a little fundamental support.
- It does not include variable valve actuation.

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

- Drop project.
- Try to obtain more guidance from the OEMs.
- Establish a clear definition of HECC that differentiates it from the other combustion systems.
- Consider cetane number and fuel volatility effects on achieving HECC.
- Explore a broader range of conditions on the load/speed map for this technology. What are its limitations and benefits to LDVs over an FTP75 and US06 cycle?
- Sensor development recommended and/or more detailed exchange with suppliers needed.
- Redesign the EGR system to obtain good EGR distribution and EGR effects cylinder-by-cylinder without having to resort to individual cylinder trimming. The compression ratio seems high compared with the latest industry thinking. Investigate whether lowering the CR will help extend the HECC range.
- Devise strategies to extend HECC operation to higher loads.
- They should conduct modeling of the combustion process at some important representative conditions.
- Evaluate the relative merits of a long-route versus short-route EGR-system.
- Investigate combustion mode transition from HECC to conventional.
- Revisit HECC emission/BSFC potential in the areas of operating conditions 4 and 5.
- Check to see if this was linked to modeling.
- Focus future research on specific versus general issues; add a more analytical ingredient to future efforts.
- Expand the scope to study effects of variable valve actuation.
- Not sure what the baseline engine model year is. May be worthwhile to benchmark HECC fuel economy and emissions against state-of-the-art and/or on a "newer" base engine.
- Continue effort to verify / address "transient" performance via excursions between conventional and HECC operation.

In-Cylinder Combustion Studies and Modeling

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



Brief Summary of Project

In this project, the team is developing and applying chemical kinetic modeling techniques to the analysis of key combustion processes in diesel, HCCI, and spark-ignition engines. The team is continuing the development of surrogate fuel mixtures for diesel and HCCI engine development, and refining the understanding of soot formation mechanisms. This team is continuing to work closely with the engine combustion team at Sandia.

Question 1: Relevance to overall DOE Objectives (Written responses from 15 of 17 reviewers)

Comments on the relevance of this work were quite good. Kinetic modeling can provide better understanding of the basic combustion processes in HCCI, LTC and diesel engines, which can enable better designs to improve efficiency and emissions, said a reviewer. Another reviewer said that this work appears to be connected to the understanding of fuel burning in HCCI engines. One reviewer noted that the fidelity with which modelers can hope to capture the chemistry of combustion, be it gasoline or diesel, lies in the hands of people like Charlie Westbrook and his co-workers. Developing capability to describe the combustion of practical fuels can help overcome key technical barriers to develop of advanced engines, said a reviewer. A further review comment was that this was very useful work, and we need to continue these efforts. The project is focused on developing a necessary element for understanding and developing clean combustion systems, noted a reviewer. Another said that the work was outstanding, and the fuel modeling lays the foundation for designing fuels and for building better chemical kinetic models. The team has made a remarkable contribution to developing an understanding of low-temperature chemistry of HCCI combustion and chemistry of soot formation for oxygenates, in a reviewer's opinion. A reviewer thought that this effort is a core contribution needed to maintain a current understanding of reaction mechanisms in what promises to be a fast-changing area in combustion/fuels research. This is an outstanding project that is critical toward development real fuel surrogates that can be used in practical engine combustion CFD codes and thus will aid engine manufacturers in developing new, low-sooting combustion systems, said a reviewer. This is a very heavy/complicated topic, noted a reviewer, and Dr. Westbrook does a good job of explaining his approach, and explaining results in an understandable and useful manner. A reviewer said that these investigations help in all chemical controlled combustion processes: HCCI as well as soot formation. This fundamental research compliments more practical DOE experimental and modeling efforts, and is critical to developing accurate combustion sub-models that will run in reasonable computational times, observed a reviewer. These simple fuel models have great potential for engine combustion models. This work is always designed to support the DOE goals, offered one reviewer: this reviewer had trouble understanding that the work on explosive materials is relevant to this review. Finally, a reviewer offered the opinion that although the work has been excellent, understanding kinetics is not a major barrier to development of clean, efficient engines.

Question 2: Approach to performing the research and development (Written responses from 9 of 17 reviewers)

Approach comments were generally positive. A reviewer commented on the very good comparison of simulation and experiment. Another noted that choosing representative compounds and studying them has been very effective. The approach is very well-thought-out and rigorous, in one reviewer's opinion. Charles is probably is offering the best expertise of SI, CI and HCCI combustion kinetics presently available. The general approach of developing simple model fuels is excellent, said a reviewer. Comparison of results to various types of experimental models is also good, noted this reviewer, who wondered if it is always possible to separate the effect of the fuel model from other physical inaccuracies present in the model. The development of surrogate fuels is an appropriate approach to address realistic topics, noted one reviewer. Apparently there are working groups that are addressing the identification of surrogate fuels. A reviewer suggested that the team refine models for HCCI fuels, look at soot formation from practical fuels, tie to experimental studies, and build practical surrogates/mixtures that satisfactorily mimic in-use fuels. Finally, a reviewer said the technical approach generally seems good; however, this reviewer questioned the relevance of work done in high explosives to that of basic engine combustion. This reviewer would also have appreciated a better explanation of why time and effort was spent developing a surrogate fuel: if the surrogate fuel was developed because gasoline was not appropriate for the test equipment, this is acceptable, but if the researchers are looking for new fuels for improved combustion, that ought to be a different project.

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

Responses to technical accomplishment questions were generally positive. One reviewer commented on the good progress so far, while another said progress was excellent, providing new insights into combustion reactions. Another reviewer thought progress was excellent, and said the team made a good presentation of a variety of results that have been achieved. The overall theme, combined with a focus towards a surrogate fuel formulation, makes his findings valuable to many researchers, said a reviewer. The work has produced significant results in advancing the development of better fuel reaction kinetics, said another reviewer. There has been great progress made in developing diesel and gasoline surrogates for predicting ignition delay and soot formation during the last couple of years. The PI should be commended for his team's efforts, in this reviewer's opinion. A reviewer observed that continuous improvement on development of surrogate fuel models was demonstrated, and that the analogy of soot formation between high explosive combustion and CI combustion of HC fuels was interesting. Different fuel compositions and comparison with model fuels was highly appreciated by a reviewer. A reviewer singled out the completed model for methyl cyclohexane, the continuation of work on toluene, the development of an HCCI model fuel description, and expanded descriptions of oxygenates in his comments. A reviewer noted that there is a history of developing the kinetic models for new fuels, identifying the controlling kinetic factors that control the combustion of specific fuels, identifying the measurables that are amenable to kinetic analysis, and applying these kinetic mechanisms to these problems. This work continues in their typical successful mode. Finally, a reviewer said that although progress has been good, kinetic modeling of fuels will have a relatively small effect on DOE program technical barriers.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 11 of 17 reviewers)

Review comments here were somewhat mixed. One reviewer noted that the team is very well connected with industry, universities and other laboratories. Another noted that collaborations have been very good. A third reviewer said that this work is integrated into other National Lab programs, modeling and engine testing. Collaborations have been very good, said another reviewer. Links to experimental studies and the combustion modeling community is providing broad impact of this work on the field, in a reviewer's opinion. Finally, a reviewer said that various industry representatives, national labs, and universities are using kinetic mechanisms developed by this team and more than likely will continue to use any new mechanisms developed by this team.

On the other hand, several reviewers noted areas for improvement. One noted that in the past the technology was good: there is little in the presentation to indicate the technology transfer. The formation of working groups to develop surrogate fuels seems to be a very positive development in this reviewer's opinion. The level of collaboration is significant according to a reviewer, but development of test fuels should perhaps extend beyond the labs and support specific interests of industry research in LTC. A reviewer said that there was good collaboration with Sandia, but the team needs to do a better job of explaining collaborative efforts. A reviewer highlighted that detailed chemistry needs reduced reaction schemes before implementation into industrial use: this work is unfortunately not conducted by LLNL. A reviewer noted that the presentation does not list any collaborators and only mentions in passing that existing collaboration is with DOE working groups. Finally, a reviewer said that there was room for some improvement here, as pointed out by Charlie himself.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 9 of 17 reviewers)

Future work relevance comments were generally positive. One reviewer saw no way to improve the plan: this work is extremely valuable and this reviewer encouraged its continuation. Another noted that surrogate fuels should be the high-priority work, while to a third reviewer soot formation and understanding of HCCI kinetics are the key issues in the future. A reviewer suggested that the work was very good, but the team needs to develop a better plan to incorporate fuel models and reaction mechanisms into practical CFD models. It would be beneficial for the diesel community to learn some more kinetics of soot formation in an oxygen-depleted charge in order to improve the NOx/soot trade-off of low NOx combustion, noted a reviewer. Another reviewer thought that more activity is needed in these areas to support LTC research, such that next-step fuel considerations can be identified and addressed (combustion system effects, toxics emissions, certification issues, etc). A reviewer commented on the continuing diesel and gasoline surrogate kinetic model development, and the consideration of other oxygenates as needed. Finally, a reviewer said it is unclear from the presentation what the future plans are, or if future funding is planned for this project. The only mention of future plans states that work is not funded for the current year. It is unclear if this applies only to the modeling work identified on the slide or all work in the research area.

Specific Strengths and Weaknesses (Written responses from 15 of 17 reviewers)

- Specific Strengths
  - Long reliable history.
  - Many years of experience.
  - Strong PI with record of accomplishments.
  - Systematic approach.
  - An experienced researcher is making good progress on understanding kinetics of fuel and additive combustion.
  - The knowledge base of combustion kinetics mechanisms is important to establishing leadership in the government labs on this particular issue.
  - Solid understanding of the chemistry.
  - This is the only work in this important area.
  - Broad impact of the outcomes from the work.
  - Excellent computational resources.
  - Detailed chemistry is a fundamental work and is highly appreciated in the simulation research community.
  - Charlie's presentation and explanation allow even someone who forgot chemistry many years ago to understand.
  - Chemical kinetic modeling is important research for DOE and the FreedomCAR program. It appears that good work has been done in the past, but question what future plans and direction are.
  - Solid technical contributions to the engineering community.
  - This team is performing unique chemical kinetics R&D that is critical for the continual development of the understanding of kinetics on soot, ignition, and heat release in diesel engines. The team's members are incredibly valuable sources of knowledge for the community.
  - Charlie is excellent at explaining how kinetics and chemistry can explain what we see in other programs. Collaboration to test surrogate mixtures quickly against available data is outstanding at generating VALUE to industry as well as other National Lab projects.
  - High potential to improve combustion modeling results.
  - The effective adaptation of the fundamental approach to practical application.
  - Developing model fuels that can be kinetically modeled.
- Specific Weaknesses
  - The amount accomplished this year seems smaller than in past years. I assume that is due to funding limitations.
  - More leadership in this area is needed to more broadly support other DOE programs.
  - Reducing detailed chemistry into practical usage of codes is not conducted by LLNL.
  - Should check consistency of kinetics with midroscopic reversibilty requirement.
  - I question the relevance of work done in high explosives to that of basic engine combustion. I would also have appreciated a better explanation why time and effort was spent developing a surrogate fuel. If the surrogate fuel was developed because gasoline was not appropriate for the test equipment, okay, but if the researchers are looking for new fuels for improved combustion, that ought to be a different project.
  - Industry collaboration could be improved.
  - How will the work improve the combustion improve fuel economy, etc? Appears to be more basic science in nature. Long-term research that will require many years to pay off. It was unclear if sufficient progress

can be made in a reasonable amount of time.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 11 of 17 reviewers)

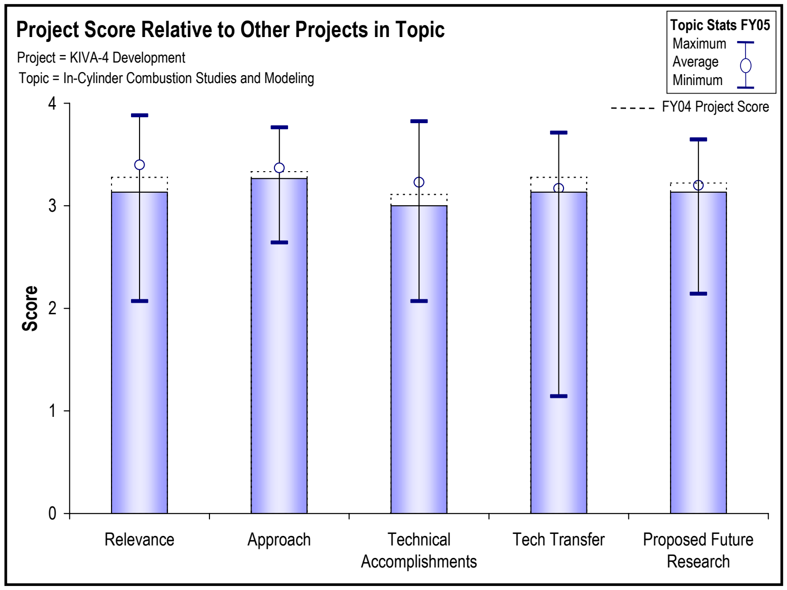
- I would appreciate more detail in next year's presentation on the collaborations.
- May be worthwhile considering (from the chemical kinetic standpoint) whether PRF fuels are good models for HCCI fuel or whether other model fuels would serve better to represent HCCI combustion behavior. Many researchers work with PRF fuels for simplicity, but perhaps this is overly limiting.
- No additions/deletions, just more of it. Also, more fundamental input of this type is needed to improve CFD/KIVA models.
- Increase the number of the correlation data points. Under "Objectives", obtain a consensus on the surrogate fuels for gasoline and diesel, by defining and agreeing upon the test criteria. Then Charlie should offer a selection of fuels which should be tested against these criteria, and agreement reached as an industry.
- Increase emphasis on hydrocarbons vs. oxygenates.
- Effort should concentrate on matching the low temperature combustion important to HCCI engines.
- Although high explosives seem to be an area of expertise for the research staff, I would like to see a better explanation of why work done with high explosives can help to understand ICE combustion.
- Keep up the good work.
- I would recommend extending these methods to aftertreatment chemistry.
- Based on improvement in understanding of soot formation kinetics, are we ready for new soot model to be developed and implemented in KIVA?
- Try to integrate more engine data into the ignition mechanisms validation process.

In-Cylinder Combustion Studies and Modeling

KIVA4 Development, David Torres of Los Alamos National Laboratory

Brief Summary of Project

This project team is working on refinements to the KIVA open-source code for transient, three-dimensional, multiphase, multicomponent analysis of chemically-reacting flows with sprays. A new version of KIVA, KIVA4, accommodates unstructured meshes and multi-component fuels, and will be available for parallel processing soon. Beta versions of the software have been distributed to several users, and converters for meshes in previous versions of KIVA have been developed.



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

Responses to this question were very positive. The project is focused on developing a necessary tool in developing clean combustion system, said a reviewer. Another reviewer said that KIVA and tools like it can enhance the effectiveness of combustion system design. Another stated that KIVA development is critical to the progress of future advanced combustion studies, as well as ultimately improving the standards for commercial CFD codes. A further reviewer said that the project was clearly relevant, and if KIVA4 development is successful, the routine will significantly improve engine efficiency. This software gets significant application within the industry, said a reviewer, who continued by stating that this work is a pre-competitive tool development, and the selection of improving the meshing technology to improve the accuracy of the calculations is an excellent choice. A reviewer said that the project team is developing a useful tool. KIVA is extremely relevant in the opinion of a reviewer, who said that it is extremely important that the code continue to be developed to provide an analytical platform. A reviewer offered that enhancing the computational capabilities of KIVA, an open-source multi-dimensional tool for combustion modeling, is likely to aid in the development of advanced combustion processes and engines and is thus in support of DOE's overall objectives. Finally, a reviewer acknowledged that constant improvements to KIVA are necessary, and that the benefits of this work are definitely "long term."

Reviewers had several suggestions for improvement. The implementation of advanced combustion models could be addressed and simplified, in the view of one reviewer. One reviewer said that unfortunately the presenter did not relate his presentation back to the DOE objectives. Certainly this code is being used by many in the industry but a few examples of why the work of going from KIVA3 to KIVA4 would be helpful. It was not clear why the problems were important, in this reviewer's opinion. The thought of providing a research-type of CFD-code available to the public domain is fundamentally good, but it is questionable in one reviewer's mind whether this effort will reach sufficient maturity before being overtaken by other methods. Combustion simulation is a critical tool for developing refined advanced combustion systems to meet DOE cost/performance goals, said a final reviewer, who also said that the focus seems to be to convert CHAD to KIVA4. This reviewer suggested more industry interaction to focus efforts.

Question 2: Approach to performing the research and development (Written responses from 11 of 15 reviewers)

Reviewers had several suggestions for the project team relative to their approach. One reviewer said simply, "I have no recommendations for improvement." A reviewer said that the team is focused on traditional limitations of CFD for engines, and it was not clear that objectives are focused on the latest challenges such as implementation. One reviewer said that the approach is focused in continuously improving the tool. Others said that these improvements are incremental and obvious but are absolutely necessary. Nothing here is revolutionary and would not necessarily be expected to be revolutionary. A reviewer commented on the open source code being further developed to have better efficiency and to parallelize, while another highlighted the new meshing options that seem to accelerate application significantly, as well as the compatibility of current efforts with KIVA3 grids. Another said that upgrading aspects such as meshing and parallel computing capabilities as well as turbulence models was necessary to keep KIVA current with commercial code advancements, but this reviewer believed that the research team should be working more closely with the labs to enhance or improve the efficiency and allowable sophistication of the advanced combustion models. A final reviewer offered that before exploring alternative turbulence models, the standard models for turbulence, combustion, spray, and heat transfer should be implemented, tested, and validated.

Several reviewers felt that the approach was reasonable, but one suggested that the project team should do a better job of justifying where time is spent. Another said that modifying the code to include unstructured meshes and to allow parallel processing will likely result in improved accuracy and a decrease in computational cost, which is significant for computing complex advanced combustion processes. A reviewer felt the approach seemed sound but it was difficult for the reviewer to determine what other options are available: this reviewer said that the project was primarily code modification and improvement.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 14 of 15 reviewers)

Reviewers were generally approving of the technical progress, but offered some suggestions for improvement. One noted that there is a clear sense of accomplishment from year to year, while another said that the KIVA model was being significantly improved. The improvements are important to maintaining KIVA's position, in another reviewer's opinion. Excellent progress, offered a reviewer. The implementation of a new turbulence model (from Paul Miles) seemed like a very good idea to one reviewer. A reviewer commented that the team tested benefits of enhanced gridding capabilities to overcome KIVA-3V mesh limitations, fixed some bugs in the beta version of KIVA4, and examined improvements of turbulence model in KIVA. Another reviewer noted that "code development always takes longer than people think it should!" A final reviewer thought that progress was good, but the priorities may need to be shifted (but did not offer suggestions for shifting priorities).

Several reviewers offered suggestions for improvement. One said that further studies and comparison with previous code still remain to be performed. Another said that good progress is being made but the "official" release of KIVA4 seams to be a long time in coming. A reviewer stated that KIVA4 seems superior to KIVA-3V, but the project team needs to do a much better job of demonstrating that results are more accurate compared to KIVA-3V in predicting experimental results. It appears that progress has been made, in the opinion of a reviewer who continued by noting that it is difficult to determine from the presentation where the principal investigators are in the total program and what the overall objectives of this effort are. A reviewer said that in general, the progress has been good, but perhaps the incorporation of state-of-the-art KIVA-3V sub-models should be the next logical step after the base meshing issues are resolved and parallel processing implementation is accomplished. A final reviewer was not sure KIVA4 will make the needed impact to justify a return on investment, and suggested a much more active survey of what the current KIVA4 needs are to meet 2010 combustion modeling needs.

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

Several reviewers were enthusiastic about the technology transfer of the project. One noted that the software had excellent beta distribution, while another said that the team is working well with universities and companies. A reviewer echoed that comment by noting the good collaboration and communication with industry and academic experts. A reviewer highlighted the option to use parallel processing as a big step. By using an open source approach and collaborative development of the code, said a reviewer, very effective partnerships have formed. This is an excellent example of DOE leading development and dissemination of R&D tools that have broad practical benefits for education and technology evolution. A reviewer said that technology transfer is very good: it is hard to transfer software without actually being a software company, and the software rollout seems to be as successful as can be expected for a project which is directly funded to accomplish this.

Several suggestions for improvement were provided. One noted that many contacts have been established, but the work would benefit from further guidance and focus. Another said that the team needs to collaborate more with universities and particularly industry: beta testing of product by external testers is a start, but more substantial collaboration is needed. A reviewer commented on significant interest in this project from industry partners, universities and National Laboratories, but felt it was not apparent how the other stakeholders are collaborating in the development effort. This is a revolution occurring with combustion modeling and hopefully soon we may have new spray model techniques, said a reviewer, who felt that the new KIVA4 should be more than integrating CHAD benefits and should look forward to how new developing techniques can be integrated. A final reviewer felt that the presenter did not offer sufficient information about collaborations in his presentation, and this reviewer provided a lower score as a result.

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

Reviewers had several comments and suggestions regarding future research. The approach should significantly improve a valuable tool for advanced combustion research, said a reviewer. Another said that KIVA will remain competitive with other codes due to its open design. Another said that the presenters need to do a better job of explaining project goals: what clear advantages will KIVA4 offer compared to KIVA-3V? This was reflected in another's question about how the relative advantages of KIVA4 versus KIVA3 will be evaluated and validated against experimental data. A reviewer suggested that the principal investigator validate the new KIVA4 and evaluate new turbulence models, enhance meshing capabilities, and complete the parallelization of the code. One noted that there should be a stronger focus on implementing and testing state-of-the-art models. Incorporation of advanced sub-models should be the next logical step, said a reviewer, and this should be followed by rigorous validation and benchmarking against KIVA-3V and experimental data. A reviewer suggested that mesh generation and parallelizing are key features to aid in the wider utilization of KIVA, and that the team should move to combustion simulation. A reviewer thought that the future research was tough to assess since it was not clear what timeframe in which these activities might occur. Finally, a reviewer thought the future research plan was "fair to poor", and asked the team to survey what the research community needs are, as the current enhancements are starting to compete with commercial tool development.

Specific Strengths and Weaknesses (Written responses from 13 of 15 reviewers)

- Specific Strengths
  - A very large user base makes this work have a strong impact.
  - Open source approach, KIVA "community" to collaborate in development and application.
  - Open-source code.
  - The position of KIVA is somewhat unique in academia and research labs. Improving these areas of recent concern will help sustain its position.
  - Competitive code that is commonly used in the research arena.
  - Unique code.
  - The continuous improvement of the tool.
  - KIVA is a great tool, but we are only seeing an evolution of current capability.
  - LANL strength in CFD.
  - Builds on fairly successful KIVA history.
  - Impressive versatility, know-how, and enthusiasm of PI (virtually a "one-man show.")
  - Extremely valuable work to provide the platform for our analytical ability.
  - This is clearly a software development project with high potential for engine improvements and the support of engine development collaboration using a common open-source code.
- Specific Weaknesses
  - This is a developmental project. It does not seem as if any of the approaches attempt to find revolutionary solutions.
  - To an outsider, KIVA would appear to have an enormous learning curve to begin using it.
  - Documentation and ease of implementation of combustion subroutines may still be improved.
  - KIVA is computing power hungry.
  - Would like to see a timeline/project plan on what will occur when.
  - Apparent lack of organization and specification of goals.
  - It is simply not feasible for a single person to develop a complete CFD-code with state-of-the-art pre-processing, numerics, physical models, and post-processing.
  - Insufficient industry input.
  - Commercial codes are now relevant contender for in-cylinder combustion modeling.
  - How does this compare to commercial models? Are there any? What is the competition? How is it used to improve engine performance? Too detailed in the changes to KIVA without a clear definition of why is

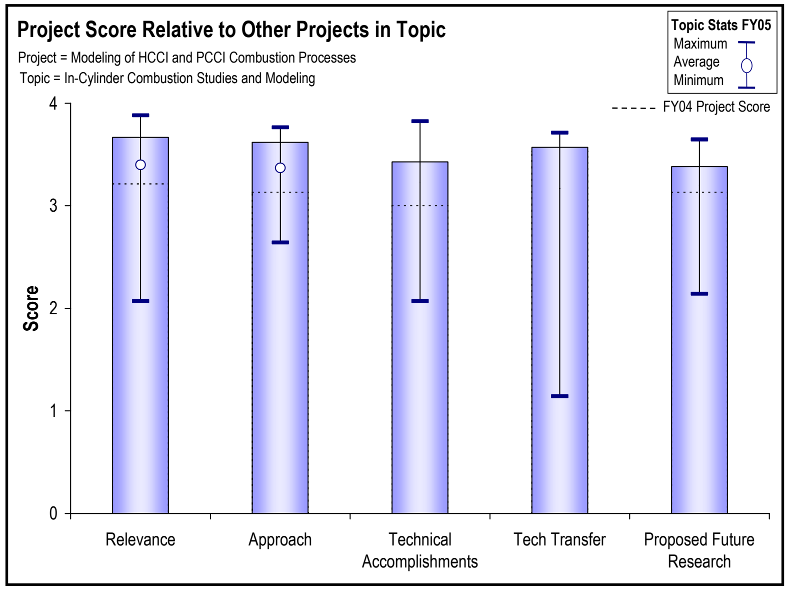
this important.

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

- The approach is satisfactory. It would be helpful if it moved along a bit faster.
- Work toward fully parallelizable code since this is the trend in the CFD community.
- In my experience, the first approach to the mesh strategy appears more useful than the second, so why make the second strategy also a development priority? Also, I would like to see more concentration in looking at conditions where reaction kinetic time scales may be closer to turbulence time scales, and whether a simplified approach can be developed to address such conditions.
- Further detailed parameter studies to prove compatibility with previous results to be extended before distribution.
- Include combustion work.
- Take Dave up on his offer to come up with ways to accommodate larger combustion chemistry mechanisms.
- They should focus more on combustion, in addition to fluid dynamics.
- Consider integration of advanced combustion and emissions sub-models followed by a comprehensive validation effort.
- Could it be beneficial to consider using KIVA4 in Dan Flowers' work as back-to-back comparison with KIVA3-MZ-MPI?
- Just an observation/thought, but is there any opportunity to utilize efforts from commercial CFD vendors to provide some of the mesh generation and remapping capability? If so, the available development efforts may be able to be focused on KIVA unique areas. How do you assess the "make vs. buy" decision?
- Target more complex geometries, where the advantages of the unstructured mesh capability become more obvious. Simulate a suite of test cases involving diesel- as well as gasoline combustion.
- The KIVA4 team needs to think about what is their niche and leverage this.
- I would guess the access to National Lab results is a huge advantage, but KIVA is not leveraging this. This is a major lost opportunity.

In-Cylinder Combustion Studies and Modeling

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



Brief Summary of Project

In this project, the team is applying chemical kinetic modeling and experiments toward solving technical barriers of HCCI engines. One goal is to develop numeric tools that can predict HCCI combustion with complex fuels in reasonable computational times.

Question 1: Relevance to overall DOE Objectives (Written responses from 17 of 21 reviewers)

Comments were positive in general. A reviewer simply noted that the program will aid with both fuel efficiency and emissions. Advancing the modeling capabilities to couple chemical kinetics and multi-dimensional CFD is important to understanding and developing advanced combustion processes and is thus relevant to DOE's overall objectives, noted a reviewer. One reviewer stated that the work is addressing a very relevant problem. Another noted that the program is focused on understanding the clean combustion process. One person commented that this is a timely topic with a nice approach with analytics, tests, understandings, and chemistry. Another added that such work is an invaluable companion to the other experimental work. One reviewer commented that the relevance of this project is indirect; the major benefit is the development of a tool to help shed light on future HCCI-like combustion system development questions and issues. One person stated that HCCI has good potential, and simulation is important to understanding the design changes necessary to make a practical engine. Another added that this modeling approach is an effective way to simulate the combustion occurring in the cylinder of an engine employing low-NOx technologies. Another person approved of combining CFD and detailed chemistry to better understand HCCI, which in combination with experiments can provide an essential understanding of combustion processes. Another felt that the proposed methodology will potentially allow HCCI to be modeled rather accurately. One reviewer noted the very accurate simulation of model fuels, which will significantly help the understanding of HCCI combustion. One person commented that chemical kinetic modeling is not very glamorous, but is an important part of the HCCI scheme, while another praised the great tool to design HCCI/PCCI combustion systems. Another felt that very good numerical modeling capabilities were demonstrated, and that the presenter did a good job of linking with other DOE and external engine experiments. One reviewer commented that the work contributes to improvement of understanding of physics and kinetics of HCCI process—especially by using a multi-zone chemistry model. The final reviewer noted that the development of a low-cost reliable combustion sensor is a must for HECC engines.

Question 2: Approach to performing the research and development (Written responses from 13 of 21 reviewers)

Comments were generally positive. One reviewer saw no room for improvement. Another commended the very good approach with computer times that were still reasonable. Others noted the excellent structured approach that has been well-tuned, as well as the effective integration of experimental and modeling efforts. One person commented on the impressive leveraging of unique National Lab resources to which industry simply does not have regular access. One reviewer stated that the CFD-chemistry split approach is an effective way to simulate both the chemistry and the fluid flow. One reviewer felt that the approach has been generally proven, while the addition of the multi-zone kinetics model, although less well suited for non-homogeneous turbulent reacting flows, provides the necessary insight. Approach of coupling multi-zone modeling for chemical kinetics with multi-dimensional CFD seems a reasonable attempt to one reviewer to achieve a trade-off between computational cost and physical representation. This reviewer suggested an increased emphasis on comparisons with experimental data followed by "applications" to understand and address technical barriers to practical application of advanced combustion processes. Another person noted that the researchers applied the multi-zone models on a range of mixedness conditions. One reviewer felt that the research approach and modeling (multi-zone interactive model, parallelization) appear to be state-of-the-art. Another added that the high-resolution CFD with low-resolution (but still multi-zone) chemistry improves computational efficiency, which can be used by industry in product development process. A reviewer highlighted the excellent illustration of the difference of timescale and length scale for chemical reactions and mixing, and the good mix of use of experimental data and detailed calculations from molecules to ensembles to systems. The final reviewer commented that this tool has been in the "works" for years and its approach has really not changed throughout the last couple of years. It provides a semi-simplified approach for linking fully chemically reactive CFD to multi-zone models that is a practical tool for developing HCCI-like combustion systems.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 16 of 21 reviewers)

Comments were generally positive. Good progress with the use of different models and the implementation of parallel code to increase efficiency, said the first reviewer. Reasonable progress seems to have been made, in one reviewer's opinion, who also felt this was an interesting study to evaluate the impact of turbulence on HCCI combustion. One person noted that the LLNL-group has already published a number of significant papers, first on the sequential-, and later on the fully-coupled approach. Another reviewer commented that whether their results will overcome practical technical barriers is hard to assess; however, the results help tremendously in elucidating the fundamental phenomena which control HCCI. One reviewer noted that the researchers characterized turbulence effects on HCCI, developed multi-zone model linked to KIVA, and showed that chemical timescales are too short to be affected by turbulence, providing validity to the multi-zone model. Another added that the calculations on a complex combustion bowl technology with complex chemistry are a significant technological step for the combustion technology development. One person commended the excellent combustion insights to combustion and explanation of phenomenon. Others noted the validation against experimental results is impressive, and the activity in the literature is an example of establishing the leadership of the combined modeling-experimental efforts. Good agreement between experiment and model in CO_2, CO, HC and OHC conversions as the function of phi effectively validates both the CFD and chemistry of the KIVA3V-MZ_MPI tool. It will be interesting to see how this tool performs in diesel-like PCCI combustion. One reviewer felt there was excellent progress with the remapping approach, while another commented on the useful study of the effect of turbulence on an HCCI engine. One person commented on the very impressive results developing a tool so we can analytically design HCCI combustion systems and therefore engines for 2010 challenges. Another felt that there was excellent modeling progress, but need to do a better job of showing coordination with broad DOE goals and with experimental researchers. The final reviewer commented that the need for extensive computing power is still a problem and will limit the widespread use of KIVA-MZ.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 17 of 21 reviewers)

Several reviewers noted the good collaboration with the all of the appropriate participants, including industrial, academic partners, and national labs, adding that all the major companies are involved. Others noted that the ACE MOU is an excellent collaboration team/resource and that the group has published many papers. A reviewer noted the excellent dissemination of information through publications, presentations and thorough leverage of interactions with industrial, academic and government laboratory collaborators. One person commented that the integration of this work with the other national laboratory engine measurements is great, adding that the results of this work have been well communicated within the engine manufacturer community. Another person added that there are direct and tangible partnerships with lots of signs of productive external collaboration. Others noted the good tie-in with John Dec's study and with other modelers and experimental research groups. One reviewer felt that among the collaborations in the group, the coordination in the HCCI efforts is perhaps the most impressive. One reviewer commented that it is difficult to overcome computer limitations, but the efforts for parallelization of code are well acknowledged. One reviewer acknowledged that the good job of collaboration was identified, but this may reflect the longevity of project. They suggested that the researchers need to do a better job of showing collaborations with industries and usefulness/relevance of LLNL capabilities on engine design. One person criticized that the "Long Standing Partnerships" listed are in the past, and the membership and participation in the ACE MOU needs to be emphasized and expanded upon. A number of collaborations between National Laboratories, universities and industry partners seem to exist as part of this project, but this reviewer was not sure how this effort is related to the KIVA-4 development work. The final reviewer simply stated that industry interaction could be improved.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 11 of 21 reviewers)

One reviewer stated that the researchers presented a very good plan, while others added that this is a key technique for further work and is well structured program which is integrated with the industry. One reviewer summarized that the work plan includes extending models, providing modeling support to experimental studies, and investigate fuels effects and combustion timing control. Another reviewer commented that there is nothing revolutionary about the future plans; however, the plan to continue this work is appropriate and encouraging. One reviewer felt that the application of KIVA3V-MZ_MPI as the guiding tool towards high BMEP HCCI/PCCI combustion optimization will be of very high practical value for industry. Another commented that the work seems to mostly support experimental work, instead of providing direction for experiments. Another reviewer agreed with this, but had a different perspective, stating that this tool is at a state of validation and thus future research is focusing on this area of development. With time, the confidence in this tool's ability to reach a predictive state will rise and such future validation efforts will be important. Another person commented that now that the tools for modeling HCCI and PCCI have been developed, the group needs to think about how to use it in optimizing the combustion process, i.e., what metrics to use, etc. A reviewer suggested an increased emphasis on experimental validation and then parametric applications to correlate fundamental in-cylinder characteristics with global in-cylinder control and calibration parameters. The final reviewer suggested that DOE needs to integrate its various experimental and numerical HCCI activities so that they support each other and follow a clear path to practical applications.

Specific Strengths and Weaknesses (Written responses from 19 of 21 reviewers)

- Specific Strengths
  - The high-end computing at LLNL, the proximity to the Westbrook group, and the SNL engine experiments make the location of this work a major strength.
  - Combining CFD and detailed kinetics to address HCCI research needs. Partnerships.
  - Nice approach combining multi-zone chemical kinetics modeling with multi-dimensional CFD.
  - Explanation of combustion process.
  - The strength of this is the development of an effective tool, validated reasonably extensively against "good" data through collaboration with experimentalists that can now be used to advance the testing efforts. Also, the resources available appear to be more than adequate to accomplish the research goals.
  - Detailed chemistry important and well included. Coordination with experiments is needed and seems to be accomplished in most areas.
  - Supports the Dec, Steeper and other SNL work.
  - Focus on elucidating effects seen in experiments useful.
  - They have addressed the need for detailed simulation of HCCI and SCCI engines.
  - Close collaboration with experimental work for validation efforts.
  - Solid conclusions and collaboration.
  - Leverage of collaborations, driving the development of theory by the use of multi-timescale, length scale models and the creation of more efficient code.
  - State-of-the-art modeling approach.
  - Excellent computational power
  - Through the interaction with Westbrook's group, the researchers have access to very detailed chemical kinetic mechanisms.
  - Strong modeling effort which maintains good contact with the experimental community.
  - Excellent modeling and computational capabilities, good use of exploiting physics and chemistry to reduce run times.
  - The effective integration of modeling and experiments.
  - Excellent modeling and approach to modeling through parallel processing and splitting the problem into two areas. Good coordination with John Dec.
  - Availability of computational resources for chemistry calculations is a major strength with this effort and also the close relationship with other partners that have experimental capability to validate this tool.
  - It supports the Sandia work (Dec et. al)
- Specific Weaknesses
  - Computer power extraordinary at Argonne. Application in the industry may take several years.

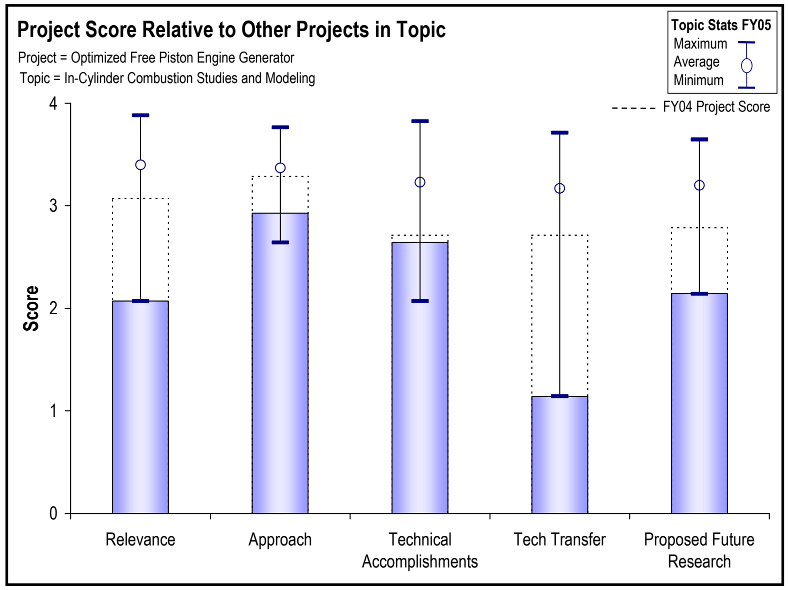
– Needs extensive computing power to utilize KIVA-MZ, even with parallel computing.
– Large computational time requirement may be an issue for industrial partners.
– Expensive computers are needed.
– Not much originality.
– A clear plan of how to utilize the analytical tool in optimizing the combustion process is lacking (e.g. how do we go from a desired fuel-temperature-equivalence ratio distribution in phase-space to the injection- and valve strategy rendering this distribution?)
– Can this assist in the transient behavior that engines are required to operate? Everything is steady state. How will transitions be managed?
– Need increased emphasis on experimental validation under “realistic” HCCI and PCCI combustion processes.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 10 of 21 reviewers)

- Continue on this path.
- Include consideration of transient operation, shifts in combustion regime (HCCI,PCCI, etc.)
- I think it would be illuminating to better understand the limitations, if any, to the MZ approach in non-homogeneous operation, and perhaps also at higher engine speeds where certain species formation time scales may be larger. In such cases, the interaction between the flow turbulence and chemistry is non-negligible.
- Comparison of results with different number of zones for stability and accuracy recommended. Influence of fuel properties should be investigated later in this project.
- Look for further ways to reduce the computing power required, otherwise the National Labs. may be the only places to run these calculations.
- Seek ideas for system improvements from simulations.
- Continue to push to establish a tool that will allow industry to make these calculations in a reasonable time.
- The computational burden may be lifted somewhat by avoiding re-initialization of the Chemkin-code and describing mixing in the multi-zone code.
- Consider further simplification of detailed chemistry computations to enable eventual integration into typical industrial computational tools.
- Utilize validated model to develop control strategies and concepts for control of combustion phasing.

In-Cylinder Combustion Studies and Modeling

Optimized Free Piston Engine Generator, Hans Aichlmayr of Sandia National Laboratories



Brief Summary of Project

The goal of this project is to demonstrate a prototype high-efficiency, low emission engine-generator suitable for hybrid vehicles or distributed power generation. The engine will use HCCI combustion in a free-piston design. A linear alternator will be employed to produce electric power from the motion of the free piston.

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

While interesting in concept, several reviewers characterized this project as being of high-risk. One noted that, although it was high risk, it was reasonable to have such a project in the portfolio, and characterized the project as having an interesting, but not unique, approach. One thought the project had relatively unlikely feasibility and another said it had a modest probability of merit (this reviewer did not see a clear potential to overcome barriers.) Another thought that, while risk was high, the payoff would be high if it were successful, and that only a government can afford to support such research and should do so. A reviewer suggested that very fundamental studies on high compression ratio may be conducted, and noted that the potential of overall fuel economy was not demonstrated. A final reviewer simply summarized the project as advanced combustion studies in free piston (variable compression) engines for use in a hybrid vehicle system.

Several issues were noted with the project. One reviewer noted that a two-stroke free-piston engine stands little chance of being clean, and the approach seems to be deficient in promising high efficiency. This reviewer felt that this particular program needs to re-evaluate its technical goals in the context of the overall program. Another noted that scientifically, the free piston engine concept for secondary power generation is interesting, but practically there are many challenges including load management, power density, packaging, and cost. The planned electronic/electrical synchronization of the two pistons will be a significant challenge, noted a third reviewer. OEM projects on two-cycle engines with conventional mechanical control of the breathing (the equivalent of the valve events on a four-cycle engine) have recently been cancelled as they failed to meet the required emissions levels. Having electrical control of the valve events will complicate this problem still further. Primarily because of its dimensions, one cannot think of an automotive application, in this reviewer's opinion. A reviewer questioned how an entirely new and radical engine geometry can prove viable in hybrid vehicles considering the changes to vehicle architecture that would be required to implement it. While the design may be viable for stationary power generation, the share of total U.S. oil consumed by stand-alone, small-output gensets is a minor percentage of overall oil consumption. So while the idea may be novel and intellectually intriguing, it appears to have little value in addressing the energy independence goals of DOE or the vehicle efficiency improvement needs of the FreedomCAR program, in this reviewer's viewpoint. Finally, a reviewer thought that this project represents a very interesting approach, but many issues remain to be answered: control of "valve events" and benefit over alternative approaches, e.g., diesel generator sets.

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

Reviewers were mixed on their views of the approach. One noted the well-acknowledged efforts for electric motor control and simulation approaches considering the minimum funding. Another thought that the approach was systematic, the analysis was good, and progress was good in developing the hardware. A reviewer said that the approach seems well thought out and follows a good long-term plan. A reviewer noted that the approach toward studying and developing this experimental engine is very good. The PI has been very clever utilizing available hardware to study/develop a linear alternator and has been attempting to simulate the engine thermodynamic cycle. Research appears to be thorough, in another's view, but it has been ongoing for 10 years and another three years are needed. In the auto OEM environment, new powertrain concepts are normally given 6-8 years to prove their merit and move into the prototype phase, or be dropped for higher priority research. A final reviewer simply summarized the approach as development of an opposed piston engine, using a linear alternator for electromagnetic coupling of pistons for timing control and to generate power, and noted that the team is also using modeling of the synchronization of the pistons for design purposes.

Reviewers offered several areas for improvement. One noted that free-piston engines can play an important role, but this one seems to have little promise to fill that role, as the technical approach does not properly address fundamental issues relating to efficiency, controllability, startability, emissions, etc. Another reviewer said that the quality of the experimental facilities related to the electric drive system is modest at best. The notion of using a resistor bank instead of an active, programmable load, for example, is inconsistent with the typically state-of-the-art approach of the national labs. This reviewer thought that some aspects of this project give the impression that very bright people with little background in electric drive systems have decided to reinvent the wheel. A reviewer offered that a significant weakness is the lack of overall system modeling to establish probable performance potential. A final reviewer thought that the electrical modeling work was good, but there was no thermal and structural modeling and material selection is unknown.

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

Several reviewers noted positive technical accomplishments, including the completed linear alternator test facility and the measured performance of a prototype, as well as the development of a model of the linear alternator and a model for opposed-piston synchronization. Another noted that progress is good, and that model results compare well to measurements. Another reviewer highlighted that the development of a linear electric generator is significant, provided that it can lend a pathway to an efficient system, and that it can provide the control that will be needed for this system.

Reviewers offered several suggestions for improvement to the technical progress. One noted that progress seems slow by OEM standards, while another noted that they seem to be making progress with the linear alternator, but the engine development status is unclear. Another offered that the project has so far been a demonstration of simulation efforts with engine testing not yet conducted. Several reviewers noted the long timeline of the project, one mentioning that the project is progressing, but the notion of being able to project a 15-year timeline for such a project is mind boggling. To this reviewer, this looks more like a hobby than a research project, when one looks at the time line. This reviewer noted that funding levels were not well-known: perhaps this project is funded on a shoestring? Another reviewer pointed out that this is the tenth year of a 13 year project, and progress has been very slow. The project team is still in the modeling phase, with no prototype hardware for either the engine or the generator. Funding was noted by another reviewer, who said that the progress made to date is slow but appears to be indirectly correlated to available funding. In particular, the linear alternator has been the main piece of hardware that has been studied to develop the power transmission power portion of this engine. A reviewer stated that it appears that this technology has a long period of time before it can be applied, and there are probably a number of technical issues yet to be uncovered in future work. Finally, a reviewer was not clear on the progress since certain aspects of the program are not being evaluated such as combustion, actual application of generated energy, overall system efficiency. This reviewer thought that the overall 55-60% "indicated" efficiency is "likely misleading" and referring to an overly simplified zero-dimensional thermodynamic analysis.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 13 of 14 reviewers)

Several reviewers thought that the collaborative aspects of this project could be improved, with one assessing the collaboration efforts as "unclear." One noted that there were no apparent commercial partners or interest, while another said that there was no mention of outside collaboration. A reviewer suggested that the team needs to do much better at finding or identifying collaborators. A reviewer thought that the team is open to transfer and collaboration, but as is typical with inventions the team is having trouble finding partners. Unlikely to obtain industrial partners in the near term, was the assessment of a reviewer. This project appears to be strictly a laboratory in-house effort, noted a reviewer, reflecting the thoughts of another reviewer who noted that most or all of the work was done in the lab, consistent with the program plan. One reviewer did highlight that there was some interaction with LANL on model development. Another reviewer thought that there is not much of an opportunity for collaboration, and so it is not surprising that this is relatively limited in scope. A reviewer suggested that this project would benefit immensely from a partnership with a potential commercialization partner with strong expertise in electromagnetics and electric drive systems. A reviewer thought that the program needs an application focus. Finally, a reviewer commented that the potential of the system not evaluated, and a benefit-risk analysis was not obvious.

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

Future work plans were felt by many reviewers to need some improvement, although one reviewer said that the research plan for next year is reasonable. One reviewer proposed that the team should work toward prototype development. Two reviewers felt that the future work plans were governed by funding, with one noting that funding is clearly an issue, and another saying that the future work plan was not clear, which could be a function of an unstable funding profile. Difficult technical challenges exist for this system from a thermal management and materials selection in another reviewer's opinion. A reviewer said that the future work will only get to the first prototype: to be successful, this type of machine will need several iterations to achieve its goals. Another observed that research is moving into prototype hardware phase. While some might question the need to do so, it is a logical extension of the R&D conducted so far. The R&D needs firm milestones and go/no go decision points to ensure valuable work continues. A reviewer felt that the plan for future research is quite incomplete: there is very little consideration of important factors, such as power electronics for grid/load interface, system control, and design optimization of electromagnetics. Their plans for the alternator are much better defined than for the engine, said another reviewer. A reviewer felt that no potential for fuel saving was demonstrated, and that indicative efficiencies that were shown in the presentation are comparable with diesel engine combustion at the same peak firing pressure levels. A final reviewer said that the project appears to have little chance for producing a successful, working engine.

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

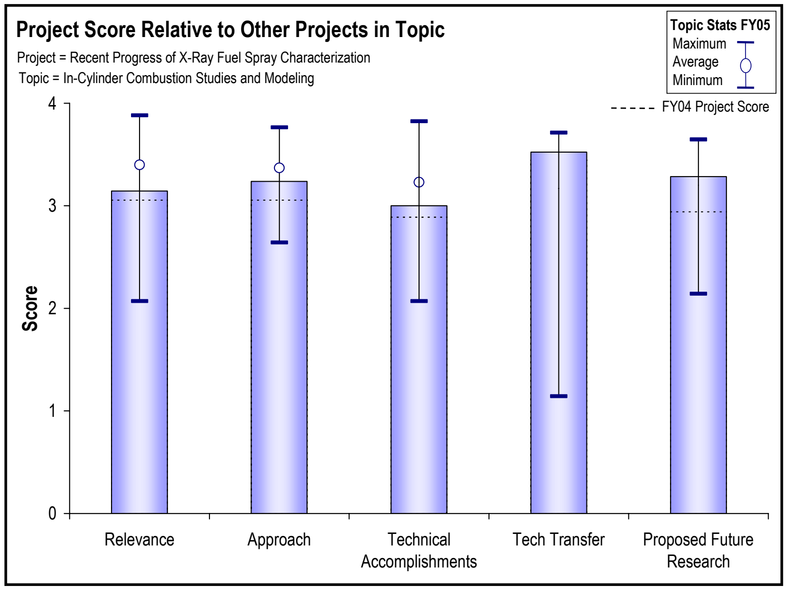
- Specific Strengths
  - Thoroughness of the approach to the design process.
  - The free-piston combustion process should offer significant benefits: low NOx, low heat loss; it should also benefit from low friction.
  - Very advanced approach with new technologies.
  - Interesting idea.
  - Interesting idea worth pursuing.
  - It is unique.
  - Very creative concept.
  - "Out of the box" concept.
  - Exploring new approach to IC engine with possibility of improved efficiency, but concerns regarding applicability in vehicle applications.
  - Development/validation of mathematical models (necessary for optimization).
  - Excellent analysis tools.
  - Some good simulation of certain aspects of the design, but oddly little to no analysis of other critical aspects.
  - Good electrical modeling capability.
  - Understanding developed with the linear alternator.
- Specific Weaknesses
  - Unclear whether there is significant commercial opportunity for this technology, but much relies on how complicated the final design will be.
  - The free-piston engine represents a substantial control challenge, yet the approach does not appear to recognize the fundamental issues. On a basic level, the two-stroke HCCI process will give significant cycle-by-cycle variability in residual gas composition and temperature (during steady state, but especially during transients and startup) that can not easily be compensated for, least of all with a comparatively low-bandwidth actuator. Electric synchronization seems very high-risk technically and very likely will only exacerbate the residuals issue. The issues with that might distract the focus of the work in a first prototype. The results of the present approach, based on similar experience, will very likely be: poor efficiency, poor control/component damage, and difficult startability.

- High risk without demonstrated or simulated advantages (power density, emissions, fuel economy) shown. Conduct a simulation study to ensure viability of the concept. If possible, include cost estimates.
- Insufficient planning; this could become a lifetime project that never reaches conclusion.
- It is unique. It does not appear to have a "home," a potential use within the automotive sector.
- Develop conceptual designs on alternative applications with comparisons to competitive approaches to guide research (stationary vs. truck vs. auto).
- They have little knowledge or experience with the issues of opposed piston engines. Also, the electrical power from the system will be in a relatively inconvenient form.
- How will an entirely new and radical engine geometry prove viable in hybrid vehicles considering changes to vehicle architecture that would be required to implement? While design may be viable for stationary power generation, the oil consumed by stand-alone, small output gen sets is a minor percentage of overall U.S. oil consumption. So while the idea may be novel and intellectually intriguing, it appears to have little value in addressing the energy independence goals of DOE or the vehicle efficiency improvement needs of the FreedomCAR program. Also question whether the measured efficiency in the test bed experiments is sufficient enough to warrant further development considering anticipated losses as one moves from an experiment to actual engine hardware.
- Industry collaboration and funding
- Lots of new technology required, including packaging considerations in the vehicle.
- No thermal, combustion or other modeling to indicate that these systems will be able to survive the conditions. Limited information on the entire efficiency for the entire working loop. Conventional generators will be ahead of this system by the time that they are developed.

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

- Find or develop a commercial partner or University partner with a long term interest in this project to give the continuity of support and effort that this project appears to require. Should begin targeting a commercial niche for this device so that design can incorporate "system" design requirements (e.g., the "balance of plant" requirements may affect performance requirements and thereby influence design).
- I do not believe a prototype is justified, unless the approach can be simplified to a design that mitigates some of the technical risks. The present approach will likely result in more "tinkering" and less useful data. I would recommend more modeling that looks at controllability during transients (a free-piston engine is, effectively, always in a transient, since it has no inertial energy storage) and control robustness/disturbance rejection.
- Even to prove the concept of this approach, packaging studies, sizing, power density, etc. need to be conducted. Potential experiences from TACOM or FEV-engines (see SAE Congress 2005) may be used for this.
- The project should include a "best case" estimate of the potential overall efficiency of such a system. Is the cost worth the potential benefit? In addition, this project requires a serious injection of expertise in areas where the investigators do not have sufficient expertise (electric machine design, power electronics, control systems). A comparison should be made with similar projects, e.g. the West Virginia University Stirling engine linear alternator. This project should not continue without input and participation from commercial partners.
- Do not continue funding.
- They need to get an engine expert familiar with opposed piston engines.
- Need firm milestones and go/no go decision checkpoints to ensure research is directed toward specific objectives and is aligned with DOE and/or FreedomCAR goals.
- Come up with more detailed projections on perceived benefits regarding fuel economy and emissions. This may increase the incentive for funding the project.
- Provide a more accurate estimate regarding pros and cons of electromagnetic synchronization vs. mechanical.
- The PI should spend much more time addressing combustion and packaging (power density) issues.

Recent Progress of X-Ray Fuel Spray Characterization at Argonne, Chris Powell of Argonne National Laboratory



Brief Summary of Project

The goal of this project is to study fuel spray geometries from diesel injectors using x-ray techniques. The techniques are being used to provide visualization of mass distributions within sprays. Industrial collaborations have been pursued with DaimlerChrysler, Caterpillar, Visteon, and General Motors.

Question 1: Relevance to overall DOE Objectives (Written responses from 18 of 21 reviewers)

Majority of the reviewers agreed that this work is relevant to DOE objectives. One reviewer stated that the approach is unique and the application of the APS to injector flow characteristics can/will have a major impact on the injector technologies that are so important for implementing new engine combustion. The topic is critical to the understanding of clean DI engines, in another reviewer's opinion, and more importantly, is focused on providing relevant data to "real" combustion systems. A reviewer pointed out that the team is directly addressing fuel efficiency with peak performance of diesel engine. Another reminded that fuel spray research is fundamental to improving the efficiency and emissions from advanced diesel engines; therefore, the subject area is highly relevant. He added that the goal of helping the DOE improve injector design and performance is not clearly linked. He asked how the knowledge of the near-nozzle region will translate into improvements. According to him, more accurate modeling of the process is not a guarantee for improvement of the system performance. Enhancing the understanding of fundamental fuel spray characteristics is critical to advanced diesel combustion and engine development and is thus very relevant to overall DOE objectives, noted a reviewer. However, the benefit is likely to be significantly limited (according to this reviewer) unless it would be possible to apply these advanced diagnostic techniques at operating conditions (e.g. injection pressures and ambient pressures) that are representative of typical diesel conditions. One person thought that modeling and understanding the benefits lines up with the DOE objectives. Another thought that important information about high density area of spray is being produced. According to one reviewer, injector spray characterization is important as it is an integral component of combustion. Someone mentioned that the researchers need to demonstrate a new insight, which has not yet been the case. A reviewer found this work interesting, but thought that it will only indirectly lead to overcoming technical barriers (by improving models). Another person found this work extremely valuable to get a better understanding of the conditions in the near field of the spray as well as inside the injector. One added that a solid understanding of the spray dynamics is highly relevant to DOE's objectives of supporting programs aiming at developing clean and efficient internal combustion engines. One person stated that this work clearly identified early measurements of injected sprays near the nozzle tip which are critical to improving diesel injector designs. One comment was that this program would enable better understanding and improving the needed elements for clean combustion. Another mentioned the qualitative and quantitative (to the degree based on resolution) insight into physical characterization of liquid spray break-up. A mention was made that a systematic parametric study of the cause-effect relationship for a selected set of parameters could further qualify the full potential of X-ray spray characterization. Someone felt that the assumption has to be made that this work has direct merit to the development of clean and efficient engines. One reviewer thought that this spray measurement tool has the potential of aiding engine manufacturers and fuel system suppliers in developing and designing future diesel combustion systems. According to him, such a technique can address certain spray characteristics in which other techniques have shortcomings, including possibly local air-fuel ratio deviations. He added that such understand is important for choosing nozzle designs and fuel injection timing strategies that will be part of an engine system approach to meet future emission standards. Another stated that this project may yield a better process to characterize fuel spray.

Question 2: Approach to performing the research and development (Written responses from 15 of 21 reviewers)

Comments regarding the approach of this work were mostly positive with a few suggestions. One reviewer felt this work is very successful in utilizing all the expertise at the APS to solve the complex problems involved in applying the beam spectroscopy for injector and engine technologies. Another stated that this work is clearly a world-leading technology that has brought good publicity to ANL and DOE. Another added that the excellent x-ray capability and engineering are being utilized in this project. A reviewer indicated that the approach appears headed in the right direction to examine the effects of expected in-cylinder temperatures and pressures. A comment was made that this research team has taken past reviewer comments and improved their approach from an application viewpoint through more engine representative boundary conditions. One thought that the X-ray method is a novel approach to solve the difficult problem of characterizing fuel spray near the tip of a nozzle. Another said that the X-ray imaging approach is unique and can provide unique information about the mass distribution within a spray. A comment was made that progress on achieving realistic conditions and obtaining meaningful data is being made. A reviewer said that the approach seems to be on the right track, now that the test environment is approaching more realistic engine conditions. A suggestion was made to compare the results with other methods whenever possible. One person mentioned that, although it was not discussed in the presentation, the issue of the dopant effects on the properties and behavior of the fuel during the spray process remains a concern. It was added that higher chamber pressures and temperatures may be difficult to achieve using polymer windows. Someone felt that the test conditions currently being used are far from representative of those found in the combustion chamber. A comment was made that an expansion of the investigation into multiple-orifice sprays and an increase in ambient pressure is definitely needed to better reflect spray development conditions in an actual engine. While the approach uniquely applies a challenging technology to improve understanding of near-nozzle sprays, it is currently limited to low injection and ambient pressures, noted a reviewer. The team stressed the complementary nature of the X-ray study to optical-based analytical tools, said a reviewer, who continued by noting that these studies are critical to the modeling/simulating programs and that fundamental science was rapidly applied to the diesel engine application.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 15 of 21 reviewers)

Reviewers pointed out several technical accomplishments of this project, but also expressed a few concerns. One reviewer felt there was not enough technical content presented. He did recognize many good technological accomplishments of this work from the past several years, but unfortunately could not identify any recent accomplishments. A comment was made that moving to higher ambient pressures is a major and significant accomplishment. One reviewer mentioned recent accomplishments including grinding technique effects of injector internal structure on spray structure to affect spray penetration, the added capability to study multi-hole injectors at relevant pressures, and the possibility for measurements at elevated pressures. He also noted progress on expanding capabilities for more relevant measurements for multiple shots via a project specific monochromator. According to him the researchers have made continuous improvements over the past 6 years. It appears that some progress has been made, noted a reviewer, who felt, however, that it was not apparent how this work has specifically influenced the development of spray sub-models, the process of injector design and/or eventually combustion and emissions enhancements. One person found the comparison of hydro-ground to sharp-edged nozzles very interesting. Another felt that there has been excellent progress in getting the data more closely connected to engine conditions. One person commented that this work seems to be maturing quickly and he is very glad to see links with modeling activities. A comment was made that the techniques developed are rather sophisticated, but the link to how the work will assist in developing cleaner and more efficient engines is still largely missing. Another comment was that a lot of the accomplishments were tested as capabilities were put in place but there was not much information given on interpretation and any new information uncovered. Someone mentioned that good recognition and response to earlier reviews shows the need to move toward commercial engine conditions. One comment was that it seems better to look at single x-ray shot images rather than average images of several shots. One person stated that since X-ray spray characterization pertains only to the liquid phase of diesel spray formation, its full practicality can only be validated through close coupling to modeling and/or engine-based complementary testing. To one person it was not clear how the information relates to combustion processes, performance and emissions. Someone thought that good experimental progress has been made within the last year. He added that in particular, the spray chamber operating pressure was doubled and now chamber density is approaching TDC conditions under lighter loads in a small automotive engine. According to him, future efforts are aimed at continually increasing chamber pressure (density) and also chamber temperature to more accurately capture evaporation effects. One comment was that work seems very slow and the team is only now looking at multi-hole injectors and higher fuel pressures. A final reviewer indicated that it would be extremely useful to have a timeline for the work: it is not always clear what was done in the last year. This reviewer thought that moving to a high-pressure regime was significant.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 16 of 21 reviewers)

Reviewers recognized good industry interaction at several levels. One reviewer stated that this group is doing an excellent job in technology transfer. It was added that the partnership with Bosch on hardware and personnel represents an excellent level of collaboration. On-going collaboration with several other companies was mentioned as well. A comment was made that close cooperation with Bosch and others will allow the latest technologies to be examined and will encourage improved interest from industry for valuable inputs. A reviewer pointed out that there were several collaborators in the industrial sector, and interactions with numerous government labs and universities. The team has a strong synergistic relationship with model developers, and does a good dissemination of knowledge through presentations and publications. One person mentioned that with improved spray ambient conditions, this is a very interesting new technique that industry may use together with ANL. Another said that collaboration with industry for injector development and with universities for modeling of diesel sprays has been very good. A comment was made that the high level of interaction with industry shows the relevance and potential significance of this work. One person stated that this project is starting to draw excellent industry collaboration, including a major fuel system supplier (sending a guest researcher), a major heavy-duty engine company (signed a CRADA), and other industry and university partners (aiding with measurement efforts). Another mentioned that this work could produce an excellent tool for nozzle development and novel data for modelers. A suggestion was made to highlight how this work applies to the modeling and how it changed the models. One reviewer commented that ANL interacts with plenty of partners on this and seem to have established good working relationships; however, the interaction with spray model developers needs to be intensified. To one person it was not clear how the collaborations with the industrial “partners” were implemented; how this is done should be outlined. It is good that a number of collaborative efforts with industry and academia seem to have resulted as part of this work, noted a reviewer, though it was not obvious to this reviewer what the specific outcome of these various collaborations has been.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 13 of 21 reviewers)

One reviewer stated that this project is headed in a very useful direction. A reviewer said that there was a clear plan for the future and a drive to conditions closer to diesel engines. The team has a solid grasp of the next big hurdles on how to operate at higher temperature and pressure. Another summarized the current approach, including development of high-pressure windows to permit higher pressure operation, consideration of X-ray exposure on window durability, and developing a new monochromator to improve sensitivity of the measurements. The approach is outstanding, said another reviewer, but may be improved somewhat by correlating with more mature optical visualization methods. If there is an opportunity to include this in the scope, or collaborate with another group doing such measurements on an equivalent system, this would be a significant step. One person suggested studying individual injections, different injectors, and operation at higher pressures. Another suggested putting stronger emphasis on how the results from the measurements can guide engine developers. One reviewer recognized that the researchers performing the work are becoming more aware of practical and fundamental aspects of sprays as shown in the future work plans. Another mentioned that focusing on synergistic correlations with dynamic measurements of injector internal geometry using phase-contrast imaging seems to be very important. A comment was made that the work plan is well thought out and there are no obvious missing elements. Another comment was that in this early stage, mostly fundamental understandings are being provided. It was added that more advanced results and specific parameters will be required for future development. Someone thought that future work should be better defined than just one simple slide. According to him, more information would probably have got a higher rating. The overall plan seems to be directionally consistent with the broader objectives, in a reviewer’s opinion. It would help if the specific plan and vision of how this data would be applied to spray modeling improvement/combustion enhancement could be emphasized. This reviewer was not sure how this effort synergizes with Wang’s work.

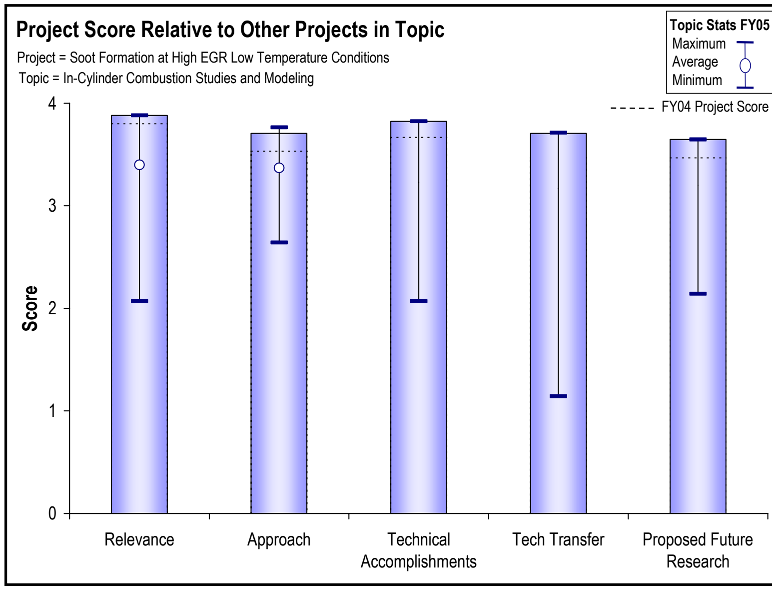
Specific Strengths and Weaknesses (Written responses from 19 of 21 reviewers)

- Specific Strengths
  - Great utilization of the APS source.
  - Unique ability to see the mass distribution.
  - Unique technology application.
  - It applies to current needs.
  - It uses a unique facility.
  - A unique capability that is delivering key insights to the engine community.
  - Uniqueness in ability to measure in-nozzle flow.
  - Opportunity to improve understanding of near-nozzle sprays.
  - They are obtaining information that has not been available previously.
  - Technology stretch, attacking of the tough problems, getting valuable unique data.
  - Augments historic and parallel visible light spray characterization.
  - A novel approach for observing spray mass distributions close to the nozzle has been developed. This represents a significant accomplishment.
  - Appropriate focus of near-nozzle region. This is a unique capability that can uncover processes occurring within the spray that have not been accessible to date. It has potential to be extremely valuable.
  - Outstanding one-of-a-kind spray imaging technique.
  - Outstanding effort to collaborate with industry and universities.
  - Good publication effort.
  - The utilization of a useful tool in understanding and visualizing the spray characteristics.
  - Excellent collaboration with many industries.
  - This research team should be commended for sticking with the development of the X-ray technique given the historical criticism of its inability to address realistic engine boundary conditions. Today this team is very close to simulating TDC operating conditions in an automotive type diesel engine. It will be interesting to see if this technique will resolve local air-fuel ratio.
  - Excellent method for evaluating certain parts of the spray.
- Specific Weaknesses
  - Need for dopant, inability to measure spray at the actual conditions (both temperature and pressure) present in an engine (so far).
  - Progress has been slow.
  - Progress towards migrating to realistic operating conditions seems to be slow.
  - From the data presented, the parts tested to date have been "obsolete."
  - The test conditions are not yet representative of actual operating conditions.
  - Use of expensive national facility for what is not yet shown to be of high value for this research.
  - Quite facilities intensive.
  - Still not up to real-world conditions, but they are making very good progress.
  - The question of how this project will help us develop cleaner and more efficient engines needs to be answered.
  - There does not seem to be a clear strategy addressing the use of the measurements to develop more sophisticated spray models.
  - Limited comparison to previous methods.
  - Not really a weakness, but is it possible to combine x-ray and conventional techniques to give a fuller picture of entire spray?
  - Need to do a better job of discussing fluid mechanical measurements near nozzle tip (or explain why it is not possible), e.g. velocities, turbulent intensities, etc. that would be useful to modelers. Maybe this is not possible. Could x-ray tracers be used?
  - Unclear how information is being used in the models and improving engine efficiency. Need to tie back how this is being used in industry. Engine combustion occurs in a highly transient environment.
  - Need to develop a comprehensive spray characterization method that is usable for the entire spray field.
  - Not sure if/how the results are being specifically utilized either for spray modeling enhancement and/or injector design.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 12 of 21 reviewers)

- Next year, give us a bit more technology in the presentation.
- Stay on track for expanded testing—work closely with industry.
- Additional techniques may be considered: Mie and Schlieren technique when higher pressures and temperatures are possible with the spray chamber in use.
- The Review Panel should be given some sort of indication of how this information is being used to improve combustion. Without it, we are unable to judge how effective it is.
- Look at reproducibility, i.e. test several samples of the same part. The differences seen between hydro-ground and non-ground appear to be small. Are they part-to-part differences or really due to the process?
- Determine if this approach can address an important specific question not currently answerable by other methods.
- Would like to see more of the counterpart modeling work.
- A sharing of data with the optical methods of looking at fuel would generate a complete picture between the complimentary techniques.
- Apart from addressing the concerns expressed above, the project would benefit from bringing together findings from other studies, utilizing various spray diagnostics (spray momentum measurements, Schlieren, Mie-scattering, PIV, LDV, PDA etc.), and present them alongside the x-ray measurements.
- Maintain or increase the interaction with colleagues who are spray experts.
- I hope that the data from this project can be combined with the findings of Siebers et al. and other spray-related research to provide an overall emerging understanding of diesel sprays.

Soot Formation at High EGR Low Temperature Conditions, Lyle Pickett of Sandia National Laboratories



Brief Summary of Project

These researchers are working to quantify soot levels within reacting diesel fuel jets at high EGR (low ambient oxygen) conditions. The team is looking at whether factors other than equivalence ratio and temperature govern the soot formation.

Question 1: Relevance to overall DOE Objectives (Written responses from 12 of 17 reviewers)

Panelists reviewing this project agreed that this project is very relevant to the overall DOE objectives. One reviewer felt that this research is well done and the PI does a great job of explaining combustion and engine processes that apply to 2007-10 emission standards. Another added that this work is fundamental to an understanding of PM-NOx tradeoffs, and makes an important contribution. This was echoed by a comment that understanding of fundamental NOx/soot formation is essential for fuel economy development. Another comment was that characterization and understanding of partially premixed combustion was highly appreciated. One person thought that this is an excellent project and a very important topic to future clean, efficient engines. Another stated that diesel engines can provide improvements in fuel efficiency and reduce CO_2 but at a risk of tailpipe emissions that may exceed future standards. He added that in order for diesels to remain viable, more needs to be learned about the science of emissions. According to him, research into soot formation at high EGR is a key enabling technology that will allow combustion improvements to make diesels viable in many US markets. Someone stated that this is terrific work that addresses a key area of interest, achieving a more fundamental understanding of mechanisms responsible for emission reductions, especially soot, in low-temperature diesel combustion concepts. He added that such an understanding enables devising improved combustion strategies. Another reviewer felt that this project is highly focused on understanding and analyzing the clean combustion process. Someone said that the results of the SNL investigation of a mixing-controlled diesel spray combustion fundamentals continue to be impressive in the depth and creativity of the insight provided in the presented work. A reviewer felt that this is critical work directly related to DOE's objectives. Another agreed, adding that this is a very fundamental project that is focused on explaining the impact of EGR on soot formation in diesel-like jets. He also said that it is too early to assess whether the understanding developed will lead toward a new combustion control strategy to meet future PM emission standards. According to this person, to date, this project is raising questions concerning the exact physics and chemistry responsible for PM trends observed with varying EGR mass fraction and also charge intake manifold temperature.

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

Comments regarding the approach of this research were positive. One comment was that the "path" to follow for air-fuel ratio, temperature, and EGR is clearly explained. Another was that the approach is very good for a fundamental study. One reviewer stated that the use of equivalence ratio versus temperature maps for NOx and soot formation and the influence of specific engine operating parameters on this allows a fundamental understanding of combustion systems. Another felt that this was an excellent approach and that the year-by-year plan outline is appreciated. A comment was made that important questions are being asked and experiments are conducted in a way to answer these questions. Someone commented that this research is highly regarded in technical community and uses test facilities and techniques that provide unique insight into soot formation inside cylinders. One person felt that this is an outstanding, well-formulated, and executed research project. This was echoed by a comment that the overall approach is very systematic and thorough; however, the modeling could be improved because the TSL-model clearly cannot replace a thorough CFD-analysis. One reviewer said that this project has a clearly-defined goal, as well as a good combination of experimental and computational methods.

Another pointed out good utilization of the experimental resources. One person felt that the approach is in general correct and effective. According to him, comments that come to mind based on presented material are: how the increased level of turbulence related to bowl/squish geometry (vs. injection pressure/orifice diameter) could improve highly-EGR-diluted spray mixing and prevent related migration of soot islands toward lower temperatures? He also questioned if there is any way to device a constant-volume vessel based experiment that could address this issue. A reviewer felt that this approach is a fantastic use of spray optical measurement tools toward addressing an important diesel jet issue.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 8 of 17 reviewers)

The reviewers felt that this project has made excellent progress. One comment was that progress made over the past year in clarifying the mechanisms for soot formation at lower ambient oxygen concentrations has been excellent and that this understanding is critical to meeting 2010 standards in a cost-effective manner. A reviewer felt that the investigated parameters (load, temperature, EGR, injection pressure) are the key issues for combustion. Someone said that characterization of soot formation inside combustion chambers with varying levels of EGR is valuable information and important to improve engine emissions. Another echoed the previous comment by stating that this is great information, not just experimental data, but also a well-formulated explanation of the data based on fundamental principles. One person commented that good measurements of sooting have been made in a model combustor. He added that this project involves interesting modeling work with a simple mechanism. Another felt there has been excellent progress and continuous improvement of the analysis technique. It was also mentioned that the PI and colleagues have made substantial experimental progress to date that has led toward more refined experiments to answer questions concerning jet PM formation as a function of EGR rate and level of EGR cooling.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 11 of 17 reviewers)

All the reviews regarding technology transfer and collaboration were very positive. They agreed that this project was very well connected with a wide range of entities in the research community. One reviewer stated that combustion insights and explanation are great technology transfers to all. The reviewers acknowledged participation of the engine manufacturer community. They also felt the cooperation through the AEC MOU group and other universities is very beneficial. A comment was made that this project involves good collaboration and information exchange among light-duty vehicle manufacturers, heavy-duty engine manufacturers, and several universities. Someone said that the researchers effectively collaborate with industry and academic combustion experts. Another viewed this as an excellent cross-functional collaboration. A comment was made that there seems to be an excellent interaction with industry through related projects and also good interaction with other PIs from the PI's host lab. Someone felt that the role of collaborators needs to be better explained.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 7 of 17 reviewers)

All of the people reviewing this project agreed that future plans are relevant and well-laid-out. One reviewer said that he is looking forward to seeing the results at future meetings. Another thought that the future work has good scope and application. Another comment was that the future work is well-thought-out and addresses the necessary mixing and higher BMEP effects on PM formation. A comment was made that the plans for future work seem to focus on relevant parameter studies. Someone mentioned that the researchers have identified important areas for further research. According to a reviewer, this work builds on past progress and is directed at continuing to address basic understanding of combustion tradeoffs among soot formation, smoke production, and NOx at high EGR. Another added that fundamental investigation of the effect of multiple injection strategies on mixing-controlled low-temperature spray combustion is of very high importance. He also said that there is significant lack of basic understanding of these fundamentals which may create a barrier in effective optimization of diesel HCCI and PPCI combustion.

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

- Specific Strengths
  - Understanding of the mechanisms and sensitivities of soot formation to salient operating parameters. The close collaboration with industry maintains the relevance of the primary areas of focus outlined in the presentation.

- Fundamental basis for understanding new combustion concepts like LTC, HCCI, etc.
- Very sound methodology.
- Thorough methodology.
- This work ties in well with other aspects of the AEC MOU.
- Good combination of experimental and modeling approach.
- Important subjects are being investigated and significant understanding is being developed.
- An excellent presentation of materials and research. Soot and NOx formation maps are easily understood and are great tools for education and understanding. Continues to be good research providing unique insight into soot formation and is highly valued by the engine community. Future plans are reasonable.
- Solid combination of well designed experiments along with analytical approaches to build a fundamental understanding.
- Reproducible experimental data.
- Good experimental technique.
- Interesting conceptual approach.
- Good utilization of experimental investigation with the collaboration of detailed modeling.
- Basic fundamental work that improves the understanding of soot and NOx formation.
- Excellent experimental facility and interaction with other researchers working on related issues.
- Excellent study of NOx/Particulates trade offs.
-

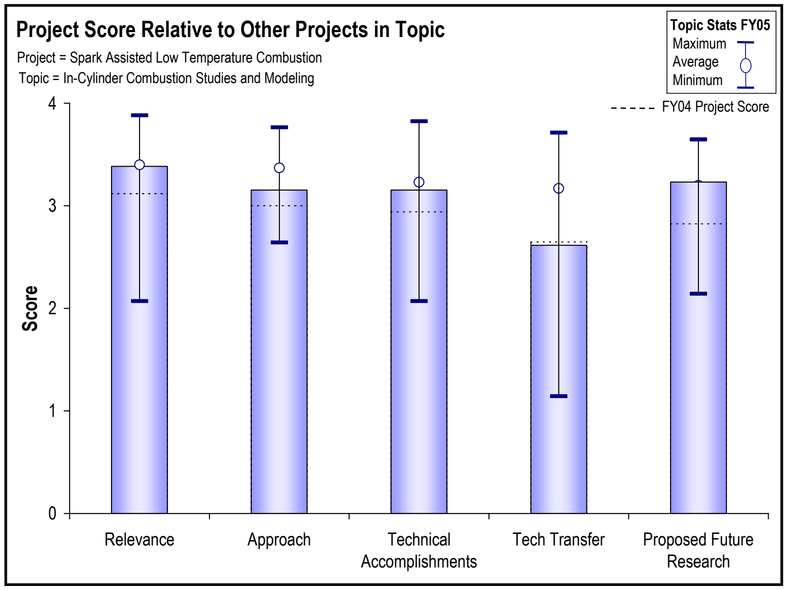
- Specific Weaknesses
  - The correlation of the reactor vessel (unbounded, stationary) with in-cylinder (wall-bounded, unsteady) results would limit broader application to effects seen in running engines.
  - Presentation was not as clear as it could be.
  - No engine experiments directly linked to the study. Musculus' engine experiments are not tied tightly enough to this research.
  - Inaccurate computational model.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 8 of 17 reviewers)

- The relative effects of hole size and injection pressure need to be clarified in a range expected for advanced common rail or intensified injection systems. Significant improvements have been seen with injection pressures in excess of 2000 bar. This effect, I believe, would be a more important contribution than multi-pulse injections.
- Focus of this study was n-heptane fuel. Further studies with different fuels including gasoline HCCI recommended.
- Look for ties between the fundamental results and their applicability to recursive semi-empirical models that could help shape EGR and injection control inputs during transients to avoid entering undesirable regions.
- Extend studies to understand nature of combustion in high pressure injection highly mixed high load diesel combustion.
- Continue the excellent work.
- Accompany research with engine experiments + CFD.
- Provide better guidance of engine experiments.
- The PI should consider adjusting dwell time for the future multiple injection work to further assess charge oxygen concentration and bulk temperature effect on jet PM formation.
- Expand the scope of the project to address EGR cooler deposits.

In-Cylinder Combustion Studies and Modeling

Spark Assisted Low Temperature Combustion, Bruce Bunting of Oak Ridge National Laboratory



Brief Summary of Project

This project is looking at achieving advanced combustion control and stability through spark augmentation. In particular, can spark assist be used to improve stability and increase operating range of the engine without detrimental effects to fuel economy or NOx emissions?

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

Two reviewers felt that the research is related directly in with DOE's road map. Another reviewer remarked that the investigation of the means to improve LTC is important. One reviewer stated that improving the stability of HCCI, dealing with transients, and understanding fuel requirements are all essential to overcoming barriers to practical use of HCCI. Another went on to add that spark-assisted HCCI may help overcome particular issues of homogeneous combustion. Another reviewer had similar comments, adding that investigating the use of a spark plug to facilitate the transition between combustion regimes is very worthwhile. This can provide the combustion stability that will be needed for a production engine utilizing these types of technologies. Others were less sure; one reviewer commented that the role of spark-assisted combustion in advanced LTC engines is unclear. It assumes combined-mode operation, with transitions in and out, which limits developers to a smaller range of hardware configurations (especially cost-effective ones). One person simply stated that the work is moderately relevant, and research as a modestly funded program. The final reviewer felt that the program needs to be more focused and generic in its nature. Investigating effects of spark augmentation and fuel on HCCI will likely require a close collaboration with not only the "major oil company," but also others, e.g., Charlie Westbrook's group at LLNL.

Question 2: Approach to performing the research and development (Written responses from 12 of 13 reviewers)

One person noted that the comments of last year's review were well-taken and acknowledged. Another felt that the researchers have used a good approach and methodology, but that the project is limited by the use of the AVL engine. However, another felt that the use of the AVL single-cylinder engine gives very good flexibility for this investigation. One person stated that the choice of subcontract was a good way to get started. One reviewer summarized the work, stating that very carefully identifying the conditions at which the spark assist is required to give stable operation is most helpful. Also crucial to understand is the combustion variation with different fuels and implicitly different fuel qualities. Investigating this in a single cylinder engine at this point is an appropriate choice. Their last point was to urge the researchers to "drop the darned RASP plug!" Another added their observations that the work is being done at AVL for the research engine and that the team will be using a new 2-cylinder variable compression engine using internal EGR at AVL, and will use external EGR in new engine. They noted that the researchers are considering HCCI and LTC (wherein slow combustion exists and supplemental ignition is required). One reviewer suggested to include the results (and relevant details) of the analysis based on the fuels work at the next review. One reviewer appreciated the presenter did a good describing the fundamental approach, because others have been more vague; however, they felt that a better job explaining and justifying spark research was still needed. Other reviewers were critical of the research progress. One reviewer said that the program needs to be more focused. Another person felt that the researcher team should have picked a modern 4-valve/cylinder engine instead of the 2-valve/cylinder engine. One reviewer thought that the approach needs to include CFD models or optical-access engines to give a more basic understanding of what is being seen with the spark-assisted engine data. The last comment was that the researchers need to develop deeper insights into effects observed; e.g. why spark effectiveness varies with fuel and speed/load conditions.

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

One reviewer felt that some interesting results have been obtained. Another went on to add that the experimental study has been adequate to give a basic characterization of the engine behavior with this approach to LTC. One person felt that the work is interesting in that it develops a possible strategy for HCCI type of engine operation. A reviewer stated that the results were very useful and the insights were interesting. Another reviewer felt that the slide on the percentage of test points that can be achieved with the spark plug versus a spark-less system is a very helpful accomplishment. One of the reviewers commended the good presentation and explanation of results, but felt that the role of "spark assist" was underestimated. They were somewhat confused by the mention of fueling study and how it fits "spark-assisted" LTC and HCCI research. One person commented that the influence of fuel properties has yet to be elaborated. The final reviewer commented that the RASP spark plug did not provide benefit for HCCI combustion. Depending on fuel, load and speed some operation is possible without spark (HCCI) and some requires spark (LTC) to achieve stable combustion.

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

One reviewer noted the team had presented at the MOU and other venues, had discussions with engine companies, and had collaborated with a fuels company. Another reviewer added that information is getting out to industry through DOE reviews and DEER. One reviewer noted that further collaboration with simulation activities is to be included. The remaining comments for this question were unified in noting that the researchers need to improve in this area. One reviewer felt that the technology transfer and collaboration is quite weak. Certainly the information is regularly communicated; however a close collaboration with an OEM that would be also test some of this technology would greatly enhance the value of the work. One person cautioned that the researchers should not count the subcontract with AVL as "collaboration," and felt that the researchers need to do a better job of attracting (and naming) collaborations and identifying their role. Another added that wider collaboration is required. It was suggested that future work is coordinated through the AEC MOU Working Group. One reviewer noted that further collaboration with CFD and/or flow visualization groups would enhance the fundamental understanding of the spark-assisted mode. The last reviewer felt that the project will likely attract more partners if it focuses more on the fundamentals of HCCI.

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

Comments to this question were mixed. One felt that valuable input from this investigation for HCCI combustion was expected. Another commended the plan to install and set up a new platform at ORNL, but cautioned that this group needs to be able to control the experiments. Another noted the complete installation of new engine, explore combustion regimes, and consider an additional matrix of fuels. Another reviewer stated that they believe that going to a more "modern" appropriate engine for this work is very worthwhile, but that the talk did not give a lot of detail on the engine planned. They went on to suggest that the researchers stay with a standard spark plug and the attendant electronics. Another reviewer added that the future research needs to work to provide a greater understanding of the flame initiation and flame spread process. This can be gained from CFD models or optical access, but may also be better understood through more conventional experimental methods. Another added that the researchers need to do a better job of identifying future research plans, but comparing conventional EGR to early-exhaust valve closing EGR will be important. One reviewer simply stated that the work plan needs better definition for more comment. The last comment was that the researchers should consider subcontracting for combustion visualization work.

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

- Specific Strengths
  - ORNL is a good place to do this type of work.
  - Capabilities of AVL engine facility, fuel matrix design, wealth of experience available for analysis and interpretation.
  - Spark-assisted combustion could be an important contribution, provided that certain enabling technologies can be identified to make it a cost-effective, while still giving acceptable performance.
  - Spark assistance may help overcome some of the tolerance and sensitivity issues with HCCI combustion.
  - Potential to aid in solving the major problem of controlling HCCI ignition timing.

- They are investigating interesting engine combustion conditions.
- Relevant hardware available (e.g. VCR, fully-flexible VVA-system, various ignition systems)
- Plenty of know-how available at AVL (however, it is uncertain to what extent this is being utilized in the project).
- Involvement of major oil company.
- Interesting exposition and exploration of various combustion regimes within the same engine.
- Information was presented in a very understandable format that places HCCI in perspective.

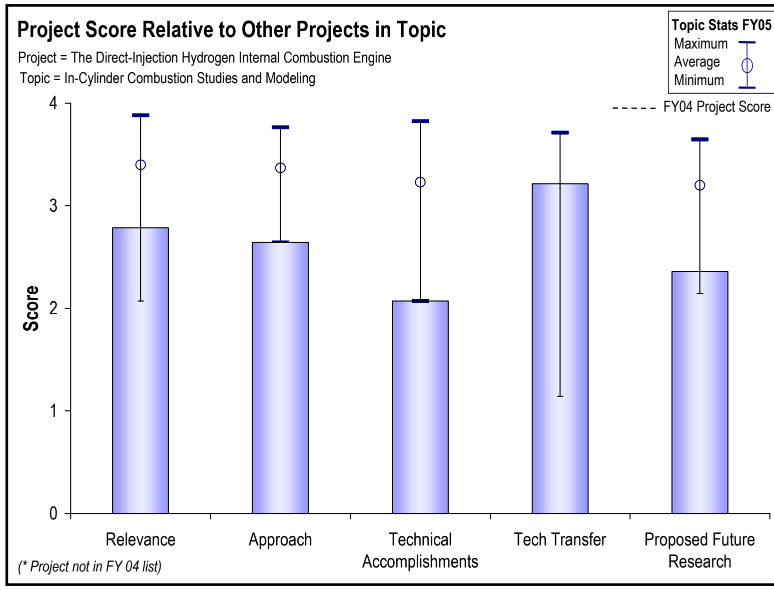
- Specific Weaknesses
  - Not a close enough collaboration with industry.
  - Need to use external facilities, potentially competing for access.
  - The scope needs to be expanded to gain a better understanding of the flame initiation and spread. It seems unlikely, based on what is shown here, that this is typical flame-front combustion.
  - Already noted in last year's review comments; include external EGR.
  - The partnership of AVL and ORNL. The AVL single cylinder engine.
  - Need to develop deeper insights into effects observed; e.g. why spark effectiveness varies with fuel and speed/load conditions.
  - They do not have the facilities and must create them.
  - Lack of theoretical analysis.
  - Lack of focus (what is the fundamental physical problem you are trying to solve/explain?)
  - Confusion between "fuels" research and "spark-assist" or combustion mode research.
  - Needs to be tied into industry a little better.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 9 of 13 reviewers)

- More collaboration with industry would focus this work more closely on the correct aspects of the application of spark assist that may be utilized in industry.
- Develop internal facilities to achieve capability to meet project objectives using in-house experiments.
- Expand the instrumentation capabilities of the engine to gain a fundamental understanding of what happens in mixed mode, and perhaps initiate a CFD study of a well-characterized, single point of operation.
- With VVA, compression ratio sweeps may be conducted (Miller cycle!). External boosting and boosting recommended. Include simulation to understand fundamentals of fuel properties.
- The results of this study are very dependent on how the engine experiments and combustion strategy are configured. Perhaps with a new platform at ORNL it will be possible to look at a broader range of combustion strategies.
- Work with the AEC MOU Working group to coordinate the project into the bigger scheme. Define the Work Plan more thoroughly.
- Explore A/F effects.
- Good idea to consider lean-burn as an alternative to EGR.
- Expand discussions with HCCI researchers in automotive companies

In-Cylinder Combustion Studies and Modeling

The Direct Injection Hydrogen Engine: A Worthy Choice for Transportation Power, Steve Ciatti of Argonne National Laboratory



Brief Summary of Project

This project, a joint operation between Argonne and Sandia, will be focusing on pre-ignition/knock and NOx reduction for hydrogen internal combustion engines. Combustion imaging will be used to identify locations of preignition, and multiple injections may be used to reduce or eliminate combustion problems.

Question 1: Relevance to overall DOE Objectives (Written responses from 13 of 14 reviewers)

A number of positive comments were offered regarding the relevance of this project. One noted that certainly the concept of a hydrogen fueled engine fits with the national goal to go to a hydrogen economy, while another noted that there is some promise for spark-ignition engines using hydrogen. The project is exploring a possible clean combustion concept, said another. A reviewer thought this project was a good addition to the review. Though this project is controversial, it is important for offering a potential practical alternative to fuel cells assuming the hydrogen economy surfaces in the future, in one reviewer's comments. Considering the finite availability of fossil fuels, research in the area of hydrogen combustion is obviously strategically important, noted another reviewer. This is a relatively new project, which makes it difficult to assess, but it appears to have some potential in this reviewer's opinion.

Some reviewers offered dissenting views. The project addresses one of DOE FCVT goals so it gets a "good" rating in one reviewer's book, but the work itself is not overly significant. One noted that he remained skeptical, based on earlier H_2 engine results, that this engine (in its final embodiment) has potential as a more cost-effective, power-dense and efficient concept. However, this reviewer believed that research in this area is important, and recognized that this is a significant component of DOE's research plans. Another said that while hydrogen ICEs have some potential advantages and the project addresses advanced engine development, this project is unlikely to lead to achieving one of the primary objectives of the DOE, displacing petroleum. Hydrogen production is highly energy intensive, noted another reviewer. Depending on how hydrogen is produced, this may help the U.S. become less dependent on energy imports. A reviewer asked to see a clear comparison of goals and objective for this vs. the work at SNL and any other lab cited as participating in this effort: the project appeared to this reviewer to have the potential for the duplication of effort. A reviewer said this project has not really started yet, so it should not be evaluated along the same lines as other projects. Similarly, this presentation did not describe a project to one reviewer: it did nothing more than present data from other sources, e.g., Ford and BMW, some unsubstantiated. The work being proposed belongs with Ford and BMW, continued this reviewer.

Question 2: Approach to performing the research and development (Written responses from 11 of 14 reviewers)

Reviews on the approach to this project were mixed. One reviewer noted that the approach is good in nature but it would be helpful to see more effort on engine system simulation. This was reflected in a reviewer who recommended a simulation effort to target performance goals, noting that there was no clear strategy mentioned and that only DOE goals were discussed as a target. One reviewer said that no significant project plans were presented. Another suggested that this engine has a reasonable chance of meeting objectives for efficiency (maybe) and emissions, but it is difficult to fully assess the approach from the limited information given. This viewpoint was reflected in the opinion of a reviewer who said that there was not much information in this talk: it contained mostly justification for the approach. There appeared to be only three slides with data from this program. There was little technical background. It is difficult to judge the approach with so little information, said several reviewers. A reviewer continued by saying it was hard to tell from the presentation just what the approach is going to be, but it looks like an experimental cut-and-try approach. This reviewer reflected other comments by noting that the project should have a modeling/analytical connection to get the most out of any test data. A reviewer suggested the use of chemiluminescence optical techniques to study multiple-injection H_2 DI: another noted that multiple injections may allow for an engine with low NOx emissions. Finally, a reviewer noted that this technology is more than 15 years away from going into production, and that a "technology monitoring" activity may be sufficient. Specific investigations may wait until HCCI combustion is well-understood with conventional fuels.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 10 of 14 reviewers)

Several reviewers noted that the project was just starting and was difficult to review for progress, although one reviewer thought much progress should be made during this fiscal year. One reviewer noted the project was just getting started, but the team should have a plan that shows what unique technical problems are going to be addressed and what specific methods will be used. Another reviewer said that it doesn't make sense to start with engine testing. A reviewer suggested it may be a technical accomplishment to get the hydrogen engine to run, but the issue of multiple injections is interesting. A reviewer commented that he is looking forward to seeing the initial results, but did not see much concern expressed over the reliability of the DI injectors. Is the proposed workaround strictly a focus on PFI? If so, then the scope of the testing may become much more limited. This reviewer also asked if the scope were limited in this fashion, then what would be the fallback test? More detailed literature survey and simulation prior to experiments may be sufficient in one reviewer's opinion. Another said that the project appears to rely heavily on the work performed by Wallner, et al. at the University of Graz in Austria. Progress there appears to have been very good. Now it's up to ANL (according to this reviewer) to reproduce this data and then move on. A final reviewer said that "this was an arrogant sales pitch for work. This was an inappropriate venue for such a pitch."

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 12 of 14 reviewers)

Partnerships with Ford and BMW were mentioned by several reviewers, with reviewers noting that these partnerships were inferred. The significant existing hydrogen ICE activities at Ford and BMW were acknowledged. One reviewer was unsure as to BMW's role, but noted the involvement of the University of Wisconsin-Madison Engine Research Center. Another reviewer acknowledged the cooperation with the University of Graz (although one reviewer did not see any universities mentioned). A reviewer inferred the collaboration with HyICE as well. One reviewer thought the collaborative efforts appear promising at the start. Another thought the team had a good plan for collaboration with industry partners. On the other hand, a reviewer said that by virtue of being a new project, the amount of collaboration is limited (but presumably this will pick up as the project progresses). In terms of the relatively few groups working in this area, a reviewer thought the level of collaboration is very good. This reviewer also suggested more academic collaboration, perhaps especially in modeling the heat transfer effects during the compression stroke. The final reviewer said that the direct benefactors would be Ford and BMW, and that this work belongs back inside the OEMs, and should not be funded by DOE money.

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

Several reviewers felt the future research plan was in need of revision. One simply noted that there are many issues that need to be resolved, while another said that the program creates additional barriers to be overcome. No targets other than DOE goals were mentioned, said another reviewer who also observed that no real strategy was mentioned other than Ford's or BMW's. One noted that the approach is good and appropriate, but this reviewer was not familiar enough with the program technical barriers with regard to hydrogen to assess whether the work plan fully addresses these. This reviewer believed that the main focus of this program's approach should be on achieving high energy efficiency and a fundamental understanding of the major factors involved, and from there, determine what tradeoffs need to be made to meet NOx standards. Another reviewer stated that it is not really clear what the proposed future research is. It seemed to another reviewer as if this project is proceeding without a firm test plan and is more exploratory in nature from an experimental viewpoint—it was not clear if system-level simulation was being performed a priori to the experimental effort. This was reflected in another's comments: "this is all future work but looks like a true plan is missing." This reviewer also asked "What are the deliverables and milestones other than getting an engine up and running and grabbing some images?" A reviewer observed that an engine will be operated in FY05, including in-cylinder visualization in UV and multiple injection strategy. Detailed testing at current knowledge is too early, in one reviewer's mind, however. Finally, one reviewer stated that "The talk was a sales talk, not much of a technical presentation. The last slides were still sales talk without a clear indication of the plan." This was echoed in another's comment that "This presentation was nothing more than a PR exercise."

Specific Strengths and Weaknesses (Written responses from 12 of 14 reviewers)

- Specific Strengths
  - Close coordination with Ford's program.
  - Popularity of H_2 and the lure of the H_2 economy.
  - This remains an important area to explore as a potential option for meeting 2010 emissions, particularly in light- and medium-duty applications.
  - Hydrogen direct injection for IC engines to build up hydrogen infrastructure understood and acknowledged.
  - Uses DOE fuel of choice in a practical ICE engine.
  - It is a different approach to a clean, efficient engine.
  - High potential.
  - Builds on a successful approach.
  - Contacts with injector suppliers established.
  - Exploring alternative methods for clean combustion systems.
  - Experimental capability is a key to completing this work—PI has nice facility that is under development and will be operational in a few months.
- Specific Weaknesses
  - No clear plan for the Argonne work.
  - Impracticality of widespread H_2 use, energy efficiency penalties of H_2 generation and low probability of displacing petroleum.
  - The focus on improving the pre-ignition characteristics does not indicate a coherent plan for addressing the main issues in that area, particularly the heat transfer.
  - Depending on future emission regulations, fuel cell development may overpass this approach.
  - What was outlined is not research, it is development.
  - It is not clear that the pre-ignition problem can be solved.
  - It is too early to tell, but right now I would say the lack of a plan is a weakness.
  - Projected benefits are speculative at this point.
  - No strategy presented.
  - No simulation effort suggested.
  - The detailed injection simulation mentioned is good, but a hydrogen engine requires a unique air system, etc.
  - No discussion on how they will address the injector issues that were mentioned in the presentation. No discussion of the infrastructure on how to obtain the hydrogen for these engines. High NOx levels with current engines.

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

- This needs to be re-reviewed to identify exactly what the Argonne contribution to this project would be.
- Include in the comparison against other engine strategies the option of "hythane" or hydrogen-enriched natural gas, which can also provide very low emissions, particularly for DI HCNG.
- Detailed literature survey from past experience recommended. Use simulation to show potential of technology requested. Plan for introduction of this technology including production strategy for hydrogen has yet to be demonstrated. On-board hydrogen production should be included into this study.
- It is hard to give recommendations on the basis of what has been shown.
- Don't fund this project.
- First adopt some targets/priorities.
- Run a full engine hydrogen cycle simulation and compare strategies to hit targets.
- Validate simulation strategies on the engine.
- Considering more modeling effort.

- High risk effort that seems to have limited path to commercialization since the hydrogen infrastructure does not exist.
- Consider more engine system simulation work to explore potential experimental test matrices that will address ignition issues and NOx formation propensity.

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 2005 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

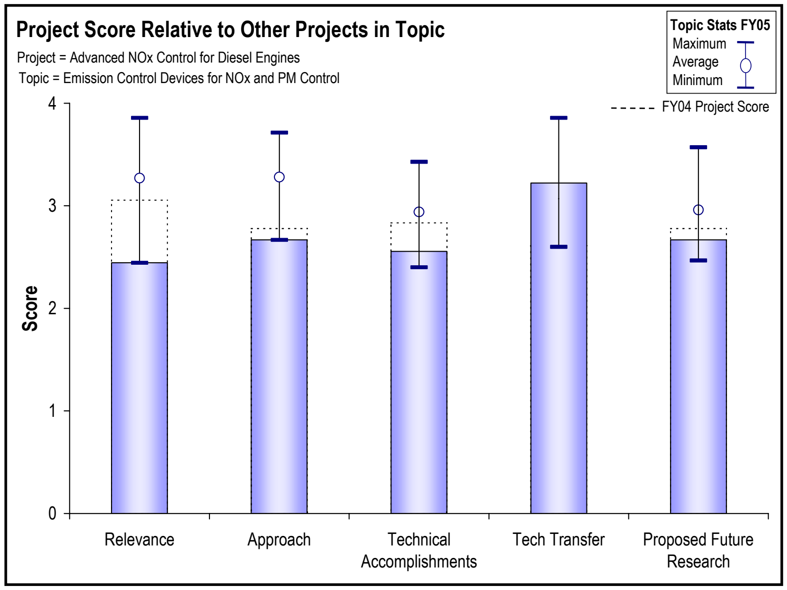
Page Number for Project Summary	Research Project Title	Q1 Relevance Score	Q2 Approach Score	Q3 Technical Accomplish-ments Score	Q4 Tech Transfer Score	Q5 Future Research Score
62	*Advanced NOx Control for Diesel Engines:* Darryl Herling, Pacific Northwest National Laboratory	2.44	2.67	2.56	3.22	2.67
65	*Characterizing NOx Adsorber Regeneration and Desulfation:* Shean Huff, Oak Ridge National Laboratory	3.40	3.67	3.27	3.07	3.13
68	*CLEERS Activities and Progress:* Stuart Daw, Oak Ridge National Laboratory	3.86	3.71	3.43	3.86	3.57
70	*Development of an Advanced Automotive NOx Sensor:* Larry Pederson, Pacific Northwest National Laboratory	3.39	3.39	2.77	3.08	2.77
72	*Diesel Soot Filter Characterization and Modeling:* Mark Stewart, Pacific Northwest National Laboratory	3.43	3.57	3.07	2.93	3.21
76	*Fundamental Studies of NOx Adsorber Materials:* Chuck Peden, Pacific Northwest National Laboratory	3.40	3.30	3.10	2.90	2.70
79	*Fundamental Study of Lean NOx Trap Deactivation:* Todd Toops, Oak Ridge National Laboratory	3.40	2.90	2.70	3.20	3.00
82	*Hydrocarbon Based DeNOx Catalysis using Diesel Fuels:* Chris Marshall, Argonne National Laboratory	2.60	2.67	2.40	2.60	2.47
87	*Intra-channel Evolution of Carbon Monoxide and Its Implication on Regeneration of Lean NOx Traps:* Jae Soon Choi, Oak Ridge National Laboratory	3.50	3.70	3.10	3.20	3.30
89	*Mechanisms of Sulfur Poisoning of NOx Adsorber Materials:* Chuck Peden, Pacific Northwest National Laboratory	3.56	3.22	3.22	3.22	3.11
	Average Score for This Category	**3.27**	**3.28**	**2.94**	**3.07**	**2.96**

Overall Program Scores

	Q1 Relevance Score	Q2 Approach Score	Q3 Technical Accomplishments Score	Q4 Tech Transfer Score	Q5 Future Research Score
Overall Program Average	3.36	3.34	3.14	3.14	3.13
Overall Program Maximum	3.88	3.77	3.82	3.86	3.65
Overall Program Minimum	2.07	2.64	2.07	1.14	2.14

Emission Control Devices for NOx and PM Control

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



Brief Summary of Project

This project, in conjunction with General Electric Global Research, seeks to develop NOx control options for off-highway (locomotive) diesel engines. The system being examined uses hydrocarbon oxygenates over lean NOx catalysts to achieve low NOx emissions at very high flow rates.

Question 1: Relevance to overall DOE Objectives (Written responses from 7 of 9 reviewers)

Reviewers were generally positive regarding the relevance of this project. One noted that the project is working on both emissions reduction and fuel savings by changing engine operation. Another said the team has chosen a potentially important research area for future engines. Another commented that the project has good relevance, is highly needed, and is appropriate for DOE funding. This project is reasonably directed toward solving a significant emissions problem, said a final reviewer. The primary drawback is that the approach is high risk; however, the payoff is also high. Consequently this reviewer agrees that government funding for a high risk project such as this is appropriate. A final reviewer said that this technology is limited to engine applications needing NOx conversion at high temperatures.

Others had questions about the relevance of the research within the DOE programs. One said that while this is a worthwhile project for off-highway and railway locomotives, it is debatable whether it should come under the umbrella of FreedomCAR and Vehicle Technologies. This work belongs neither to the FreedomCAR nor to the 21st Century Truck Partnerships. Another questioned the relevance of research sponsored by DOE on locomotives, since their fuel consumption is only a little over 1% of total U.S. oil consumption. Research funding might better be spent in areas (this reviewer continued) that constitute a significantly larger opportunity for reducing total US oil consumption.

Question 2: Approach to performing the research and development (Written responses from 7 of 9 reviewers)

Several reviewers felt the approach was appropriate. One noted that the approach is reasonable and unlike many other projects, is tightly integrated with industry requirements: the team made a good response to last year's ACE review. The idea of an onboard reformer, particularly for a locomotive where weight and space are not so much of an issue, has merit in one reviewer's opinion. Another thought the approach to reform, then synthesize the optimum reductant was interesting. Another mentioned the use of "High Throughput Technology." A reviewer commented that, given the constraints of a locomotive powerplant, this approach is possible. This reviewer suspected that the technology advances necessary to implement this technology will be far greater than the difficulty of adding a urea tank to the locomotive powerplant in this reviewer's limited experience. It seemed to one reviewer that the system will be fairly complex. The final reviewer questioned the viability of on board reformation as an effective aftertreatment system: this reviewer was not sufficiently familiar with the rail industry to be able to comment about viability of storing two hydrocarbons on board the locomotive: one as a fuel and one as an emissions control enabler.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 7 of 9 reviewers)

A number of positive comments were made regarding technical progress, including that the team is showing some promising results and that the team has done a good job making DME and determining its reduction potential. A reviewer said that solid progress is being made to accomplish the goals, but a bit more evidence that the researchers have selected the correct oxygenated species to "tune" the reformer for would be good. Is DME the correct choice? The inconsistent conversions using DME raise some questions as to the selection of that oxygenate as the correct reductant. Another reviewer said that the team has made good progress but appears to need some assistance on POx and lean NOx reduction chemistry. No improvement has been to the baseline alumina lean NOx catalyst, said another reviewer who also noted the limited HC-SCR data. To one reviewer, it was unclear what "key DOE program technical barrier" this research was addressing. A final reviewer noted that the team is almost two-thirds through the project, and it appears that there are multiple paths still being pursued. Some tough decisions on what technology to pursue need to be taken in this reviewer's opinion.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 6 of 9 reviewers)

Several reviewers noted the strong and good collaboration with General Electric, with one noting that the close coordination on this project with GE is the best way to get implementation of a high-risk technology. This reviewer thought the team is doing a great job with the collaboration. Another thought the team has a reasonable teaming arrangement. A reviewer thought there appeared to be an effective collaboration between the national laboratory and industry. Another suggested that collaborations with industry needed to be developed. The final reviewer acknowledged the limited field of collaboration, but this reviewer thought having other catalyst suppliers involved would probably help.

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

Reviewers had several suggestions for the future research. One suggested the team age the prime lean NOx catalysts ASAP and test under realistic engine conditions (high space velocity). With only 16 months to go, there are still too many avenues being investigated, in one reviewer's view, and more focus is required. Another was unclear what "key DOE program technical barrier" this research is addressing. Starting to use the combinatorial materials developed from the GE combinatorial project is a must at this point, offered a reviewer. More evidence that DME is the correct choice would be helpful. Certainly methanol has a known track record as a good reductant, noted this reviewer. The final reviewer said the plan was reasonable and the project appears near completion in the next year or two.

Specific Strengths and Weaknesses (Written responses from 8 of 9 reviewers)

- Specific Strengths
  - Good coordination with the industrial partner. A reasonable approach.
  - Good teamwork.
  - They are investigating a different approach to NOx aftertreatment.
  - Project has conducted good research and made progress toward identifying several alternatives which may prove viable in addressing the problem at hand, but question the relative value of R&D into such a small part of the U.S.'s energy consumption challenges.
  - Capability of using of High Throughput Technology but limited results for now.
  - Good coordination of research with industry users that should result in useful, near-term product.
- Specific Weaknesses
  - It does sound as if GE has put almost unrealistic demands on the technology. However, since they are directly involved in the technology development, I am assuming that realistic demands will be quickly tempered by data from the team working on the project.
  - Too much of a "shotgun" approach.
  - Scheme proposed is very naive and has too low a probability of success to warrant pursuit.
  - R&D is technically intriguing but has little applicability outside the locomotive and possibly stationary gen set industries. As these constitute an insignificant portion of the energy consumption in the US, DOE R&D ought to be redirected to areas where there are more significant opportunities to reduce oil consumption.
  - Durability. Durability. Durability. Sulfur attack on alumina and hydrothermal durability of the lean NOx catalyst!!! No improvement to the baseline alumina the lean NOx catalyst. Limited HC-SCR data.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 6 of 9 reviewers)

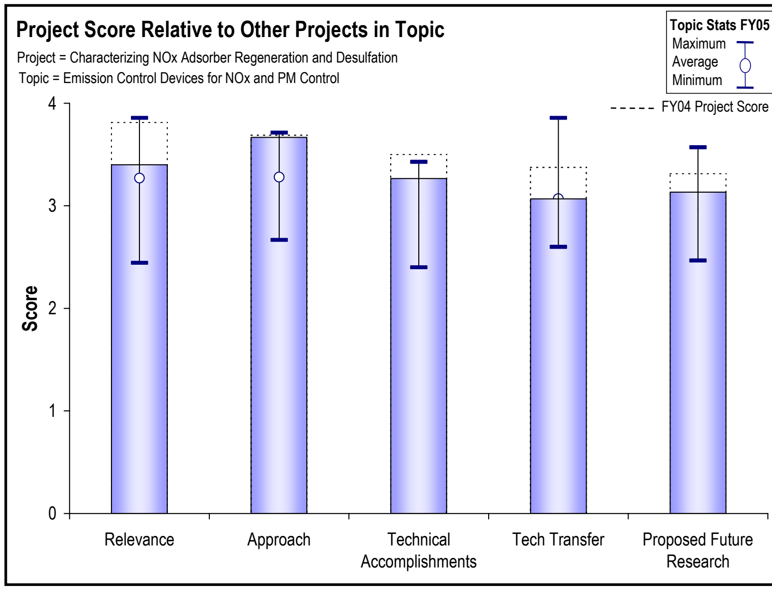
- Get some measurements on a good candidate catalyst with the syngases as soon as possible.

- It would be nice to see more evaluation of various catalyst/reductant systems rather than the standard Ag/Al_2O_3.
- Either "pick a horse and ride it," or be prepared to extend the project.
- Discontinue project.
- Aside from questions about the focus of the research, PNNL has good test facilities that allow high-throughput evaluation of many catalysts. If possible, redirect R&D to light- or heavy-duty road transportation vehicle R&D.
- More work on formulation development and testing of lean NOx catalysts.

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

Brief Summary of Project

This project team is working to characterize several aspects of diesel engine operation, including NOx adsorber performance and degradation and engine-out emissions. The idea is to develop a stronger link between bench and full-scale system evaluations.



Question 1: Relevance to overall DOE Objectives (Written responses from 9 of 15 reviewers)

One reviewer commented that this project represents a valuable topic to industry and the author provided good insights to application of LNT calibrations. Another reviewer noted that the project supports the DOE and national needs to achieve substantially lower NOx emissions and noted that this work is probably "too risky" for industry, so it complements industry activity. One person commented that meeting future emissions standards is critical for future engine technologies to be viable in many markets in the U.S. These technologies support achieving the DOE goals of improved fuel efficiency, resulting in reduced demand for imported oil. A better understanding of NOx adsorber operation is a key enabling technology for HCCI and diesel ICEs. One person felt that this is an excellent study that can have immediate impact on the efforts of the OEMs to implement the engine strategies that will allow the successful use of LNT devices. One of the reviewer commented that NOx adsorbers offer chance to meet 2010 emissions without a secondary fluid like urea, and this project seeks to overcome several of the key technology barriers. Another agreed that NOx absorbers are a possible technology for future engines, while another added that improved NOx regeneration and DeSOx strategies help to improve fuel economy. The final reviewer stated that LTC looks like a good approach to increase fuel economy, but will it have the NOx reduction, but asked whether it will break even with the other methods in the end.

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

Several reviewer commented that the researchers have used a good overall approach and use of analytical tools with a good understanding of NOx reduction versus fuel economy trade-offs. Another person agreed that the approach is fine, the team approach is excellent, and improvements can come through the advice and guidance of industry partners. One person added that the researchers are addressing important issues. Another person noted that the work includes probing reductant chemistry, desulfation of adsorber, combining bench and engine tests. Another reviewer added that the detailed HC composition, even if not shown in the presentation, is highly appreciated. One reviewer felt that the technical approach is solid, but results yield no significant new information. The catalyst formulations evaluated are not the latest technologies. The final reviewer commented that the presenter needs to do a better job of outlining and justifying overall approach rather than quickly jumping to details.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 11 of 15 reviewers)

One reviewer commented that this work shows great strides from year to year in answering relevant questions. Another felt that the researchers are making good progress on improving understanding of lean NOx trap regeneration, but another noted that the reasons for LNT deactivation still needs to be understood. One reviewer acknowledged that some good findings regarding LTC, but much more work to be done. Another reviewer agreed that the detailed analysis of the LTC technique for NOx regeneration was well conducted; however, LTC is very sensitive to production tolerances, tolerances in ambient conditions, as well as EGR distribution. One reviewer acknowledged the researchers had developed a good method for eliminating ammonia. Another felt that the one key accomplishment/approach is where the researchers changed engine strategies to evaluate feed gas. One person noted that the researchers found that multiple injection strategy suppressed NH_3 formation without N_2 formation penalty, as well as examining NOx adsorber regeneration during LTC operation, by combination of EGR and injection control. They also noted that this technique resulted in a PM spike during lean-LTC to rich-LTC transition, and that the researchers found better fuel-specific NOx reduction with LTC. One person's impression is that this project is effective in generating useful answers, but realistically, this work is very personnel- and dollar-intensive. They acknowledged that the team has done well in focusing on the suggestions put forward by the 2004 ACE reviewers' comments. Another person commented that the presenter showed good specific results but need to do a better job of inferring generalized conclusions. The conclusion that an NCO mechanism is implied by results seems shaky; need to focus on more detailed analysis of exhaust speciation (e.g. NCO and O_2). The final reviewer noted that numerous papers and presentations document the work in this area.

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

Reactions to this question were varied. One reviewer felt that the collaborations have been multiple and substantial. Another acknowledged the cooperation with Sandia. One reviewer felt that the group is well connected through the CLEERS effort. Others agreed that through CLEERS, the team has connections to industry and partners and that CLEERS is a good model for National Lab/industry collaboration. Others were more cautious about the CLEERS involvement. One person commented that using CLEERS to provide direction and guidance is good; however, the project team needs to get more aftertreatment suppliers involved. They acknowledged that this is hard work but that it is mandatory. Another person stated that the PI mentions presentations to and collaboration with CLEERS and Diesel Cross Cut Team, but it is unclear from the presentation how much collaboration goes on. One reviewer commented that the technical data is valuable to engine and catalyst firms; continue to make efforts to share as much as possible. One reviewer stated that they would like to see a much closer interaction with the OEMs or the heavy-duty engine manufacturers. Another expanded this desire to include interactions with the major OEM car manufacturers. Others just suggested the group needs to do a better job of collaborating with industrial partners.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 7 of 15 reviewers)

One reviewer felt that the layout of future work seems very effective and promising. Another reviewer agreed with this, assuming that research can move into new areas that are not already being investigated by industry; this reviewer also recommended expanding catalyst work beyond model catalysts. One reviewer noted the future plans include considering the temperature dependence further, examining new catalysts, and continuing desulfation studies; however, they felt it was unclear where the most critical hurdle lies between current status and practical/robust operation. One reviewer cautioned that the researchers need to know what they are testing, i.e. what materials are in the catalyst. Another person stated that the researchers need to do a better job of demonstrating/explaining a cohesive and comprehensive research plan. One of the reviewers commented that the talk did not specify the future plans; however the PI has a good track record of picking the right issues on which to focus study. Another agreed with this, adding that the "Future Plans" are not specific enough. The terms "Investigate Potential" and "Improve Understanding" used by the presenter are too vague and have no real meaning in this context. The team needs to be more focused, and set out a plan to answer specific questions.

Specific Strengths and Weaknesses (Written responses from 13 of 15 reviewers)

- Specific Strengths
  - Very excellent engine application work and very powerful use of unique ORNL instruments.
  - Broad capabilities being brought to bear on NOx adsorber use and regeneration. Tremendous control capabilities to probe operating regimes and their impact on the adsorber.
  - SpaciMS in collaboration with the engine.
  - Modern diesel engine and close cooperation with Sandia helps develop a system integration.
  - Team effort, outstanding experimental capabilities. Willingness to take advice and focus research effort on industry-driven needs.
  - ORNL has the equipment and the expertise for this work. The connection to CLEERS is important.
  - Speciation data.
  - They are making good progress in improving understanding of lean NOx traps.

- Good focused work. Measurement capability of gas compositions.
- Good experimental capabilities demonstrated along with some provocative results.
- Systems viewpoint which is very good.

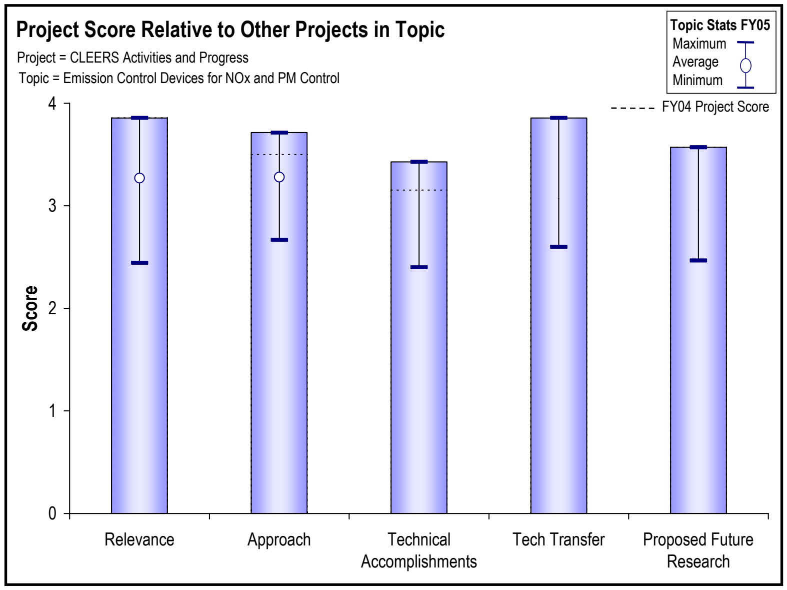
- Specific Weaknesses
  - Better characteristation of the catalysts in use in the studies. They are not black boxes and they are not all kinetically similar devices.
  - To some extent, the project seems to focus so much on engineering strategies that opportunities to learn more on fundamental combustion chemistry and catalyst chemistry are getting lost.
  - Focus on HSDI engine may limit the applicability to heavy-duty industry (high load operation missing).
  - None that can be attributed to the researchers. The scope of this work is so broad that it is a real challenge to do more than look at a few key problems at a time.
  - Trying to cover regeneration AND desulfation may be too much for this one project.
  - Recommend that PI not try to cover so much information in the presentation. Presentation was 38 slides and PI needed to rush too much and skip over too much in order to fit a 20 minute time frame. He should identify one or two areas of prime research results and cover those in more depth rather than trying to cover four different aspects of the research.
  - What is happening to the catalyst on a fundamental basis by characterizing the sulfur poisoning and thermal durability?
  - Appears to be weak in terms of collaboration and in terms of developing a clear research strategy with specific goals.
  - Not using advanced technologies in a timely manner. Toyota DPNR should have been analyzed a long time ago.

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

- Spend more time relating the properties of the LNT to the engine regeneration strategies. Specifically, I believe that the ceria content in these catalysts are going to have a major impact on your regeneration
- In terms of objectives, it may help to consider and clarify whether getting to a "system" design is the main goal, or to understand the fundamental interactions between the combustion process and the chemistry in the adsorber. The latter topic may be better served by narrowing consideration of materials and strategies, rather than expanding to more catalysts and operating conditions.
- Your title mentions rapid desulfation, but I didn't see any times in your presentation for desulfation.
- Less focus on LTC approaches recommended.
- Keep doing this work!
- Look carefully as to whether the regen and desulfation work aspects should be split.
- Work with the CLEERS group to define specific questions to be answered by the research. Then set out the necessary Work Plan.
- Need further studies to determine conditions needed for more complete desulfation by post injection. Special attention needed for sulfur balances.
- Need closer work with industry to understand the current state of the art in the technology and to try to obtain most current technology & formulation to evaluate.
- Work on the sulfur balance and recording H_2S, SO_2, and COS as the function DeSOx time. Please report the details of the DeSOx event you use.
- If you do study model catalysts, please try to incorporate your analytical facilities to understand/characterize on a funadametal basis the sulfur and thermal durability.
- If 90% NOx conversion is required over the FTP75, can you really avoid releasing NH_3 over an aged catalyst and at all the different exhaust temperatures?
- Please report more information on how the LNTs are aged and evaluated for NOx conversion such as lambda, exhaust composition, SV, temperature range, and DeNOx frequency (such as grams NO2/liter catalyst).
- Please comment how and if you it is possible to achieve Tier II Bin 5 requirements after 120k miles on light-duty vehicles (both on the from the catalyst and engine point of view).

Emission Control Devices for NOx and PM Control

CLEERS Activities and Progress, Stuart Daw of Oak Ridge National Laboratory



Brief Summary of Project

The overall objective of CLEERS is to maximize energy efficiency and acceptability of lean-burn engines through development of chemistry information for emission control materials, development of analytical tools for device performance modeling, and use of tools to identify sources of energy inefficiency and potential solutions to emissions control technology bottlenecks.

Question 1: Relevance to overall DOE Objectives (Written responses from 5 of 7 reviewers)

One reviewer felt that the project was a great concept and is highly important to DOE in terms of research goals as well as the coordination of research. Another added that lean exhaust aftertreatment is a major issue for future clean, efficient engines. Two reviewers stated that this is a very well-coordinated program on a real-time basis through ORNL. The last comment was that CLEERS is necessary to extend the pre-competitive knowledge to make aftertreatment control possible.

Question 2: Approach to performing the research and development (Written responses from 3 of 7 reviewers)

One reviewer stated that the researchers have taken a good methodical approach. Another noted the excellent experimental and modeling methodology. The last reviewer commented that the approach appears good, but need to avoid too much focus on existing technologies (LNT, SCR, DPF) that might inhibit emergence of novel technologies.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 4 of 7 reviewers)

One reviewer noted the good progress, while another stated that it was great to see movement to commercial samples. Another reviewer commented that the researchers are significantly improving the understanding of lean NOx absorbers. The last person commented that the workshop and partner participation growth and success indicates good progress towards goals. Good evidence of progress evident from other presentations at this review as well as this presentation.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 5 of 7 reviewers)

Several reviewers noted the excellent collaboration and coordination within DOE as well as industry and academia and noted the good dissemination of information on web and workshop. One reviewer noted that the project is concentrating on collaboration and coordination, and there is a great deal of interest in their activities. The last reviewer summed the project up by saying that this project is a model for other collaborative efforts involving the Labs, industry and universities.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 2 of 7 reviewers)

One reviewer felt that the team had an excellent long-term plan, but added that they really need to develop standards in these systems (i.e., round robins, etc.) and need to develop common procedures. Another reviewer commented that the researchers have a reasonable plan for next year, but felt that they need to specifically pursue improvement of understanding of NH_3 and N_20 chemistry.

Specific Strengths and Weaknesses (Written responses from 7 of 7 reviewers)

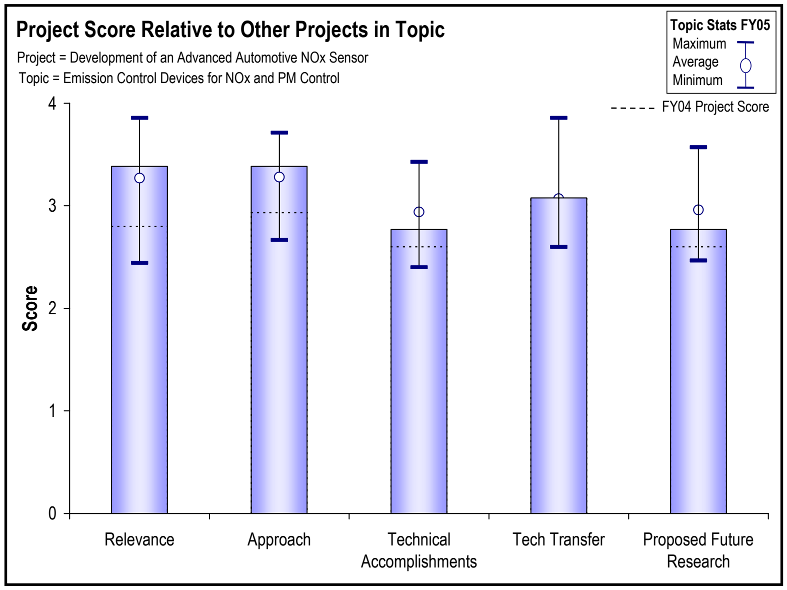
- Specific Strengths
  - Large group working together with somewhat realistic catalyst from supplier.
  - Broad collaborative nature and excellent integration of experiments and computation.
  - Seems to have all the "players" involved.
  - Main contribution is as serving as focal point for industry dialogue.
  - The cooperative nature of the research seems to be providing substantial benefits.
  - Good clearinghouse and control center for the DOE lean exhaust emission treatment research programs.
  - Good source of coordinated data for model building.
  - Coordination among various laboratories in the US and outside the U.S. Great that information on real world catalyst is now becoming available. Excellent that we are now being able to relate observations back to the microstructure.
- Specific Weaknesses
  - Need to drive to a conclusion for the various systems available. It is not clear what is positively known and what is left that is needed to apply these catalyst systems.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 5 of 7 reviewers)

- Is there a plan to perform TEM on the catalyst to determine aging effects on dispersion?
- Continue!
- Could reduce effort and get most of benefit.
- They need to conduct more work on sulfur poisoning and desulfation, since this is a major issue with LNT.
- How can we prioritize the information better to help engine designers? What is critical and what are the operating regimes where these systems work?

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

This project, in its final year, sought to develop a robust NOx sensor for monitoring of combustion processes and emission control effectiveness. The work in the final year focused on evaluating the cross-sensitivity of the sensor to other exhaust gases and on exploring alternative electrode compositions as a means to enhance sensitivity and selectivity at lower cost.

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

The reviewers generally agreed that NOx sensors will probably be very important to monitoring and control of future low NOx engines. One reviewer stated that the goal of this project was to develop a U.S. produced NOx sensor. He added that unfortunately it is not clear if Delphi will actually produce this sensor. One person mentioned that the need for a NOx sensor is very high for feedback control of NOx control systems, whether urea-SCR, lean NOx or LNT. He added that this is an enabling technology for low emissions advanced combustion engines. Another reviewer felt that a NOx sensor is needed. Someone said that OBD requirements force a need to have NO sensors available. This person went on to say that operating the engine at the emission limit helps reduce fuel consumption in avoiding or minimizing production safety margins. One reviewer mentioned that a good NOx sensor was defined as a "need" at the meeting at Berkeley back in the late 1990's. It was acknowledged that NOx sensing is critical to accurate emission control systems feedback loops to ensure that emissions regulations are met. Also, the development of an inexpensive, accurate and durable NOx sensor is important to advanced combustion engine systems. One person felt that it is rather questionable whether this will be an enabling technology in developing clean and efficient ICEs. According to him, there was no indication whatsoever in the presentation given.

Question 2: Approach to performing the research and development (Written responses from 6 of 13 reviewers)

Reviewers agreed that this project had a very sound technical approach to performing the research and development. One reviewer thought that this was a reasonable approach to develop a NOx sensor. Another pointed out that this project involved building an amperometric sensor for NOx that is robust, sensitive and accurate. He also acknowledged the collaboration with Delphi to develop performance criteria for the components of the NOx sensor. Another stated that the reaction cell was designed in a very interesting way. A comment was made that cross-sensitivity is a key investigation for emission sensors. It was added that this is only part of the whole development and that it is assumed Delphi conducts most of the missing development efforts. Good laboratory support from the industrial partner was praised by one reviewer. Someone thought that this was a good technical approach for development of a cost effective and durable NOx sensor that is critical for the automotive industry.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 7 of 13 reviewers)

All of the reviewers agreed on the significant accomplishments and pointed out some commercialization issues. One reviewer thought that the materials developed in this program are not sufficient to produce a marketable NOx sensor. Another reviewer stated that PNNL researchers have done what Delphi asked of them. He added that technically, this sensor is not "perfect" but is "pretty good." He also said that it appears that Delphi is planning to offer this sensor to the OEMs; hence, one can characterize the work as a success. Another person said that the NOx sensor is a key enabling technology for future ICE systems. The reviewer noted some inconsistencies in the presentation materials, but did not dwell on them since the project is ending. One reviewer said that this was good work. He added that now the usual cost and durability questions need to be addressed. A reviewer mentioned that the researchers have assessed cross-sensitivity and examined alternate electrode materials but ammonia is seen to bias the results if present with oxygen. He suggested determining which materials appear best for some stages of the sensor. Two reviewers commented about how the ammonia cross sensitivity can not be solved and remains a key challenge if the sensor is used for NOx reduction aftertreatment devices.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 6 of 13 reviewers)

The comments regarding industrial collaboration were very positive. All of the reviewers for this project acknowledged the close collaboration with Delphi during the project. A comment was made that if there is a chance for commercialization, this project could have made that happen. Another comment was that it is encouraging to hear that Delphi is considering this technology for production.

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

Reviewers acknowledged that the work is complete and that the project will be finished soon. A comment was made that there does not appear to be a continuation plan. One reviewer added that Delphi will take over results and put the sensor into production. Another comment was made that there seem to be no plans to improve the NOx sensor. One person suggested that more work on NOx sensors could be beneficial because there are still some questions and issues with the research results that need to be answered. He added that it is not clear if continued research into this area is warranted through the auspices of DOE or if industry ought to move the technology onward. He recommended that DOE consider additional funding for this research in the future.

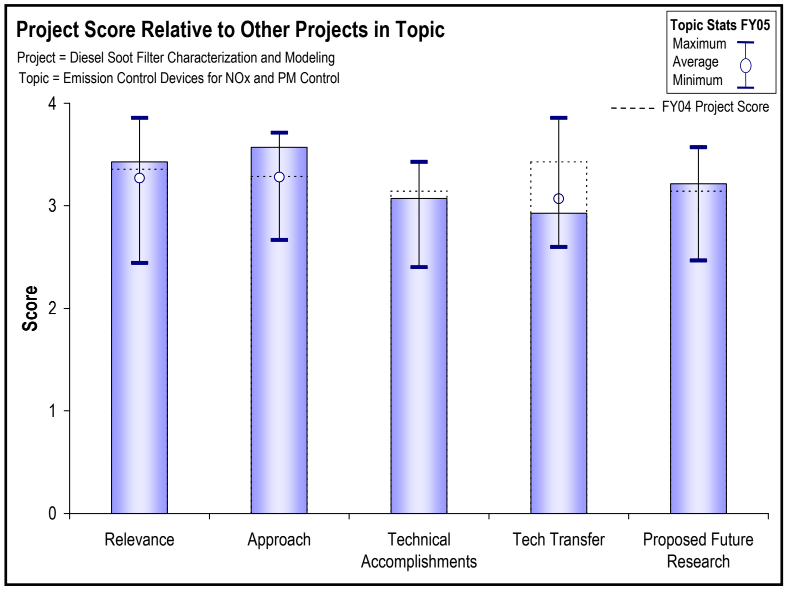
Specific Strengths and Weaknesses (Written responses from 8 of 13 reviewers)

- Specific Strengths
  - Close developmental collaboration with Delphi.
  - Close collaboration with Delphi, benefits to NOx control system operation in the field.
  - Electrochemistry capabilities.
  - Close to product development and high volume production: a "success story."
  - NOx sensing is a key technical enabler for advanced combustion emissions systems.
  - The outcome of the project is an effective tool in emissions control.
  - The objectives for the project are great.
- Specific Weaknesses
  - A lot more work needs to be done to develop a reliable sensor.
  - It does not seem to work (too large of an uncertainty).
  - Due to being so close to product development, fundamental work is missing.
  - It is unclear whether this project made progress toward development of a practical NOx sensor by Delphi.
  - High risk for commercialization.

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

- Let the project terminate as planned.
- Apply sensor to real engine-out emissions (if not already performed by Delphi).
- Project is over.
- None, research is being wrapped up. However, it appears more work on NOx sensors could be beneficial because there are still some questions and issues with the research results that need to be answered. It is not clear if continued research into this area is warranted through the auspices of DOE or if industry ought to move the technology onward. I would recommend DOE consider additional funding in the future.
- With this project coming to an end, the review seams to be a moot point, but given the technical problems encountered, it does not look like it will ever be incorporated into commercial product.

Diesel Soot Filter Characterization and Modeling, Mark Stewart of Pacific Northwest National Laboratory



Brief Summary of Project

This project team is looking at the modeling of soot deposition in diesel particulate filters as part of the CLEERS activities. This modeling has been combined with experimental procedures with single channel soot loading and regeneration as well as micro-scale interrogation of soot deposits.

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

Reviewers felt strongly that this project is very relevant to the overall DOE objectives. One reviewer noted that this basic information about the soot filtration is important to developing models for the device regeneration. He added that detailed control of regeneration is a major issue for automotive application of the DPF. According to him, the information provided by this work is important for that task. According to one reviewer, enhancing the understanding of DPF loading and regeneration characteristics is beneficial, both for emissions control as well as overall fuel consumption, and is relevant to overall DOE objectives. Another reviewer stated that PM filters are essential to meet upcoming PM emissions regulations and their understanding and improvement are critical tasks to overcome challenges of implementation. It was also mentioned that DPFs will become the standard aftertreatment system, but little is still known about soot and ash layer build-up and modeling. Someone pointed out that this project fits the CLEERS DPF Sub-Team's # 1 priority. One person mentioned that this is very relevant work and models are needed for PM filter soot layer build-up. Another called this research a solid building block supporting ICE goals. This was echoed in the comment that this is highly important work for allowing efficient diesel engines with minimal particulate emissions. In addition, this work ties in well with the health effects of soot as well as the engine industry's need to comply with 2007/2010 regulations. Someone thought that the presenter needs to state why this information is critical, because it was not clear that the pressure drop across the filter relates to engine efficiency.

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

Most of the reviewers praised the approach to R&D in this project. A question was raised if the model can be validated. One person stated that the approach with detailed physical modeling seems to be more profound than Konstandopoulos rough approach. He added that this technique allows an understanding of the phenomena at the end of the project. Another commented that this is a very systematic approach with an excellent methodology. This was echoed by a comment that the work seems to be well planned. Someone particularly appreciated the challenge of getting the experimental data for the model validation and called it "nice work." One reviewer pointed out the use of the latest methods to improve the understanding. He added that there is a lot of dialogue and industry interest considering 2007 and 2010 pressures. He also liked the approach despite a broad team. Someone thought that the fundamental approach is very refreshing. It was pointed out that the DOE patience is justified in this approach and it will bear good fruit over time while offering better long-term potential than more empirical methods. He also said that it is good to see supporting experimental work accompanying modeling. One person summarized the approach as very novel and creative for evaluating a difficult problem that of pressure drop in a particulate filter and the oxidation of the soot. A reviewer said the team had a reasonable approach, but they should increase emphasis on experimental validation. This reviewer was not sure how that can be effectively accomplished at the micro-scale level, but it perhaps can be attempted at the 1D system level with respect to global metrics such as pressure drop and soot mass balance.

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

A question was raised if deep bed filtration is the highest priority information that is needed at this point. One reviewer stated that evidence seems to suggest that the deep bed filtration does not impact the pressure drop or the regeneration kinetics. Another pointed out that linking modeling and experimental studies of cake formation and particle deposition in the filter. Someone commented that this project is adding to knowledge of diesel particulate filters and that a lot of good progress has been shown. Nice progression of results was also mentioned in one of the comments. One reviewer thought that very good progress has been made to date, including modeling and experimental characterization of soot accumulation. A suggestion was made to considered elementary filter pores to better understand pore structure-pressure drop response. Someone thought that good progress was made on the models, but expressed concern about the validity of the model. It was added that more detailed studies and comparisons with experiments would be beneficial. A comment was made that by comparing the Accomplishments/Progress to the “Feedback from 2004 ACE Review” slide, the progress has not been as great as one would have expected. One person felt there was good progress in understanding soot deposition and modeling, but the presenter needs to link more strongly to DOE’s goals by clearly stating how it relates to diesel engine efficiency. The team has made reasonable progress on micro-scale DPF modeling, said a reviewer, who continued by suggesting the project needs increased emphasis on experimental validation against global DPF system metrics.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 12 of 14 reviewers)

The reviewers thought that collaboration was good in general but involvement of a DPF manufacturer would be beneficial. One comment was that this research is very active, probably the DOE benchmark for technology transfer and industry collaboration. One person stated that this work is regularly reported to industry; however, it would be beneficial if it was continued by modelers within the industry to ensure that the properties studied in this project are clearly focused on the properties that are impacting DPF regeneration studies. A reviewer said that there is good collaboration with the labs and CLEERS, but there is no filter manufacturer on the CLEERS team. He added that the engine manufacturers are not going to modify a filter pore shape/size. According to him, the Dow CRADA is good, but Dow material is not used by any engine manufacturer yet. Someone commented that the current focus on one specific material helps to understand the basics but further investigations in particular into SiC material are urgently required. One person felt that the presentation did not list specific collaborations. Furthermore he said that it appears there was a strong interest in this work among attendees. A comment was made that work with suppliers (outside of the CLEERS meetings) is required and that Corning offered to help. That comment was echoed by a statement that there is insufficient participation from the manufacturers of DPF. Another reviewer stated that the project seems to have fairly good collaboration through the CLEERS working group. Another comment was that the researches need to interact more with aftertreatment manufacturers. Someone said that there is a good collaboration identified within DOE, but a better job of pointing out collaboration with industry and academia needs to be done. One reviewer mentioned that information is disseminated very well through publishing.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 10 of 14 reviewers)

Reviewers generally agreed that the future research plan was appropriate. According to one reviewer this research is an outstanding, natural progression toward other materials. He also mentioned that there is a nice balance between fundamental studies and items of curiosity. In general, the proposed future work is consistent with overall program objectives, said a reviewer. Perhaps, at some point, the focus of the modeling effort as well as the CLEERS working group should transition to be more applications-related. Another stated that the research plan was reasonably well explained and justified. He also said that better coordination with industrial DPF manufacturers and users is needed. Someone thought that this work is very helpful; however, he would like to see more industrial collaboration and would hope that the work could be efficiently focused on the issues that strongly impact regeneration. One person thought that good effort is being made to consider how this work can be applied to program’s technical barriers. Suggestions by the reviewers included enhancing the discrete particle model, continuing modeling soot layer structure effects, considering other substrate materials and observing regeneration events experimentally. One person pointed out that understanding the (local) soot loading of a DPF helps to improve ECU strategies for regeneration strategies, thus improving fuel economy. A comment was made that some of the tasks from the 2004 ACE Review are still incomplete. Someone suggested a single-channel experiment to investigate if there are any interactions between the channels.

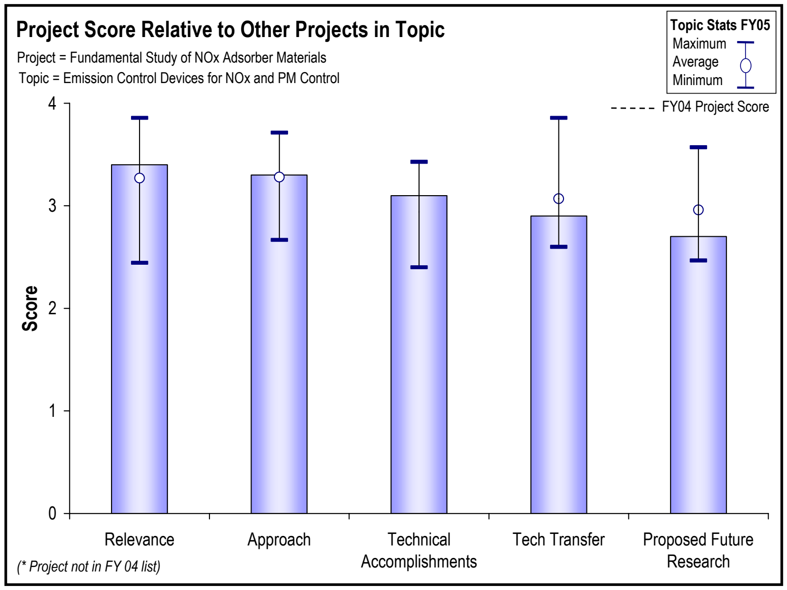
Specific Strengths and Weaknesses (Written responses from 13 of 14 reviewers)

- Specific Strengths
  - This work does a great job of utilizing national laboratory technology to investigate soot.
  - PNNL's SOW focuses on what they do extremely well and leverages National Lab capabilities that do not exist in the industry. Excellent discipline to leverage capabilities of the entire industry/National Lab team.
  - Range of scales of work from pore scale to device-like components.
  - Detailed simulation of soot particles allows physical modeling instead of phenomenological approaches.
  - Excellent methodology and strong relevance to DOE and supplier objectives.
  - Good team, good equipment.
  - Tie-in of modeling with experimentation.
  - Good results thus far from model effort.
  - The presentation was very well done.
  - Model filling a gap in our current analytical capabilities.
  - Good characterization of soot through experimentation. Please continue to capitalize on unique DOE resources such as the APS.
  - Novel methods, excellent ties between modeling and experimental approach.
  - Various "dimensions" of modeling being attempted, including fundamental micro-scale as well as global system level.
- Specific Weaknesses
  - It is not clear that deep bed filtration will have a small effect on trap regeneration.
  - Considering only uncatalyzed substrates, when most practical devices are moving toward catalyzed substrates.
  - It is difficult to validate the model.
  - Lack of adequate experimental validation.
  - Time consuming buildup of simulation code and validation.
  - Low funding level.
  - Working too close to current technology.
  - Work on regeneration seems missing.
  - Apparently, not enough emphasis on modeling regeneration processes.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 13 of 14 reviewers)

- Focus on soot cake filtration and soot cake oxidation kinetics.
- Consider regeneration and the impacts of practical regeneration strategies. Consider SOF content effect on deposition process, rather than just particle deposition.
- Increase emphasis on modeling regeneration processes.
- Need to work on the regeneration and thermal methods that they just initiated. Even though the fiber composite media has been stopped it may be worthwhile to evaluate that system for future understanding of the effects of various media on engine efficiency.
- Interesting model but it appears it does not account for soot agglomeration prior to the deposition due to the simplifications. Is there any assistance for 2007? Look at Keong Lee's work on soot morphology as a function of aftertreatment system. Also look at SOF content.
- As laid out in the scope of work: detailed flow characteristics required. Other materials like SiC to be included.
- Strengthen ties with filter manufacturers, and report on specific collaborations next year.
- Increase the funding.
- Explore stepout modules tailored to future metal catalyzed approach and address trapping efficiency of particles below 100 nanometers. Address factors important to management of internal temperature profiles; e.g soot loadings and nature of the soot.
- Just a few thoughts/questions
  - How do you handle the different forms of particulate (dry vs. SOF)?
  - How is the input modified to differentiate between the different forms/proportions of PM that occur at different engine condition?
  - How can you handle the effect of iron or cerium fuel additives?
  - How can this be extended to handle metal fiber/mesh constructions?
- Continue to balance resources between new tools and 2007 relevant applications. Great job!

- Need to coordinate more with industrial DPF manufacturers.
- Add modeling for various substrate materials.
- Increase emphasis on experimental validation against global DPF system metrics e.g. pressure drop during loading and regeneration; soot mass balance during regeneration and loading.



Brief Summary of Project

This project is aimed at developing a practically useful fundamental understanding of NOx adsorber technology operation, focusing on chemical reaction mechanisms correlated with catalyst material characterization. This project is coordinated with the ORNL program looking at the development of aging protocols as well as the LLNL modeling activities.

Question 1: Relevance to overall DOE Objectives (Written responses from 8 of 10 reviewers)

All of the comments regarding the relevance of this research to overall DOE objectives were positive. One reviewer said that this work is definitely relevant to the emission reduction goal of the EERE department of the DOE. Another added that this is necessary fundamental work and understanding NOx adsorbers is very relevant to DOE's objectives. One person stated that NOx absorbers are an important technology and the researchers are addressing important issues with them. A comment was made that meeting future emissions standards is critical so that future engine technologies can be viable in many markets in the U.S. He went on to say that these technologies support achieving the DOE goals of improved fuel efficiency resulting in reduced demand for imported oil. He also said that a better understanding of NOx adsorber operation is a key, enabling technology supporting diesel and HCCI ICE engine development. One thought that LNTs, only if durable, will help provide an opportunity for clean diesels. Someone felt that this is very good fundamental research. Another person agreed that this is fundamental work on understanding NOx adsorbers to lower the impact on fuel usage.

Question 2: Approach to performing the research and development (Written responses from 7 of 10 reviewers)

The comments on this topic were mixed. One person felt that the project has a good fundamental approach. Another reviewer agreed that they are addressing important issues with relevant techniques. One felt that this project has a well-organized research plan with goals clearly specified. Another agreed by saying that the approach appears to be thorough, utilizing world-class test facilities and equipment. He went on to state that PNNL has excellent research staff and with the new facilities, good things are expected from future work. One reviewer questioned whether this work is redundant to the work being done in Italy and Chalmers. To him this certainly is a reasonable approach, but he is not convinced that additional work in this field is necessary. He added that approach is not significantly differentiated from Chalmers and Pio Forzatti. One person did not see a reason to focus on BaO and AlO_2O_3. He added that there is no apparent structure to the test plan. Another thought that it would be important to examine more fully formulated model LNTs with aging included, not just with fresh catalysts.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 8 of 10 reviewers)

The comments on this topic were mixed. One person felt that excellent progress was made considering the funding level. Another thought that this project leverages/utilizes the DOE resources well. A reviewer considered the distribution of the barium depending on the processing as good information. He suspected that the LNT suppliers have much of this information; however, it is unlikely that it is published. Another mentioned that the video animation does provide some good insights to potential explanations of mechanisms at work here. Someone thought that a lot of work was accomplished, and good understanding is being developed. One person recognized that this project is still in the early stages of research. To him it appeared that progress has been made, but with the time constraints and the number of topics the presenter tried to cover in the available time, it was difficult to make detailed assessment of each (or any specific) area. One suggested including more representative gas composition components such as CO_2 and H_2O on the morphology observations and with the inclusion of Pt in the LNT. A reviewer said that the presentation was "poor" and did not leave him with any sense of real progress in understanding NOx adsorbers. Another agreed that the presenter needs to focus on one or two areas and a make detailed presentation about them.

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

The comments on this topic were mixed. One reviewer felt that collaboration was reasonable for the program size. Another stated that he did not see any evidence that this work has been reviewed or vetted by the catalyst suppliers. He wondered if the direction of this research may have been refined if a catalyst supplier had been included in the discussions. One thought that it is difficult to determine from the presentation exactly how much collaboration exists in these projects. A comment was made that an interface with LLNL is mentioned but with too little information to determine how extensive that collaboration has been. A reviewer pointed out a good industry representation at the October 2004 meeting. He added that this must be maintained and that more meetings than one per year are needed (increase the frequency to 2 or 3 per year). A reviewer wondered if references to various technical publications and presentations qualify for collaboration. He added that he would have liked to see a list of direct collaborators and what each contributed/received (in an appendix).

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 6 of 10 reviewers)

Reviewers that commented on the approach to and relevance of proposed future research agreed that there was no future work discussion. A suggestion was made to interact with Sean Huff from ORNL. One person stated that there was no "Future Work" slide in the presentation. Another thought that the researchers seem to be investigating important issues. One commented that although he is sure that there are future plans and that they may be well-thought-out and relevant to the goals of DOE and this research project, these plans are not discussed in this presentation. Another added that the researchers needed to do a better job of outlining plans, but that they ran out of time.

Specific Strengths and Weaknesses (Written responses from 8 of 10 reviewers)

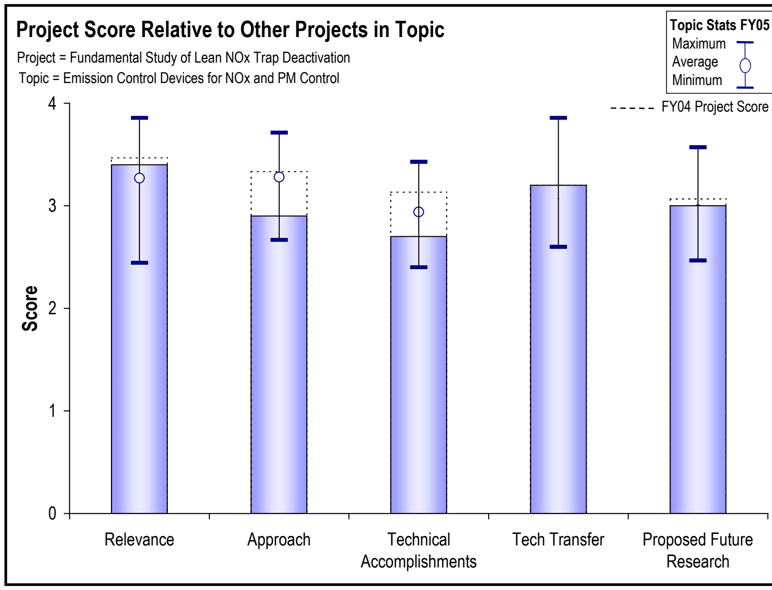
- Specific Strengths
  - Strong researcher and very competent laboratory.
  - Very good fundamental approach that some of the other programs were lacking.
  - Mechanistic focus.
  - Excellent facilities and research staff. Working on technical areas that are important to goals of DOE, FreedomCAR program and auto OEMs. Tools and equipment available in the lab are beyond that typically available in industry allowing research that permits a level of understanding that is critical to the success of aftertreatment systems.
  - Very good "bang for the buck," deserves continued funding.
  - High potential for creative developments of NOx catalytic materials.
  - Excellent use of tools in the National Laboratories and cross-laboratory cooperation. Excellent information on how the systems are responding in applications through model catalyst systems.
- Specific Weaknesses
  - No supplier collaboration.
  - Difficult presentation to follow. No defined plan. Work has focused on a material that PNNL has been "playing with" for 2-3 years. Why? The reason was not given.
  - Too close to what industry is already doing.
  - Presentation was too long for time allotted. PI tried to accommodate this by talking quickly and too superficially about several major areas of research, then by providing 60+ slides in the appendix. While it appears there is a lot of information in the Appendix, since there was no time to review the Appendix or ask questions about it, it provides little value. PI needs to find a way to focus on one or two key areas of research and report on those in more depth. If the scope of the research is so much broader than in other projects, perhaps more review time needs to be allotted to the bigger projects. No discussion of future plans.
  - Show more information and data on the new material improvement. Was it aged or was it fresh testing?

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 6 of 10 reviewers)

- I don't see a reason to continue this work without a "buy-in" from a supplier.
- The conclusions that were made regarding the melting of barium nitrate are circumstantial. The TEM you are planning on performing will give more direct proof. The melting temperature of barium nitrate is 592°C. Your data shows the material to melt at ~550°C.
- A well-thought-out plan is necessary. Chuck also needs to work on his presentation skills and format for next year. Specifically, he needs to decide who his audience is (it's not the same one he has at CRADA and technical reviews), and what it is that he needs to tell them so they get a good idea of his progress and plans. The vast majority of the reviewers are not chemists!
- Provide complete details on nitrogen balances for NOx reduction at different temperatures. Since this is a part of the same program discussed by Do Heui Kim should be presented as an integral whole to reviewers.
- Need a clearer indication of future work planned, timelines, goals, milestones, etc. for this research. There must be some, but there was no information presented that will allow comments regarding the future direction. The scope of the project seems appropriate and the researchers and facilities should be up to the task.
- Investigate your theory with Ba/Ce based LNTs. Also, what happens to the theory as your contaminate with sulfur? Where does the sulfur go during storage? Does it go to the monolayer or the bulk? Where does the non-released sulfur go after a DeSOx process? Does it go deeper into the washcoat, in the bulk, the monolayer?

Emission Control Devices for NOx and PM Control

Fundamental Study of Lean NOx Trap Deactivation, Todd Toops of Oak Ridge National Laboratory



Brief Summary of Project

This project is designed to provide a better understanding of the deactivation mechanisms for lean-NOx traps that result from regeneration and desulfation events. This effort uses multiple analytical techniques, including X-ray diffraction, DRIFTS, and mass spectrometry to perform the necessary experiments.

Question 1: Relevance to overall DOE Objectives (Written responses from 6 of 10 reviewers)

Reviewers agreed that this research is relevant to the DOE objectives. A comment was made that the sulfur poisoning of LNT catalysts is one of the limiting factors for the application of the technology. One person stated that sulfur deactivation of LNT is an important issue for future engines. One reviewer commented that a successful adoption of high fuel efficiency engines in the future in regions where there are stringent emissions standards will require NOx aftertreatment systems that are effective, durable and can easily be regenerated to restore effectiveness. According to him, this research helps to understand NOx regeneration of catalysts under several experimental conditions. Someone added that understanding and improving LNT durability (and DeSOx efficiency) will significantly help in overcoming the major barrier limiting LNT technologies. A comment was made that this research has good relevance, but the presenter needs to clarify the importance of this work relative to other LNT research.

Question 2: Approach to performing the research and development (Written responses from 5 of 10 reviewers)

Reviewers generally agreed that this project has a sound R&D approach. One reviewer mentioned that the DRIFTS technology is a unique approach to identifying the effects of surface sintering and sulfur poisoning on an active material. Another pointed out that there is data that shows that the lean/rich cycling causes increased local temperatures within the catalyst bed. He added that although the bed may be held at a particular overall temperature, the actual local temperatures may be much higher. Someone stated that important LNT issues are being investigated in this project. One person thought that the research approach seems thorough and well thought out, but questioned how the model catalysts were chosen. Another felt that good experimental test bed was developed with a well laid out plan of attack, although some objectives are likely over-ambitious.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 6 of 10 reviewers)

Reviewers made several suggestions regarding the progress of this research. One reviewer mentioned that it would be interesting to know what state the sulfur resides in after the high temperature desulfation, besides pointing out that at temperatures above 500°C there is no detectable sulfur in the exhaust. Another commented that the experiments are providing useful results. One person said that good data appears to have been collected during testing that demonstrates degradation of LNTs after operation at increasing temperature ranges; however, it does not appear that any significantly new knowledge of LNT deactivation has resulted from the research. Someone stated that the work on the aging seems slow with good observations but little analysis and hypothesis as to their reasoning. He added that a very limited number of materials have been tested. One reviewer thought that this project involves good measurement of catalyst behavior, but there are still several unanswered/unaddressed issues such as sulfur balance. Another suggested determining what happened to the missing sulfur and also reporting absolute NOx conversion instead of normalized values.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 6 of 10 reviewers)

The reviews regarding the technology transfer and collaborations were positive. One reviewer thought that obtaining catalysts from two separate suppliers is certainly a useful level of industry collaboration. Another added that Engelhard will be a good partner. One person recognized the need for proprietary information but thought that simply naming the catalyst supplier would enable the reviewers to better assess the quality of the collaboration. He also added that this information along with the data and the results of this research is shared at CLEERS workshops. A suggestion was made to try to involve car manufactures. One person thought that the PI did a good job of describing collaborative roles of other groups/companies.

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

Most reviewers agreed that the approach to future research seems reasonable. According to one reviewer, the focus on the direction to identify the stable sulfur species that occur at high temperature desulfation has good long term implications for being able to identify the most effective de-sulfation strategies. Another added that further study of desulfation is important to investigate. A comment was made that future plans seem well thought out and consistent with research plan; however, the PI needs to work more closely with industry to help understand what research direction may prove more valuable to industry. One person thought that there is nothing wrong with the presented plan, except that it needs to be better organized. Someone else stated that more focus should be given to interpreting the test results to look for the "why."

Specific Strengths and Weaknesses (Written responses from 6 of 10 reviewers)

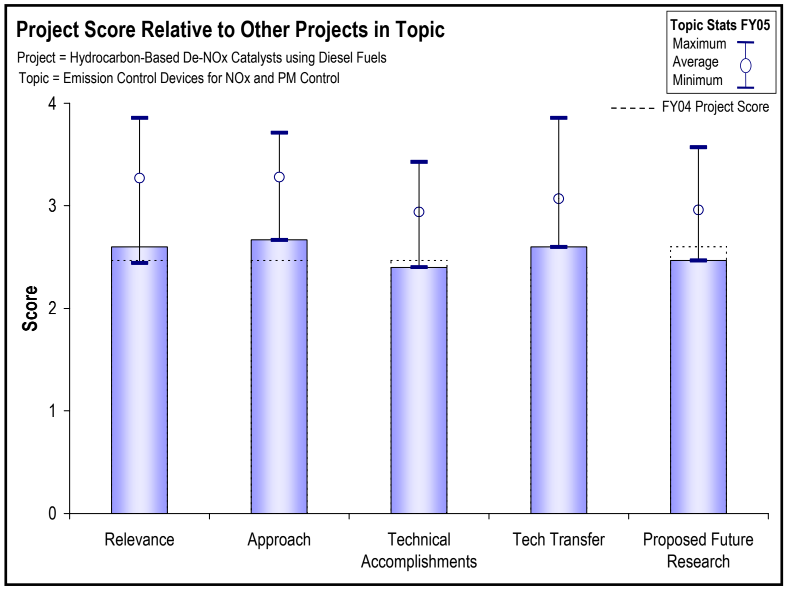
- Specific Strengths
  - A unique experimental set up and the range of national laboratory expertise.
  - ORNL's skills and equipment.
  - Goal of learning more about sulfur effects is worthwhile. However, approach to address needs improvement.
  - Supports developing basic understanding of LNT catalysts.
  - Durability. Durability. Durability. Very important to understand and improve. Important for project to continue and understand aging. Thermal versus SOx/DeSOx aging.
  - Excellent use of tools to determine what is happening to the catalyst system.
- Specific Weaknesses
  - I do not see a part of this program that attempts to identify the sulfur species on the surface.
  - Poor sulfur balances.
  - There does not appear to be a lot of new knowledge that has resulted from this research.
  - Report absolute NOx conversion instead of relative.
  - Need to evaluate the effect of space velocity on the catalyst and broaden the temperature range for the evaluation.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 6 of 10 reviewers)

- Perhaps TEM, SEM and ion probe experiments could be used to identify the sulfur species that are left on the surface at the end of desulfation at higher temperatures.
- Determine if catalyst bed temperatures are what you think they are. Modeling will help.
- Look for an "understanding" of the deactivation mechanisms, as stated in the "Objectives" slide, rather than just observing. Formulate a plan to look for this understanding.
- 1) Unravel reasons for poor sulfur balances and develop procedures to avoid associated loss mechanisms and define necessary analytical approaches. 2) Desulfation studies should be done with the short rich/lean pulsing method. 3) Determine sulfur species retained on trap after desulfation. 4) Determine impact of DeNOx temperature on extent and type of sulfur retention during subsequent desulfation.
- Study Ba surface area as it ages such as CO_2 chemisorption.
- 200g/ft^3 Pt loading is too high.
- Please describes in more detail what "sulfated" means. The sulfation was 100 ppm SO_2 but what was the duration (i.e. grams of sulfur per liter of catalyst before deciding to DeSOx)
- Important to show absolute (not normalized) NOx conversion verses temperature after each aging. Ba vs. K

LNTs have different operating temperature ranges. There is a need to know the conversion as a function of temperature.

- To achieve sulfur balance, take the catalyst to >800°C for 1 hour rich with hydrogen to measure H_2S and close the balance. However, it destroys the sample. Alternatively, XRF for Sulfur could help also.
- Try running as rich as lambda = 0.90 to more quickly DeSOx LNTs at lower temperatures.
- Check for K loss after high temperature aging. It could account for some loss in NOx storage capacity.
- Testing the activity at 250°C is good but what about at 450°C or 500°C to understand the other end.
- Determine the extent of the deactivation (what function of the LNT deactivates, NOx storage or NOx reduction) for both extremes of the operating temperature range.
- Have you considered that some of the undetectable sulfur could be platinum sulfide? If you were to run rich/lean during your DeSOx, perhaps you would see SO_2 released from the Pt.
- Please clarify the gas composition used for DeSOx in slides 17-18! Was it with H_2 only and no other gas components? Unclear to me.
- Need to use some atomic sulfur analysis method to complete sulfur balance in desulfation.



Brief Summary of Project

This project seeks to create a new set of catalysts for the reduction of NOx emissions from diesel engines by using hydrocarbons onboard the vehicle. The catalyst system will work without extra additives or changes in engine tuning. The catalysts being examined are copper-ZSM-5 formulations.

Question 1: Relevance to overall DOE Objectives (Written responses from 14 of 15 reviewers)

Several reviewers thought that this project fit well with DOE goals. One felt that NOx catalysts are essential to meet upcoming emissions targets, while another felt that this research is very valuable, as it provides another approach to NOx reduction other than NOx adsorbers. A reviewer offered that the concept is attractive if the system designers avoid the use of a reformer. A final reviewer said that this is very relevant work for industry.

Several reviewers had more critical comments. One noted that although HC-SCR certainly fits the DOE aftertreatment objectives, this particular approach is not showing strong indications of success. Another said that using hydrocarbon-based NOx reduction increases fuel consumption and with that the dependency on foreign oil imports. A reviewer noted that the program targets the reduction of emissions but also said that when the presenter was questioned on how the program aids fuel efficiency, a clear answer was not forthcoming. A reviewer offered that this system is limited to engine applications needing NOx conversion at high temperatures. This may contribute to NOx reduction in a moderate amount, said a reviewer, but C/N ratios between 6 and 22 are very high and to some engine manufacturers may be unacceptable. A reviewer noted that although NOx reduction is a key technical barrier, this work is not at all likely to add any useful knowledge, let alone succeed. HC-SCR would be ideal if high NOx reduction would be achieved at low C/N ratio, a reviewer stated. The project, if successful in significantly exceeding program goals, offers the potential to provide an alternate NOx aftertreatment system that utilizes diesel fuel as a reductant and does not require engine management for NOx reduction, observed a reviewer. However, the goals set by the program and the range of NOx reduction efficiencies currently demonstrated seem inadequate to meet 2010 emissions regulations, unless combined with significantly low engine-out emissions obtained via advanced combustion processes. Finally, a reviewer felt that the project was definitely relevant to low emissions goals, but its advantage vis-à-vis other de-NOx techniques needs to be better articulated.

Question 2: Approach to performing the research and development (Written responses from 13 of 15 reviewers)

Several reviewers offered positive comments about the approach to this research. It was felt by one reviewer that the high efficiency potential of this system with a low cost material is very important to pursue. Another noted that the approach is well formulated, and this reviewer did not have any recommendations for changes. Another felt the technical approach was sound. A reviewer noted that the team has made a good switch by moving from propylene to diesel fuel. A reviewer said that copper and silver are well known as reducing catalyst materials, and the included cerium may help.

Several reviewers offered suggestions on the approach. A reviewer suggested that the team consider setting more aggressive targets for NOx reduction efficiencies and the temperature limit for thermal durability. Some reviewers noted the approach may be too reliant on trial and error, with one reviewer suggesting the efforts were “a bit Edisonian.” Another asked for some engine data, noting that with only 40% NOx reduction on the bench, I would predict that on engine data would only go down. It would also be good to understand which components of the fuel contribute to the NOx reduction mechanisms. A reviewer had several comments on the work plan, including that it lacks focus, and that it is unclear whether the plan is to be working on the effects of fuels of various types, on reforming various diesel fuels, or on developing dopings of CuZSM-5. CuZSM-5 and all its versions have already been thoroughly investigated and found lacking. The temperature window objective is too small; the lower limit should be no higher than 200°C for automotive applications. The temperature window of 250-500°C is too narrow even for HD truck use. A reviewer thought the approach of using additives to enhance the performance of a known active catalyst is quite reasonable. A C/N ratio of 22, however, probably makes the mixture rich and is misleading in identifying the system as an efficient, lean NOx catalyst. Conversions of 40% are not much better than the conversions for the CuZSM-5 base metal catalyst. A reviewer said that there is not a clear C/N ratio or NOx reduction target that would help frame the problem. Several of the data points presented were outside the target values of % water, % oxygen, and % NOx. While this is informative, it does not drive directly to the solution of the problem. In the rapid drive to market this could open the question of whether the approach is focused on the final application. A final reviewer noted the team is developing catalysts that will require no additional reductant and be passive, with fuel/HC-based NOx SCR using CU-ZSM-5 doped with CeO_2. It was unclear to this reviewer if there has been effort put into tailoring the CeO_2 doping (e.g., crystallite/particle size).

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 14 of 15 reviewers)

Reviewers' comments were mixed on technical accomplishments. While good progress has been made in one reviewer's opinion, another thought there was nothing exciting here. A reviewer felt the team is making good progress, but many important issues remain. The project had well founded objectives and demonstrated considerable progress to the goals, said another reviewer. A third reviewer said that the team is getting lots of data on a tough problem. A reviewer noted the good presentation of achievements in a relatively short time: the team seems to be making good progress toward technical goals. Steaming of the zeolites was a good step forward, in one reviewer's comments, as was the addition of stabilizing agents to the zeolite.

Several aspects were singled out by reviewers. Results are far away from the target NOx reduction, said one reviewer. Another said that the efficiencies shown here have been known for years, and no significant breakthroughs have been achieved. No detailed aging effects have been demonstrated, nor have copper emissions (if any) been addressed. Another reviewer echoed these comments by observing that peak efficiencies of 64.2% on JP-8 and just over 50% on ULSD (both at 350°C) will not be sufficient. The team is seeing good selectivity and moderate activity (< 50%), noted another reviewer, who continued by observing that light HC's give lower temperature activity than higher boiling fuels. The approach is plagued by the same problems that HC-SCR have had in the past, in that a high C/N ratio is needed and >50% conversion is not within reach. HC-SCR base metal zeolite catalyst technology is considered as a technical stretch when targeting 70-90% NOx conversion after real high temperature engine aging and testing, said a reviewer. Current NOx reduction efficiencies demonstrated by the HC-SCR system seem inadequate to meet 2010 emissions targets in one reviewer's opinion. A final reviewer thought that with the previous experience on a similar catalyst in previous programs that the progress would have been a little better.

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

Several positive comments were offered relative to this project's collaborative aspects. One noted the good open approach with industry, while another said that the right players are involved. A reviewer pointed out that the PI mentioned project partners but did not mention how closely the team interacts with the partners. A reviewer noted the establishment of a CRADA with an engine company and catalyst company, as did a reviewer who singled out the work with a catalyst company, a substrate manufacturer, and a diesel engine company. On the other hand, another reviewer referred to the catalyst and monolith partners listed as "Future Partners" as being "lightweights," and noted that if the "engine manufacturer" believes in the program, he should "be prepared to be named." This was reflected in another reviewer's statement that the focus on one unidentified engine supplier reduces technology transfer since more details are missing. Some collaboration between engine manufacturer and catalyst manufacturer seems to exist via a CRADA, noted a reviewer, who was unclear as to what the goals of the CRADA are and how they advance the current state-of-the-art. A reviewer felt that there was no particular evidence of industry interest in these materials. A reviewer suggested that the team should leverage the diesel engine manufacturer to age and test catalysts on an engine. Another reviewer suggested the team needs to do a better job of collaborating with companies and universities, or do a better job of marketing collaboration. A reviewer had several comments, noting that there was a reference to two new papers in Catalysis Today. It was not clear to this reviewer whether this was from this work or was more related to the stationary source application. No collaborations with other government labs and no collaboration with academics were shown, according to this reviewer. Hopefully the CRADA will be announced shortly. A list of presentations would also be useful. Finally, a suggestion was provided that the project team needs to talk about applications and the relevance to 2007/2010 regulations and to other technologies to be used, such as diesel particulate traps.

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

Review comments were mixed on the future research. One noted that the key areas for future research were covered, while another pointed out the plans to consider higher space velocities and sulfur tolerance issues, as well as development of a CRADA.

On the other hand, one reviewer said the technical work plan needed to be better described and justified. A reviewer said there was no plan mentioned to improve NOx reduction, and this reviewer did not see an effective program going forward. This was reflected in another comment that no breakthrough in the low efficiency of the catalyst system is seen. One reviewer said the plans offered were “pretty standard plans for a set of not very interesting materials.” A reviewer suggested that the team define “long-term testing” and provide more representative engine conditions. The team should consider adjusting program targets to be representative of a 2010 integrated engine, DPF and NOx aftertreatment system, offered a reviewer. The test for sulfur tolerance should be done as soon as possible, offered a reviewer. Examination of components of diesel and how they affect the different catalysts may lead to a robust catalyst system that can be used all over the US with the variants in fuel. Finally, a reviewer noted that Tim Johnson (Corning) remarked in the meeting that high NOx reduction is capable with silver catalysts and hydrogen. However, the unattractive aspect is the added cost and complexity of the reformer and associated equipment. This reviewer said that lean NOx catalysts have had issues with durability on-engine. If the reformer-assisted lean-NOx system shows promise, the team should then check durability of the system on an engine.

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

- Specific Strengths
  - The project, if successful in significantly exceeding current program goals, offers potential to provide an alternative NOx aftertreatment system.
  - NOx control focus on a strategy that does not require regeneration or additional reductant.
  - Monitoring and research in this area required, but with less effort possible.
  - Catalysis background of PI.
  - Building of Argonne’s prior knowledge of reformers was a good idea.
  - It might offer a good alternative to lean NOx traps and SCR for very low NOx emissions.
  - Overall sound approach.
  - Use of diesel fuel as the HC reductant.
  - Total system cost impact if program could hit goals.
  - Could potentially be superior to other De-NOx strategies now being discussed.
  - Program gives diversity to DOE’s portfolio. It also has the opportunity to be placed into production relatively quickly and does not require infrastructure like a urea-SCR system would require. Also the catalyst system as described does not contain precious metals which should result in reasonable catalyst cost.
  - Approach may allow to tuning of engines to higher efficiency.
  - This technique, combined with optical methods, should be able to lend fundamental understanding of fuel sprays that can then be generally incorporated into CFD spray models.
- Specific Weaknesses
  - HC consumption looks very high at present.
  - Good catalyst relationship, it may be worthwhile to get more engine OEM buy-in.
  - No engine data to date, no specific mechanism to date.
  - The time-averaged absorption method alone may not provide sufficient information to achieve the prime objective of providing a better fundamental understanding of the near-field breakup. A better physical description of the transference of inertial energy to surface energy is needed, and the time-averaged

behavior can not provide it.
- I believe this approach is not in the scope of DOE and would fit better to EPA-sponsored programs. The temperature range is too low and narrow; the implied target efficiency is too low. A 4-1/2 year program to look at something that has already been flogged to death! In short, "Been there, done that!"
- Formulation is too close to what industry logically would look at on their own.
- The catalyst may not have sufficient efficiency for NOx removal and may require significant amounts of fuel.
- Looking at C:N > 6 is a waste of time that would not be acceptable if you are going to compete against a urea solution.
- Testing more practical engine conditions.
- No plans to achieve target NOx reduction.
- Results seem far away from target NOx.
- Current NOx reduction efficiencies, space velocity targets and thermal durability targets do not seem representative of a 2010 integrated system.
- Need to do a better job of justifying technical and commercial advantages of these catalysts relative to other De-NOx methods.
- NOx reduction is still a little below program objectives, high temperature stability is acceptable but limited.
- Examining N_2O emissions and nitrogen containing hydrocarbons would be beneficial. Resolving any possibility of dealumination due to sulfur interactions or conversion of ceria to cerium sulfate and its differing oxygen transfer abilities might be beneficial to probe quickly.

EMISSION CONTROL DEVICES

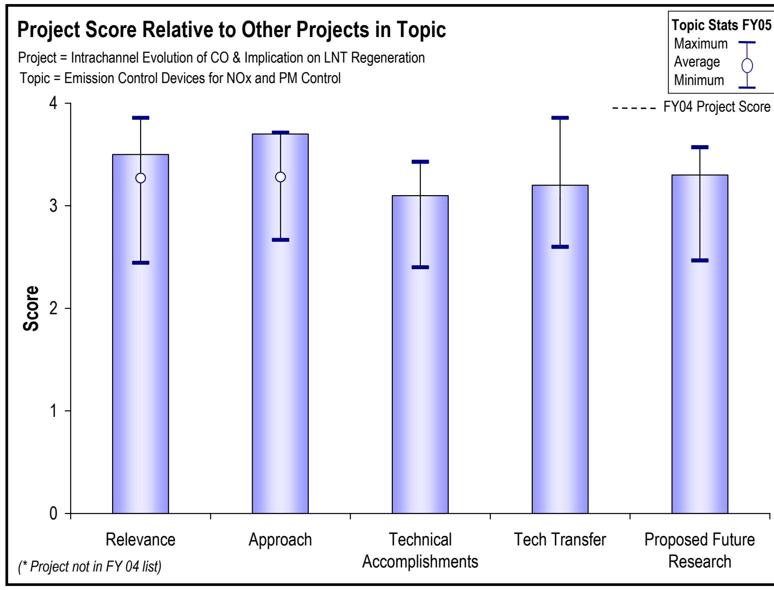
Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 12 of 15 reviewers)

- A list of presentations and publications would aid in a clearer picture in the dissemination of knowledge.
- It is not clear that there is enough potential for this material to continue the investigations.
- May want to project how this catalyst, when targets are reached, will impact the fuel efficiency (from HC consumption) and ability to meet emissions regulations.
- Add engine testing for both performance and durability if applicable. If the engine data returns less than 50% NOx reduction, the value of the work must be questioned.
- Resolving the finer scales of the hydrodynamic instability and fluid momentum transfer in the near field would add to the significance of the work. The higher-power monochromator opens up the possibility of looking into single-shot spray structure—can finer scales also be resolved by reducing target area?
- Limit the investigations to a kind of "technology monitoring" with very limited experiments.
- Drop this project.
- Need to consider effects of sulfur on Ceria. Also need concepts for thermal stability over 600°C. If not in the cards discontinue project.
- They should address sulfur tolerance first.
- I realize the targets are tough enough as it is, but for a viable solution for the industry (and to compete with a urea solution), you need to have 75+% NOx reductions with a space velocity of 50+k/hr and a C: N < 4.
- Slide 10 and 15: C/N=22, oxygen=2%, NO=1000ppm. This is about 2.2% CH_2 which requires more than 2% oxygen to oxidize completely. The experiment is carried out under rich conditions. Therefore, this case is not realistic when studying HC-SCR. I would expect NH_3 at the lower temperatures. Please report on HC oxidation.
  I suggest checking your different types of tests and/or fuel types with a blank or inactive powder to determine known autoignition behavior of long-chain alkanes. You may notice apparent NOx conversion without any active catalyst in your system. A possible reason for this is the generation of "alkyl nitrates" where chemiluminence analyzers don't detect. Try placing a Pt based catalyst downstream to see if NOx reappears.
- Slide 16 - Please relate the hydrothermal treatment to resultant effect on the NOx conversion. I suggest to study the hydrothermal stability such as aging at varies temperatures (550 – 750°C) for an extended time (>16 hours) and then performing the NOx evaluation for each case.
- The thermal durability targets should be extended to at least 600 – 650°C, to account for the possibility of active DPF regeneration occurring upstream of the SCR.
- None of the NOx conversion graphs indicate the state of the catalyst. Was it aged or was it fresh? I disagree that the catalyst is stable simply because the zeolite surface area is not lost or that that it took longer for the improved catalyst structure fall apart. I think that each aging and type of aging needs to be judged based on the NOx conversion.
- Try different zeolites in your formulations!

- Show a plan to achieve target NOx reduction on engine of 60-90% at target C/N ratio of 6:1.
- I would not do additional work that was not consistent with first identifying technology that could achieve the target NOx reduction.

Emission Control Devices for NOx and PM Control

Intra-channel Evolution of Carbon Monoxide and Its Implication on Regeneration of Lean Nox Traps, Jae Soon Choi of Oak Ridge National Laboratory



Brief Summary of Project

These researchers are working on bench-level experiments to gain insight into the nature and network of carbon monoxide lean-NOx trap regeneration reactions. In addition, they are looking to characterize reaction exotherms and heat transfer, and identifying the origin of poor low-temperature carbon monoxide lean-NOx trap regeneration efficiency.

Question 1: Relevance to overall DOE Objectives (Written responses from 6 of 10 reviewers)

Comments to this question were generally positive. One reviewer noted that developing a good understanding of the reduction mechanism for LNT systems fits the goals of improved fuel economy with reduced emission of DOE EERE. Another person commented that meeting future emissions standards is critical for future engine technologies to be viable in many markets in the U.S. These technologies support achieving the DOE goals of improved fuel efficiency resulting in reduced demand for imported oil. A better understanding of lean NOx trap operation is a key enabling technology for diesel ICEs. One reviewer commented that detailed mechanisms in adsorber catalysts help to optimize the layout of the catalysts (zone coating, flow, etc.) and thus helps to reduce the fuel economy penalty of aftertreatment systems. Another felt that LNT mechanisms and kinetics appear to be key areas of investigation, while another added that LNT research is a potentially important technology for future engines. The last reviewer was critical, stating that the project is reasonably important to meeting emissions requirements, but the team needs to do a better job of explaining specific goals.

Question 2: Approach to performing the research and development (Written responses from 8 of 10 reviewers)

Comments were positive in general. One reviewer commented that using intra-channel measurement techniques is a very necessary approach to move from inferring chemistry from sample-out results (basically the integral reactor model) to point-by-point measurements within the monolith (single-point kinetics), which is crucial for getting the technology from just a phenomenological basis to actual predictable kinetics. Several people commented on the excellent use of specialized ORNL tools in this study, which should lead to better understanding. One person noted the useful study of the details of LNT operation, while another noted that understanding CO chemistry during NOx is important. One reviewer felt that there was good use of in-situ instrumentation to resolve species and temperature profile along the catalytic converter channel, but suggested that the research team needs to do a better job of explaining the chemistry. The final reviewer commented that the researchers need to understand CO chemistry during regeneration of NOx traps as key technology that can enable successful application of NOx aftertreatment systems.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 6 of 10 reviewers)

One reviewer noted that the researchers appear to have developed considerable understanding of lean NOx trap regeneration. Another noted that there are many good results on catalysis reactions as a function of channel position. Another reviewer felt that the progress has been very good, but noted that there are issues of heating and heat loss in these measurements that need to be well-quantified; it is not clear from this presentation that those issues are clearly understood. They added that the observation that CO is more important in LNT regeneration than H_2 is very helpful. Another person also noted the good understanding of local regeneration characteristics, but questioned why there was only a visible exotherm at 0 and 0.5. They added that it would be thought to be noticeable through out the entire cross-section of the core and would guess that problems exist with not only thermal gradients in the core but also flow gradients that don't give adequate mixing of the reductant. One reviewer commented that the use of real or artificial exhaust gas with all relevant components needs to be conducted not too late in the project. The last reviewer commented that it was difficult to follow the talk, but the slides indicate some good results.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 6 of 10 reviewers)

Several reviewers noted the CRADA with Cummins was very good. Another also acknowledged the collaboration with the catalyst industry. One reviewer acknowledged that since this is a CRADA, only limited technology transfer is occurring, while another felt that the transfer should be conducted well through CLEERS. One reviewer suggested that the researchers should develop university collaborations. The final reviewer commented that the prompt dissemination of this data to the general community would be very much appreciated.

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

Comments were generally positive. One reviewer felt that the group is headed in a very useful direction, and liked all the plans, but was a bit confused by the discussion of intra-channel fuel reforming versus direct consumption. They did not find anything in the presentation that indicated that this should be a high priority. One person thought it would be very helpful if the researchers included the SOx process followed by the DeSOx for intra-channel speciation. Another commented that the researchers realistically choose the hydrocarbon(s) used as reductants. Another acknowledged the new materials and side products investigations are important. The final reviewer felt that the research teams had a reasonably good plan, but too brief and not tied to current results and project goals sufficiently.

Specific Strengths and Weaknesses (Written responses from 8 of 10 reviewers)

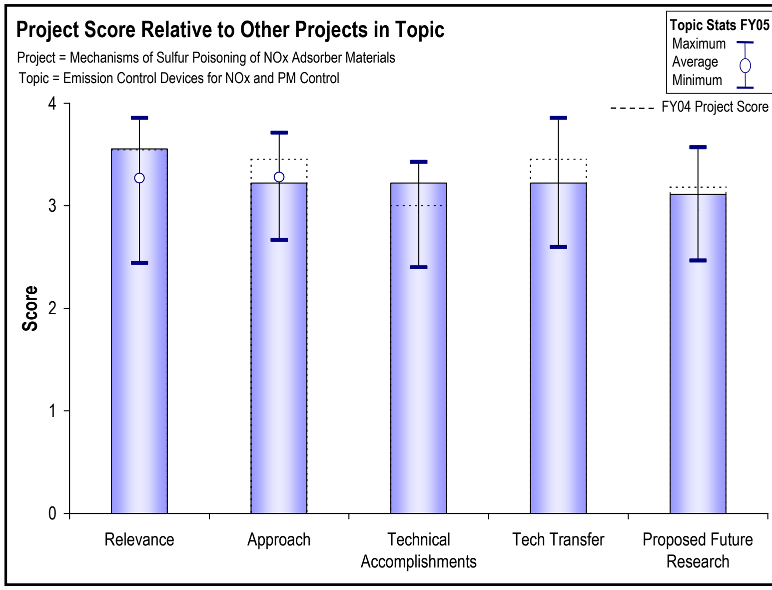
- Specific Strengths
  - The use of the ORNL-developed techniques for probing the catalyst channels is a great accomplishment, especially since it is being done at an engine laboratory where the focus is the application of the devices.
  - Uses ORNL's strengths.
  - Good use of tools.
  - Excellent tools help together with simulation to understand the micro mechanisms inside an adsorber catalyst.
  - Knowledge gained from in-situ probe of chemistry proceeding along LNT axis.
  - Good work on De-NOx catalysis.
  - Good experimental setup for detailed examination of catalysis processes along channel.
  - Unique tools that have shown to significantly contribute to the understanding of the catalyst systems.
- Specific Weaknesses
  - Issues with testing uniformity due to complex evaluation equipment.
  - One company CRADA will limit the availability of this knowledge to others.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 7 of 10 reviewers)

- Continue on the present track.
- Run a realistic exhaust mix, especially reductants, and measure the local temperature. You may find the exotherms to be dramatic.
- Apply the techniques to real exhaust gas in engines. Investigation of transient flow (temperature swing, pressure waves). The temperatures in the catalyst are not comparable to engine conditions (exit temperature higher than inlet temperature); this can be overcome easily and would make the results more valuable.
- Should add studies on effect other reductants and CO+on DeNOx chemistry and desulfation.
- They should study the multiple pulse regeneration process and shown by Shean Huff (ORNL).
- Testing with Ba-based and Ba/Ce based model LNT catalysts. Also, fully formulated LNT.
- Very good work on DeNOx. This work for DeSOx would be very helpful (H_2S, SO_2, and COS)!
- Include NH_3 and N_2O in future work.
- Please consider work on H_2S, NH_3, N_2O and SO_2 in future research.

Emission Control Devices for NOx and PM Control

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



Brief Summary of Project

The focus of this work is on identifying and understanding the important degradation mechanisms of the catalyst materials used in NOx adsorber technology. In particular, loss of performance due to the effects of high temperature operation and sulfur poisoning are being studied.

Question 1: Relevance to overall DOE Objectives (Written responses from 4 of 9 reviewers)

It was acknowledged that the NOx adsorbers offer chance to meet 2010 emission standards without a secondary fluid like urea, and this project seeks to overcome several of the key technology barriers. A comment was made that sulfur poisoning is a very important issue with NOx absorbers. One person pointed out that meeting future emission standards is critical for future engine technologies to be viable in many markets in the U.S. He added that these technologies support achieving the DOE goals of improved fuel efficiency resulting in reduced demand for imported oil. According to him, a better understanding of NOx adsorber operation is a key enabling technology for diesel ICEs. One reviewer thought that the issues of thermal aging and sulfur poisoning are interesting, but according to his belief, the suppliers seem to already know this information.

Question 2: Approach to performing the research and development (Written responses from 4 of 9 reviewers)

Comments regarding the approach were generally positive. One reviewer believed that this goes over the knowledge that the suppliers already have. A statement was made that the researchers are considering high temperature and sulfur deactivation with model NOx adsorber materials and the tools at PNNL. A reviewer thought that this project uses the available tools well to provide a fundamental understanding of the subject. A comment was made that the method of testing is not given other than the statement "Utilize PNNL's State-of-the-Art Catalyst Characterization and Testing Facilities." This reviewer though that this statement is "pure PR." He added that it does nothing to provide information on what tests were run so that they can be critiqued.

Question 3: Technical Accomplishments and Progress toward project and DOE goals (Written responses from 5 of 9 reviewers)

The comments regarding technical accomplishments were mixed. One reviewer felt that nothing new was accomplished. Another felt that good progress was made. He added that the XPS data on the enhanced model shows about 20% of the initial sulfur remained after desulfation at 600°C and data on slide 70 showed little change in NOx conversion after multiple desulfation events. To him it appears that after the initial sulfur diffusion into the structure, no more sulfur diffusion into the structure occurs. He suggested to check that with XPS. Someone pointed out that it was observed that Pt particle size growth is the primary mechanism of thermal aging. He also mentioned that the researches performed aging studies with decoupling of thermal and sulfur deactivation. He added that the initial sulfate formation does not reduce NOx. A comment was made that useful information on LNT deactivation was obtained. Another comment was that the presentation included numerous plots and graphs that meant very little to the majority of the Review Panel. This same reviewer stated that the "poor presentation" made it very difficult to assess the progress.

Question 4: Technology Transfer/Collaborations with Industry/Universities/Other Labs (Written responses from 7 of 9 reviewers)

Reviewers acknowledged that this work is a result of a CRADA with a diesel engine manufacturer (Cummins) and a catalyst supplier (Johnson Matthey). One person felt there was a good collaboration with Johnson Matthey.

Another mentioned that Johnson Matthey provided samples, but it was not clear that they had any impact on the research directions. One reviewer stated that the CRADA involves only two companies and that a wider dissemination of the results would get a higher rating. Someone stated that collaboration and technology transfer was limited because the work is a CRADA. A reviewer pointed out that a diesel engine manufacturer, a catalyst company and a National Laboratory are all working together.

Question 5: Approach to and Relevance of Proposed Future Research (Written responses from 4 of 9 reviewers)

Several suggestions were made including refinement of aging measures, incremental aging validation, and confirmation of protocol for interrogation of aged samples. Another suggestion was made to incorporate information from a catalyst company and an engine company into the future work. To one person it was not completely clear that completion of the proposed future work will ensure development of a material that meets performance needs. Another reviewer felt that the future work not communicated well to the Panel. One reviewer stated that there is nothing ground breaking here.

Specific Strengths and Weaknesses (Written responses from 8 of 9 reviewers)

- Specific Strengths
  - The availability of the PNNL instrumental services is good.
  - Techniques available for catalyst characterization. Close partnership with industry. Expanded consideration of aging cycles.
  - Good tools, fundamental understanding.
  - Showing LNT design improvements based on knowledge gained.
  - Efforts to decouple thermal vs. DeSOx durability issues are very important and addressed.
  - Work is very valuable on durability issues associated with thermal cycling and also with De-SOx processes.
  - Excellent results that assist in the understanding of catalyst deterioration factors. Able to separate effects of sulfur and thermal aging.
- Specific Weaknesses
  - There does not seem to be an appreciation of the information that the suppliers already have.
  - Very poor presentation probably obscured the merit of this work.
  - Some concern about analytical methods. Also no info on sulfur balances.
  - The thermal treatment clearly shows Pt sintering but could Ba sintering that remains amorphous also explain the loss in NOx storage and activity. What is the Ba surface area decline with thermal exposure? What about the theory of Pt separation of Pt-Ba. What happens with the Pt-Ba as it ages and is sulfur poisoned?
  - PI presented a lot of information (76 slides including appendices), but tried to present too much information for the time allotted. He needed to skip too many slides to be able to complete his presentation. The data in the appendices did not receive any attention in the meeting.

Specific Recommendations/Additions to or Deletions from the work scope (Written responses from 4 of 9 reviewers)

- Work very closely with a supplier or drop the project.
- The Work Plan needs to be properly identified to the Panel.
- Conclusions as to barium states after various treatments need confirmation. It is surprising that formation of Ba-aluminate can be reversed back to $BaCO_3$. Possibly Ba-aluminate has become more dispersed and therefore not visible (check if $BaCO_3$ restored by TPD) .Also surprising that $BaCO_3$ can not be reduced with H_2; maybe an issue of sample handling (check by in-situ defraction).
- The thermal treatment clearly shows Pt sintering but could Ba sintering that remains amorphous also explain the loss in NOx storage and activity. What is the Ba surface area decline with thermal exposure? What about the theory of Pt separation of Pt-Ba. What happens with the Pt-Ba as it ages and is sulfur poisoned?
- Please consider work on decoupling high temperature lean only aging, rich only aging, and cycling lean and rich (with O_2 in the rich pulse).
- Please consider working on K containing catalysts and their issues with volatility and S release.
- I appreciate the extra information in the appendix. However, please don't flash slides during the presentation. It is hard to follow. In general, there was too much information during the presentation.

At the end of the review meeting, the advisory held a luncheon meeting to discuss the projects and the sessions in general. The following summarizes these comments for the meeting. DOE responses are shown in italics.

April 21, 2005: Comments from Review Committee Lunch

1. Project Presentations
   - Timeline for the project was very useful but only a few presenters included it.
     - *Ken Howden: Agreed.*
     - *Kevin Stork: I have sent out a template for the presentations and some principal investigators (PIs) choose to follow it and some do not. The timeline was a part of the template.*
     - One suggestion was to ask/require the presenter to show the timeline and near-term deliverables/milestones.
   - Some presentations jump right into the data while others are 90 percent overview and with little technical content. A brief introduction is necessary especially for the first-time reviewers that have not seen the previous year's presentation.
     - *Kevin Stork: What about a general introduction of their projects by the laboratory leads?*
     - That could add a significant amount of time to the meeting.
     - *Gurpreet Singh: A brief description of projects for each national laboratory at the start of the meeting or at the start of each day by a couple of laboratories would provide a good overview of their activities and allow the PIs to focus more on the technical aspects of their projects. These introductions could be done in 15 minutes.*
     - *Kevin Stork: That would be useful but we should not cut-down project presentation time to less than 20 minutes.*
   - Another reviewer agreed and added that about 60 percent of the presentation should focus on technical work. The collaboration and general introduction should be shorter in general. The talks should be more technical, and less of the lab justifying their role.
   - Timeline of the project would be useful along with near-term milestones. It is difficult to review a project not knowing when it started and when is projected completion.
     - Original goals of the project should be made clear because some longer projects are still trying to answer the original questions. Reviewers are not aware of the original goals unless they are stated in the presentations, thus the reviewers can misunderstand the current focus of the project.
     - *Ken Howden: A copy of the R&D plan would be useful for the reviewers to better understand the history of the projects.*
     - The R&D plan would provide context for the projects.
   - *Ken Howden: The presenters should clearly state what they are going to do next.*
     - *Kevin Stork: Most presenters mentioned what their future plans are but milestones that go along with those plans would be useful.*
   - Several reviewers commented that it was helpful when the presentations addressed the last year's comments and explicitly described how they addressed them in the current year's work.
   - There was a general consensus that it would be helpful if the someone gave a short presentation about the work being done at each lab and to show the inter-lab collaborations.
     - Lab leads should give a short (10 minute) talk about the overall lab goal and a high level overview of the work being done at each lab.

2. Reviewer Panel Format
   - It was very helpful that the presentations were sent out prior to the meeting.
   - Why were the reviewers not divided into two groups (In-Cylinder Combustion & Aftertreatment) like in the previous years?
     - *Kevin Stork: This year there was more focus on the In-cylinder combustion and it would be harder to alternate the two reviewer groups. Therefore, we thought it would be easier if the reviewers would select the project that they want to review.*
     - *Ken Howden: If the fuels projects will be included in the review meeting along with in-cylinder combustion and aftertreatment, then it would make sense to have two groups of reviewers.*
     - *Kevin Stork: This year we had 24 fuels projects and combining the two programs would significantly lengthen the meeting, but will consider doing so for next year.*
     - Another reviewer agreed that splitting the reviewers into groups is not necessary since the in-cylinder and aftertreatment are so intermingled these days.
   - *Kevin Stork: Was there enough time allocated for the reviewers to write their comments (20 minutes for presentations and 10 minutes for questions)?*
     - In general, the reviewers felt that 10 minutes during the question period was sufficient.
     - One reviewer commented that the 10-20 minutes is not enough time if the comments need to be handed in at the end of each day.

APPENDIX A

- Sequential sessions of In-Cylinder Combustion and Aftertreatment would be better since the reviewers and other participants would have to spend less time at the meeting while still seeing the presentations relevant to their work. In the current meeting the presentations were mixed and people interested in only one topic had to sit through all the presentations to see the ones that are of interest to them.
  - *Kevin Stork: Sequential sessions would be good but parallel format would not be a good idea since a lot of participants are interested in both sessions.*
  - *Ken Howden: Agreed with Kevin since some companies would not be willing to send more people to cover both sessions.*
  - Grouping presentations into one day or day and a half each could work for everyone's benefit.

3. DOE Programmatic Comments
   - Program Elements
     - Poster session should be later on in the meeting since presentations stimulate discussion with the presenters during the poster session.
     - *Gurpreet Singh: That is a good idea and can easily be accommodated.*
     - Jin Wang's presentation was a proposal of a new technique and thus should be distinguished from other already ongoing projects.
     - Getting industry feedback on project proposals is a good idea, but this is not the correct forum for that.
     - *Kevin Stork: This meeting should only have presentations of existing projects and not proposals. Proposals do not belong into this meeting.*
     - Industry is interested where the money is being utilized. Where do you want our input for current projects or for proposed ones?
     - *Gurpreet Singh: Agreed with Kevin and emphasized that this meeting is peer review only.*
   - DOE Program Collaboration
     - It would be beneficial if there was a combined overall technical strategy among the national laboratories.

\- Sharing of information by PIs is very impressive.

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 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 DOE 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 DOE 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
ACE	Advanced Combustion Engine
AEC	Advanced Engine Combustion
ANL	Argonne National Laboratory
AOP	Annual Operating Plan
APS	Advanced Photon Source
CA	Crank Angle
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
DDC	Detroit Diesel Corporation
DI	Direct Injection
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
EPA	U.S. Environmental Protection Agency
FTP	Federal Test Procedure
FY	Fiscal year
HC	Hydrocarbons
HC-SCR	Hydrocarbon Selective Catalytic Reduction
HCCI	Homogeneous Charge Compression Ignition
HD	Heavy-duty
HECC	High-Efficiency Clean Combustion
HSDI	High Speed Direct Injection
ICE	Internal Combustion Engine
KIVA	Modeling code developed at Los Alamos
LANL	Los Alamos National Laboratory
LD	Light-duty
LIF	Laser Induced Fluorescence
LLNL	Lawrence Livermore National Laboratory
LNT	Lean NOx Trap
LTC	Low-Temperature Combustion
MOU	Memorandum of Understanding
MZ	Multi-zone
NOx	Oxides of nitrogen
OEM	Original Equipment Manufacturer

Acronym	*Definition*
ORNL	Oak Ridge National Laboratory
PCCI	Premixed Charge Compression Ignition
PDF	Probability Density Function
PI	Principal Investigator
PM	Particulate matter
PNNL	Pacific Northwest National Laboratory
PRF	Primary Reference Fuel
R&D	Research and Development
RASP	Rotating Arc Spark Plug
SAE	Society of Automotive Engineers
SCCI	Stratified Charge Compression Ignition
SCR	Selective Catalytic Reduction
SI	Spark ignition
SNL	Sandia National Laboratories
SOI	Start of Injection
SOW	Statement of Work
SpaciMS	Spacially Resolved Capillary Inlet MS
SV	Space Velocity
UW	University of Wisconsin
UW/ERC	University of Wisconsin Engine Research Center
VCO	Variable Configuration Orifice
VCR	Variable Compression Ratio
VVA	Variable Valve Actuation
XPS	X-Ray Photoelectron Spectroscopy

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

To learn more, visit www.eere.energy.gov

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